CO5BOLD User Manual

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1 Introduction

CO5BOLD – nickname COBOLD – is the short form of "COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with l=2,3".

It is used to model solar and stellar surface convection. For solar-type stars only a small fraction of the stellar surface layers are included in the computational domain. In the case of red supergiants the computational box contains the entire star. Recently, the model range has been extended to sub-stellar objects (brown dwarfs).

CO5BOLD solves the coupled non-linear equations of compressible hydrodynamics in an external gravity field together with non-local frequency-dependent radiation transport. Operator splitting is applied to solve the equations of hydrodynamics (including gravity), the radiative energy transfer (with a long-characteristics or a short-characteristics ray scheme), and possibly additional 3D (turbulent) diffusion in individual sub steps. The 3D hydrodynamics step is further simplified with directional splitting (usually). The 1D sub steps are performed with a Roe solver, accounting for an external gravity field and an arbitrary equation of state from a table.

The radiation transport is computed with either one of three modules:

- `MSrad` module: It uses long characteristics. The lateral boundaries have to be periodic. Top and bottom can be closed or open ("solar module").
- `LHDrad` module: It uses long characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (old "supergiant module").
- `SHORTrad` module: It uses short characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (new "supergiant module").

Recently, the code was supplemented with an (optional) MHD version [Schaffenberger et al. (2005)] that can treat magnetic fields. There are also modules for the formation and advection of dust available. The current version now contains the treatment of chemical reaction networks, mostly used for the formation of molecules [Wedemeyer-Böhm et al. (2005)], and hydrogen ionization [Leenaarts & Wedemeyer-Böhm (2005)], too.

CO5BOLD is written in Fortran90. The parallelization is done with OpenMP directives.

To get a brief overview you might want to look into the "Quickstart Sections" "How to Compile CO5BOLD" (Sect. 3.1), "Introduction to UIO" (Sect. 4.1), "How to Make a Proper Parameter File" (Sect. 5.3.1), "How to Run CO5BOLD" (Sect. 6.1).

2 Equations

2.1 Basic Equations

The hydrodynamics equations are expressed as conservation relations plus source terms for

$$\rho,\ \rho v1, \rho v2, \rho v3,\ \rho e\mathrm{ikg}\ , \tag{1}$$

the mass density, the three mass fluxes and the total energy density (per volume), respectively. Each quantity q has its corresponding flux f(q) and possibly source term s(q). For convenience,

$$\rho,\ v1, v2, v3,\ e\mathrm{i} \tag{2}$$

are chosen as independent quantities. The conserved quantities are purely algebraic combinations of these.

The 3D hydrodynamics equations, including source terms due to gravity, are the *mass conservation equation*

$$\frac{\partial \rho}{\partial t} + \frac{\partial\ \rho\ v1}{\partial x1} + \frac{\partial\ \rho\ v2}{\partial x2} + \frac{\partial\ \rho\ v3}{\partial x3} = 0\ , \tag{3}$$

the *momentum equation*

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho v1 \\ \rho v2 \\ \rho v3 \end{pmatrix} + \frac{\partial}{\partial x1}\begin{pmatrix} \rho v1\ v1 + P \\ \rho v2\ v1 \\ \rho v3\ v1 \end{pmatrix} + \frac{\partial}{\partial x2}\begin{pmatrix} \rho v1\ v2 \\ \rho v2\ v2 + P \\ \rho v3\ v2 \end{pmatrix} + \frac{\partial}{\partial x3}\begin{pmatrix} \rho v1\ v3 \\ \rho v2\ v3 \\ \rho v3\ v3 + P \end{pmatrix} = \begin{pmatrix} \rho\ g1 \\ \rho\ g2 \\ \rho\ g3 \end{pmatrix} \tag{4}$$

and the *energy equation* including radiative heating term Q_{rad}

$$\frac{\partial \rho e\mathrm{ik}}{\partial t} + \frac{\partial\ (\rho e\mathrm{ik}+P)\ v1}{\partial x1} + \frac{\partial\ (\rho e\mathrm{ik}+P)\ v2}{\partial x2} + \frac{\partial\ (\rho e\mathrm{ik}+P)\ v3}{\partial x3} = \rho\ (g1\ v1+g2\ v2+g3\ v3)+Q_{\mathrm{rad}}\ . \tag{5}$$

The pressure P is computed from density ρ and internal energy ei via a (tabulated) *equation of state*

$$P = P(\rho, e\mathrm{i})\ . \tag{6}$$

For local models the *gravity* field is simply given by

$$\vec{g} = \begin{pmatrix} 0 \\ 0 \\ -g \end{pmatrix}\ . \tag{7}$$

For global models it is given by

$$\vec{g} = \begin{pmatrix} g1 \\ g2 \\ g3 \end{pmatrix} = -\begin{pmatrix} \frac{\partial}{\partial x1} \\ \frac{\partial}{\partial x2} \\ \frac{\partial}{\partial x3} \end{pmatrix}\Phi \tag{8}$$

with

$$\Phi = -\frac{G\,M_*}{\left(r_0^4 + r^4/\sqrt{1+(r/r_1)^8}\right)^{1/4}}\ . \tag{9}$$

Here, M_* is the mass of the star to be modeled; r_0 and r_1 are free smoothing parameters.

In addition, there are equations for the non-local radiation transport. If grey opacity tables are used, the opacities κ are a simple function of e.g. temperature T and pressure P

$$\kappa = \kappa(T, P) \tag{10}$$

and the source function S is given by

$$S = \frac{\sigma}{\pi}T^4\ . \tag{11}$$

The change in optical depth $\Delta\tau$ along a path with length Δx is than

$$\Delta\tau = \kappa\rho\Delta x \ . \tag{12}$$

The variation of the intensity I with optical depth τ along a ray with orientation (θ, φ) can be described by the simple differential equation

$$\frac{\mathrm{d}I}{\mathrm{d}\tau} = -I + S \ . \tag{13}$$

The radiative energy flux is given by

$$F_{\mathrm{rad}} = \int_0^{2\pi} \int_0^{\pi} I \cos\theta \sin\theta \ \mathrm{d}\theta \ \mathrm{d}\varphi \ . \tag{14}$$

The energy change can than be computed from the flux divergence with

$$\frac{\partial \rho e\mathrm{i}}{\partial t} = Q_{\mathrm{rad}} = -\left(\frac{\partial F_{x1,\mathrm{rad}}}{\partial x1} + \frac{\partial F_{x2,\mathrm{rad}}}{\partial x2} + \frac{\partial F_{x3,\mathrm{rad}}}{\partial x3}\right) \ . \tag{15}$$

2.2 Magnetohydrodynamics (W. Schaffenberger)

The current MHD module is a reduced version of the original MHD module. The aim was to create a stable and easy to use module (see [Schaffenberger et al. (2005)]).

The module has the following features:

- Use of the HLL solver with the Janhunen source terms.
- Extension to 2nd order with linear reconstruction and a Hancock predictor step.
- The following limiters are available: Minmod, vanLeer, Superbee.
- Hybridization of 1st and 2nd order flux to ensure positivity of pressure and density.
- Flux interpolated constrained transport step.
- Small violation of strict energy conservation after the constrained transport step to keep the pressure positive.

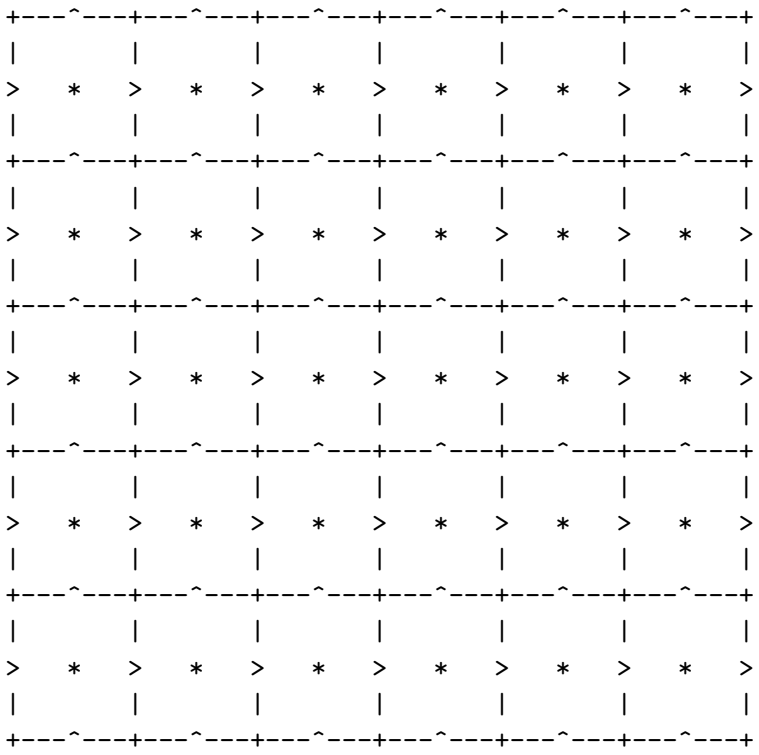
The original test version has the additional features:

- HLLC, HLLEM, and Roe solver.
- Janhunen source terms can be deactivated.
- Use of entropy equation instead of energy equation possible.
- Use of both, energy equation and entropy equation possible.
- Field interpolated constrained transport step available.
- Different choices for the energy correction after the constrained transport step: no energy correction, exact energy conservation for each cell or energy correction only if pressure remains positive.

Originally, the module included also an explicit electric conductivity and an additional energy diffusion. These were removed due to a modification of the constrained transport routine. These features may be supported again in a future version of the module.

The magnetic field is located at the cell boundaries rather than in the cell centers. Therefore, the format of the magnetic field arrays is slightly different from that of the other hydrodynamic variables.

Staggered grid representation of the magnetic field in 2 dimensions:



* hydrodynamic variables
> x component of the magnetic field
^ y component of the magnetic field

The extension to 3 dimensions should be clear. Variables at the left or the bottom boundary have the same indices as the cell.

For a box with 120×120×120 cells, the headers for the magnetic field arrays in the start model may look like

```
real bb1 d=(1:121,1:120,1:120) f=E13.6 p=4 b=4 &
         n='cell boundary magnetic field 1' u=G*sqrt(4pi)
real bb2 d=(1:120,1:121,1:120) f=E13.6 p=4 b=4 &
         n='cell boundary magnetic field 2' u=G*sqrt(4pi)
real bb3 d=(1:120,1:120,1:121) f=E13.6 p=4 b=4 &
         n='cell boundary magnetic field 3' u=G*sqrt(4pi)
```

For simplicity, the MHD module uses units such that the 4 pi factors do not appear in the MHD equations.

THEREFORE YOU HAVE TO MULTIPLY YOUR ORIGINAL MAGNETIC FIELDS IN GAUSS WITH THE FACTOR 1 / SQRT(4 PI) TO GET THE CORRECT MAGNETIC FIELD STRENGTH FOR CO5BOLD!!!

AFTER THE COMPUTATION, YOU HAVE TO MULTIPLY THE MAGNETIC FIELDS FROM THE CO5BOLD OUTPUT WITH THE FACTOR SQRT(4 PI) TO GET THE MAGNETIC FIELD STRENGTH IN GAUSS!!!

The CO5BOLD analysis tool CAT does this automatically during the reading of model data, so you can use the CO5BOLD output directly with CAT.

Positivity of pressure and density:
A special problem of MHD simulations is that pressure or density can become negative in some situations. This problem is also present in pure hydrodynamic simulations but gets worse for MHD. The original hydrodynamic version of CO5BOLD tries to fix this problem by reducing the time step. In hydrodynamics, this works in most cases. In MHD, however, reduction of the time step often does not help and other methods are necessary to avoid this problem. Therefore, the

MHD module uses a HLL solver instead of a Roe solver like the hydrodynamic module. It was shown numerically by Janhunen, that using a HLL solver together with additional source terms in the induction equation keeps pressure and density positive under all circumstances. Because the constrained transport step, which is performed after the 1D sweeps with the MHD solver, changes the magnetic field, a correction of the internal energy in each cell is necessary to keep the total energy conserved. Because this correction can lead to negative pressure, it is omitted if the internal energy would become too small. Therefore, the total energy is not exactly conserved but this affects only a few cells in the simulation box.

Concluding remarks:
The methods described above result in a very robust scheme which guarantees positivity of pressure and density under almost all conditions. However, this does not mean, that these values are accurate! The pressure and temperature distribution may be very inaccurate in regions with strong magnetic fields. This may be relevant, if one includes special chromospheric physics such as dynamic hydrogen ionization and CO formation in the simulation. A possibility to get more accurate pressure and temperature would be the use of the entropy equation instead of the energy equation for the computation of the internal energy in regions with strong magnetic field. This was included in the original test version of the MHD module. An other possibility is the use of the equation for the thermal energy itself. This is the dual energy approach, used in many MHD codes.

Due to the Courant condition, the time step can become considerably smaller than in the hydrodynamic case. This happens because the time step is also limited by the Alfvén speed which is large in regions with strong magnetic field and low density.

This module has been extensively tested. It should be able to handle many MHD flows of astrophysical interest. Bugs and problems can be reported to `werner.schaffenberger@gmx.at`.

2.3 A collection of thermodynamic relations (M. Steffen, AIP)

2.3.1 Basic thermodynamic equations

Differential relations:

$$\mathrm{d}e = T\mathrm{d}s + \frac{p}{\rho^2}\mathrm{d}\rho \tag{16}$$

where e is the **internal energy** .

$$\mathrm{d}h = T\mathrm{d}s + \frac{1}{\rho}\mathrm{d}p \tag{17}$$

where the **specific enthalpy** , h, is defined as

$$h = e + p/\rho \tag{18}$$

This implies:

$$\left(\frac{\partial e}{\partial s}\right)_\rho = T \tag{19}$$

$$\left(\frac{\partial e}{\partial \rho}\right)_s = \frac{p}{\rho^2} \tag{20}$$

$$\left(\frac{\partial h}{\partial s}\right)_p = T \tag{21}$$

$$\left(\frac{\partial h}{\partial p}\right)_s = \frac{1}{\rho} \tag{22}$$

2.3.2 Definition of often-used thermodynamic coefficients

Definition of specific heats:

$$c_p \equiv \left(\frac{\partial h}{\partial T}\right)_p = T\left(\frac{\partial s}{\partial T}\right)_p = \left(\frac{\partial s}{\partial \ln T}\right)_p \tag{23}$$

$$c_v \equiv \left(\frac{\partial e}{\partial T}\right)_\rho = T\left(\frac{\partial s}{\partial T}\right)_\rho = \left(\frac{\partial s}{\partial \ln T}\right)_\rho \tag{24}$$

Definitions of further thermodynamic coefficients:

$$\chi_T \equiv \left(\frac{\partial \ln p}{\partial \ln T}\right)_\rho \tag{25}$$

$$\chi_\rho \equiv \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_T \equiv (Kp)^{-1} \tag{26}$$

$$\delta \equiv -\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \equiv \alpha T = \frac{\chi_T}{\chi_\rho} \tag{27}$$

It can be shown that

$$c_p - c_v = \alpha^2 T/(K\rho) = \frac{p}{\rho T}\,\delta^2\,\chi_\rho = \frac{p}{\rho T}\,\delta\,\chi_T = \frac{p}{\rho T}\,\chi_T^2/\chi_\rho \tag{28}$$

Definition of adiabatic exponents:

$$\Gamma_1 \equiv \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_s \tag{29}$$

$$\Gamma_3 \equiv \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s + 1 \tag{30}$$

$$\nabla_{\rm ad} \equiv \left(\frac{\partial \ln T}{\partial \ln p}\right)_s \equiv \frac{\Gamma_2 - 1}{\Gamma_2} \tag{31}$$

2.3.3 CO5BOLD equation of state

CO5BOLD equation of state input:

$$\rho;\ e \tag{32}$$

CO5BOLD equation of state output:

$$s;\ P;\ T;\ \left(\frac{\partial p}{\partial e}\right)_\rho;\ \left(\frac{\partial p}{\partial \rho}\right)_e;\ \left(\frac{\partial T}{\partial e}\right)_\rho \tag{33}$$

All required thermodynamic coefficients can be expressed in terms of $\left(\frac{\partial p}{\partial e}\right)_\rho, \left(\frac{\partial p}{\partial \rho}\right)_e, \left(\frac{\partial T}{\partial e}\right)_\rho$:

2.3.4 Derived thermodynamic coefficients

First, the missing derivative $\left(\frac{\partial T}{\partial \rho}\right)_e$ can be found from the relation:

$$\left(\frac{\partial T}{\partial \rho}\right)_e = \frac{T}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho - \frac{p}{\rho^2}\left(\frac{\partial T}{\partial e}\right)_\rho \tag{34}$$

which is obtained from the equality of the mixed derivatives in Eq.(16), written as:

$$\mathrm{d}s = \frac{1}{T}\mathrm{d}e - \frac{p}{T\rho^2}\mathrm{d}\rho \tag{35}$$

Then

$$\frac{\partial^2 s}{\partial e \partial \rho} = \frac{\partial}{\partial \rho}\left(\frac{1}{T}\right)_e = \frac{\partial}{\partial e}\left(-\frac{p}{T\rho^2}\right)_\rho \tag{36}$$

First adiabatic exponent:

$$\Gamma_1 \equiv \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_s = \frac{\rho}{p}\left(\frac{\partial p}{\partial \rho}\right)_e + \frac{1}{\rho}\left(\frac{\partial p}{\partial e}\right)_\rho \tag{37}$$

This relation is obtained by combining Eq.(16) with the identity

$$\mathrm{d}p = \left(\frac{\partial p}{\partial \rho}\right)_e \mathrm{d}\rho + \left(\frac{\partial p}{\partial e}\right)_\rho \mathrm{d}e \tag{38}$$

The **adiabatic sound speed** is then obtained as

$$c_s \equiv \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\Gamma_1 \frac{p}{\rho}} \tag{39}$$

Third adiabatic exponent:

$$\Gamma_3 \equiv 1 + \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s = 1 + \frac{1}{\rho}\left(\frac{\partial p}{\partial e}\right)_\rho \tag{40}$$

This relation is obtained by combining Eq.(16) with the identity

$$\mathrm{d}T = \left(\frac{\partial T}{\partial \rho}\right)_e \mathrm{d}\rho + \left(\frac{\partial T}{\partial e}\right)_\rho \mathrm{d}e \tag{41}$$

and then using Eq.(34).

Adiabatic temperature gradient:

$$\nabla_{\mathrm{ad}} \equiv \left(\frac{\partial \ln T}{\partial \ln p}\right)_s = \frac{\Gamma_3 - 1}{\Gamma_1} \tag{42}$$

since

$$\left(\frac{\partial \ln T}{\partial \ln p}\right)_s = \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s \cdot \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_s = \frac{\Gamma_3 - 1}{\Gamma_1}. \tag{43}$$

Adiabatic energy changes:

$$\rho\left(\frac{\partial e}{\partial p}\right)_s = \frac{p}{\rho}\left(\frac{\partial \rho}{\partial p}\right)_s = \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_s = \frac{1}{\Gamma_1} \tag{44}$$

or

$$\left(\frac{\partial \rho e}{\partial p}\right)_s = e\left(\frac{\partial \rho}{\partial p}\right)_s + \rho\left(\frac{\partial e}{\partial p}\right)_s = \frac{1}{\Gamma_1}\left(1 + \frac{\rho e}{p}\right) \tag{45}$$

We define the coefficients c_v' and c_p' through the relation

$$\mathrm{d}s = c_v' \mathrm{d}\ln p - c_p' \mathrm{d}\ln \rho \tag{46}$$

Entropy change at constant density:

$$c_v' = \left(\frac{\partial s}{\partial \ln p}\right)_\rho = \frac{p}{\rho T}\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_s = \frac{p}{\rho T}\frac{1}{\Gamma_3 - 1} \tag{47}$$

This relation is obtained from the equality of the mixed derivatives in Eq.(16) together with Eq.(40).

Entropy change at constant pressure:

$$c'_p = -\left(\frac{\partial s}{\partial \ln \rho}\right)_p = \frac{p}{\rho T}\left(\frac{\partial \ln p}{\partial \ln T}\right)_s = \frac{p}{\rho T}\frac{\Gamma_1}{\Gamma_3 - 1} \tag{48}$$

This relation is obtained from the equality of the mixed derivatives in Eq.(17) together with Eq.(42).

Specific heat at constant density:

$$c_v = c'_v \chi_T = \left(\frac{\partial s}{\partial \ln T}\right)_\rho = \left(\frac{\partial e}{\partial T}\right)_\rho = 1/\left(\frac{\partial T}{\partial e}\right)_\rho \tag{49}$$

To derive the specific heat at constant pressure, we start from the relation

$$\mathrm{d}\ln T = \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s \mathrm{d}\ln \rho + \left(\frac{\partial \ln T}{\partial s}\right)_\rho \mathrm{d}s \tag{50}$$

from which we get

$$\left(\frac{\partial s}{\partial \ln \rho}\right)_T = -\left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s \Big/ \left(\frac{\partial \ln T}{\partial s}\right)_\rho \tag{51}$$

Using Eqs.(40) and (49), we obtain

$$\left(\frac{\partial s}{\partial \ln \rho}\right)_T = -c_v\,(\Gamma_3 - 1) \tag{52}$$

Now

$$\mathrm{d}s = \left(\frac{\partial s}{\partial \ln p}\right)_\rho \mathrm{d}\ln p + \left(\frac{\partial s}{\partial \ln \rho}\right)_p \mathrm{d}\ln \rho \tag{53}$$

or

$$\mathrm{d}s = \left(\frac{\partial s}{\partial \ln p}\right)_\rho \mathrm{d}\ln p + \left(\frac{\partial s}{\partial \ln \rho}\right)_p \left\{\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_s \mathrm{d}\ln T + \left(\frac{\partial \ln \rho}{\partial s}\right)_T \mathrm{d}s\right\} \tag{54}$$

hence

$$\mathrm{d}s\left\{1 - \left(\frac{\partial s}{\partial \ln \rho}\right)_p \left(\frac{\partial \ln \rho}{\partial s}\right)_T\right\} = \left(\frac{\partial s}{\partial \ln p}\right)_\rho \mathrm{d}\ln p + \left(\frac{\partial s}{\partial \ln \rho}\right)_p \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_s \mathrm{d}\ln T \tag{55}$$

and finally

$$\left(\frac{\partial \ln T}{\partial s}\right)_p = \left\{1 - \left(\frac{\partial s}{\partial \ln \rho}\right)_p \left(\frac{\partial \ln \rho}{\partial s}\right)_T\right\} \Big/ \left\{\left(\frac{\partial s}{\partial \ln \rho}\right)_p \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_s\right\} \tag{56}$$

or

$$\left(\frac{\partial \ln T}{\partial s}\right)_p = \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s \left\{\left(\frac{\partial \ln \rho}{\partial s}\right)_p - \left(\frac{\partial \ln \rho}{\partial s}\right)_T\right\} \tag{57}$$

Using Eqs.(23), (40), (48), (52), we finally obtain the relation for the **specific heat at constant pressure:**

$$\frac{1}{c_p} = \frac{1}{c_v} - \frac{\rho T}{p}\frac{(\Gamma_3 - 1)^2}{\Gamma_1} = \frac{1}{c_v} - T\left(\frac{\Gamma_3 - 1}{c_s}\right)^2 \tag{58}$$

Alternatively, c_p can be obtained from Eq.(28)

$$c_p = c_v + \frac{p}{\rho T}\,\delta\,\chi_T \tag{59}$$

or from

$$c_p = \delta\,c_p' = \frac{p}{\rho T}\,\delta\,\frac{\Gamma_1}{\Gamma_3 - 1} \tag{60}$$

once δ and χ_T are known (see below).

We can now express the thermodynamic coefficients provided by CO5BOLD in terms of c_v, Γ_1, Γ_3, and $\nabla_{\rm ad}$:

$$\left(\frac{\partial p}{\partial e}\right)_\rho = \rho\,(\Gamma_3 - 1) \tag{61}$$

$$\left(\frac{\partial p}{\partial \rho}\right)_e = \frac{p}{\rho}\,(1 - \Gamma_3 + \Gamma_1) \tag{62}$$

$$\left(\frac{\partial T}{\partial e}\right)_\rho = \frac{1}{c_v} \tag{63}$$

$$\left(\frac{\partial T}{\partial \rho}\right)_e = \frac{T}{\rho}\,(\Gamma_3 - 1) - \frac{p}{\rho^2}\frac{1}{c_v} \tag{64}$$

$$\left(\frac{\partial e}{\partial \rho}\right)_T = -\left(\frac{\partial T}{\partial \rho}\right)_e \Big/ \left(\frac{\partial T}{\partial e}\right)_\rho = \frac{p}{\rho^2}\left\{1 - \frac{\rho T}{p}\,c_v\,(\Gamma_3 - 1)\right\} \tag{65}$$

$$\left(\frac{\partial e}{\partial \rho}\right)_p = -\left(\frac{\partial p}{\partial \rho}\right)_e \Big/ \left(\frac{\partial p}{\partial e}\right)_\rho = \frac{p}{\rho^2}\left\{1 - \frac{\Gamma_1}{\Gamma_3 - 1}\right\} = \frac{p}{\rho^2}\frac{\nabla_{\rm ad} - 1}{\nabla_{\rm ad}} \tag{66}$$

We consider again Eq.(35), replacing $\mathrm{d}e$ by

$$\mathrm{d}e = \left(\frac{\partial e}{\partial T}\right)_\rho \mathrm{d}T + \left(\frac{\partial e}{\partial \rho}\right)_T \mathrm{d}\rho \tag{67}$$

so

$$\mathrm{d}s = \frac{1}{T}\left(\frac{\partial e}{\partial T}\right)_\rho \mathrm{d}T + \left\{\frac{1}{T}\left(\frac{\partial e}{\partial \rho}\right)_T - \frac{p}{T\rho^2}\right\}\mathrm{d}\rho \tag{68}$$

The requirement that the mixed derivatives must be equal then yields

$$\frac{\partial}{\partial \rho}\left(\frac{1}{T}\left(\frac{\partial e}{\partial T}\right)_\rho\right)_T = \frac{\partial}{\partial T}\left(\frac{1}{T}\left(\frac{\partial e}{\partial \rho}\right)_T - \frac{p}{T\rho^2}\right)_\rho \tag{69}$$

or

$$0 = -\frac{1}{T^2}\left(\frac{\partial e}{\partial \rho}\right)_T - \frac{1}{\rho^2}\left\{\frac{1}{T}\left(\frac{\partial p}{\partial T}\right)_\rho - \frac{p}{T^2}\right\} \tag{70}$$

Finally,

$$\left(\frac{\partial e}{\partial \rho}\right)_T = \frac{p}{\rho^2}\left\{1 - \left(\frac{\partial \ln p}{\partial \ln T}\right)_\rho\right\} = \frac{p}{\rho^2}(1 - \chi_T) \tag{71}$$

Comparison with Eq.(65) implies

$$\chi_T = \frac{\rho T}{p}\, c_v\, (\Gamma_3 - 1) \tag{72}$$

Similarly, replacing de by

$$\mathrm{d}e = \left(\frac{\partial e}{\partial p}\right)_\rho \mathrm{d}p + \left(\frac{\partial e}{\partial \rho}\right)_p \mathrm{d}\rho \tag{73}$$

in Eq.(35), we get

$$\mathrm{d}s = \frac{1}{T}\left(\frac{\partial e}{\partial p}\right)_\rho \mathrm{d}p + \left\{\frac{1}{T}\left(\frac{\partial e}{\partial \rho}\right)_p - \frac{p}{T\rho^2}\right\}\mathrm{d}\rho \tag{74}$$

and the requirement that the mixed derivatives must be equal then yields

$$\frac{\partial}{\partial \rho}\left(\frac{1}{T}\left(\frac{\partial e}{\partial p}\right)_\rho\right)_p = \frac{\partial}{\partial p}\left(\frac{1}{T}\left(\frac{\partial e}{\partial \rho}\right)_p - \frac{p}{T\rho^2}\right)_\rho \tag{75}$$

or

$$\left(\frac{\partial e}{\partial p}\right)_\rho \left(\frac{\partial T}{\partial \rho}\right)_p = \left(\frac{\partial T}{\partial p}\right)_\rho \left\{\left(\frac{\partial e}{\partial \rho}\right)_p - \frac{p}{\rho^2}\right\} + \frac{T}{\rho^2} \tag{76}$$

or

$$\left(\frac{\partial e}{\partial p}\right)_\rho \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_p = \left(\frac{\partial \ln T}{\partial \ln p}\right)_\rho \left\{\frac{\rho}{p}\left(\frac{\partial e}{\partial \rho}\right)_p - \frac{1}{\rho}\right\} + \frac{1}{\rho}. \tag{77}$$

Since

$$\left(\frac{\partial \ln T}{\partial \ln \rho}\right)_p \Big/ \left(\frac{\partial \ln T}{\partial \ln p}\right)_\rho = -\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_T = -\chi_\rho \tag{78}$$

we finally obtain, using Eqs.(25), (61) and (66),

$$\chi_\rho = \Gamma_1 - \chi_T\, (\Gamma_3 - 1) \tag{79}$$

and

$$\delta = \chi_T / \left\{\Gamma_1 - \chi_T\, (\Gamma_3 - 1)\right\} \tag{80}$$

The **isothermal sound speed** is then obtained as

$$c_T \equiv \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{\chi_\rho \frac{p}{\rho}} = \sqrt{\Gamma_1 \frac{p}{\rho}\left\{1 - \chi_T \frac{\Gamma_3 - 1}{\Gamma_1}\right\}} = c_s \sqrt{(1 - \chi_T \nabla_{\mathrm{ad}})} \tag{81}$$

2.3.5 Ideal gas with constant specific heats (polytropic gas)

In this case, we obtain much simpler relations:

$$e = c_v T = \frac{p}{\rho}\frac{1}{\gamma - 1} \tag{82}$$

$$h = c_p T = \frac{p}{\rho}\frac{\gamma}{\gamma - 1} \tag{83}$$

$$s = c_v \left\{\ln p - \gamma \ln \rho\right\} + \text{const.} \tag{84}$$

$$\gamma \equiv \frac{c_p}{c_v} = \Gamma_1 = \Gamma_2 = \Gamma_3 = \text{const.} \tag{85}$$

$$c_p - c_v = \frac{p}{\rho T} \equiv \mathcal{R} \tag{86}$$

$$c_v = \mathcal{R}\frac{1}{\gamma - 1} = c'_v \tag{87}$$

$$c_p = \mathcal{R}\frac{\gamma}{\gamma - 1} = c'_p \tag{88}$$

$$\chi_T = \chi_\rho = \delta = 1 \tag{89}$$

$$c_s \equiv \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\gamma \frac{p}{\rho}} \tag{90}$$

$$c_T \equiv \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{\frac{p}{\rho}} \tag{91}$$

3 Program Files, Installation, Compilation

In this section all the files and modules CO5BOLD contains are listed. The installation procedure is outlined and compiler switches necessary to compile CO5BOLD and to optimize its performance are described.

3.1 Quickstart: How to Compile CO5BOLD

If you are going to install CO5BOLD on a machine with a "known" (to setup script and makefile) operating system and compiler (see Sections 3.5 and 3.7) then the procedure should be fairly easy. The general compilation procedure is now:

If a directory for the current machine exists (in the tar ball) and the configure script is there:

```
tar -zxvf for.tar.gz
cd for/hd/rhd/YOUR_MACHINE
./configure
make
```

If the directory for the current machine has to be created:

```
tar -zxvf for.tar.gz
cd for/hd/rhd
mkdir YOUR_MACHINE
cd YOUR_MACHINE
ln -s ../conf/configure .
./configure
make
```

The compilation process is explained in more detail in Sect. 3.2. The configure script is described in its header and in Sect. 3.5. The directory structure is shown in Tab. 1. All Fortran files are listed in Tables 2 and 3.

3.2 Compilation Procedure for CO5BOLD

The installation procedure has changed significantly since the last release: now, there is a configure script (see Sect. 3.5) that creates the complete (temporary) makefile which can be used to compile CO5BOLD and produce the executable `rhd.exe`.

Installation procedure:

1. Choose/create a proper base directory. (This will usually be `$HOME`. Then the master directory will typically be `$HOME/for` – this is the default created by the tar file. Some prefer to rename it to `$HOME/HYDRO`.)

2. Put all source files and the configure script there. This will be done typically by expanding the gzipped tar file `for.tar.gz` e.g. with

   ```
   tar -zxvf for.tar.gz
   ```

   (or by copying all files from an existing installation). On a restricted UNIX you might be forced to use

   ```
   gunzip for.tar.gz
   tar -xvf for.tar
   ```

   instead. Unpacking the tar file creates a sub directory `for` in the local directory (and possible overwrites existing files!). You get sub sub directories as described in Sect. 3.3 and files as listed in Tables 2 and 3. See the Readme file '`for/README`'.

3. Change with

   ```
   cd for/hd/rhd
   ```

   into the main directory.

4. Look at the existing sub directories, e.g. with

   ```
   ls -og | grep "^d"
   ```

   to see if you find one that fits your machine. The directory

   ```
   for/hd/rhd/conf
   ```

   should not be used. It contains only the configure script. But any other directory will do. If you don't like any of the existing directories, create your own e.g. with

   ```
   mkdir YOUR_MACHINE
   ```

   Change into this directory with

   ```
   cd YOUR_MACHINE
   ```

5. Check if there is a configure script or a link to it with

   ```
   ls -og configure
   ```

   which should give something like

   ```
   lrwxrwxrwx  1  17 2002-12-04 17:39 configure -> ../conf/configure
   ```

   If it is not there, create the link with

   ```
   ln -s ../conf/configure .
   ```

6. Start the configure script to create the (first version of the) Makefile

   ```
   ./configure
   ```

   This gives you a screen output like

   ```
   Configuration script for CO5BOLD Makefile
   =========================================

   No parallelization requested, assume default:  F90_PARALLEL=scalar
   No debugging requested, assume default:        F90_DEBUG=0
   No LHDrad   module requested, assume default:  F90_LHDRAD=0
   No MSrad    module requested, assume default:  F90_MSRAD=0
   No SHORTrad module requested, assume default:  F90_SHORTRAD=1
   No CHEM     module requested, assume default:  F90_CHEM=0
   No HION     module requested, assume default:  F90_HION=0
   No dust     module requested, assume default:  F90_DUST=0
   No MHD      module requested, assume default:  F90_MHD=0
   No TWEAK    module requested, assume default:  F90_TWEAK=0
   No explicit machine requested, assume default: F90_MACHINE=local
   ```

```
List of control environment variables:
F90_COMPILER =
F90_PREFLAGS =
F90_POSTFLAGS=
F90_PARALLEL = scalar
F90_DEBUG    = 0
F90_LHDRAD   = 0
F90_MSRAD    = 0
F90_SHORTRAD = 1
F90_CHEM     = 0
F90_HION     = 0
F90_DUST     = 0
F90_MHD      = 0
F90_TWEAK    = 0
F90_MACHINE  = local
 -> MACHINE  = i686
    MACMODEL = Intel Pentium
F90_BASEPATH = /home/bf/for

Linux system with i686 architecture
  PGI compiler
  version=3.3-2

pgf90 -byteswapio -fast -Mvect=sse -Mcache_align -Minfo=inline

Write compiler name and flags into file compiler_flags.info

Makefile already exists. It is appended to Makefile_old.
New Makefile written.....................................
```

A new '`Makefile`' is produced. An existing one is appended to '`Makefile_old`'. Additionally, the file '`compiler_flags.info`' is written which contains the compiler call in Fortran format.

7. Check the output of the configure script and the header of the new Makefile. You get an overview over the relevant environment variables that control the configure script (see Sect. 3.5) with

   ```
   env | grep F90_
   ```

   Obs: at the beginning there might be none.

8. Look into the header (and if necessary the rest) of the configure script or into Sect. 3.5 to find out how to change the environment variables to control the script properly. For instance, if you want to enable debugging options, type:

   ```
   export F90_DEBUG=1
   ```

   Restart the configure script after every change in the control variables! With e.g.

   ```
   export F90_MACHINE=dummy
   export F90_PREFLAGS="-Oprettyfast +Qsomethingelse"
   ./configure
   ```

it is possible to specify all machine-dependent settings yourself (see Sect. 3.5 and Sect. 3.5). This is useful when dealing with a compiler hitherto unknown to the configure script.

9. Start the compilation with

```
make
```

to produce the executable `rhd.exe`.

A simple sample installation may look like the following (the sub directory '`for`' is put into the home directory).

```
# --- Choose base directory ---
cd $HOME

# --- Put the tar file there ---
# ...

# --- Expand the tar file ---
tar -zxvf for.tar.gz

# --- Go into (default) master directory ---
cd for/hd/rhd/YOUR_MACHINE

# --- Activate OpenMP und MSrad radiation transport ---
export F90_PARALLEL=openmp
export F90_MSRAD=1

# --- Start the configure script ---
./configure

# --- Compile ---
make

echo 'Voila!'
```

If you want to compile in a directory in a completely different place (not in a sub directory of `for` as described above), you have to set the environment variable `F90_BASEPATH` (see Sect. 3.5) to make the paths to the source files known to the configure script. That might look like

```
mkdir SOME_WEIRD_PLACE
cd SOME_WEIRD_PLACE
export F90_BASEPATH=$HOME/for
ln -s $F90_BASEPATH/hd/rhd/conf/configure .
./configure
```

The variable `F90_BASEPATH` also has to be set explicitely if the main directory `for` should have another name. Renaming the sub-directories with the source files is not a good idea – it requires modifications of the configure script itself.

3.3 Directory Structure

The files necessary to compile CO5BOLD are distributed over a few directories. A typical setup would be to put everything into the main directory `for`. Then the source files would be located as in Tab. 1.

The executables (and makefiles, object files, module information files) are usually located in subdirectories of the source code directories. These subdirectories typically have the name of the machine, architecture, or operating system the executable is compiled for.

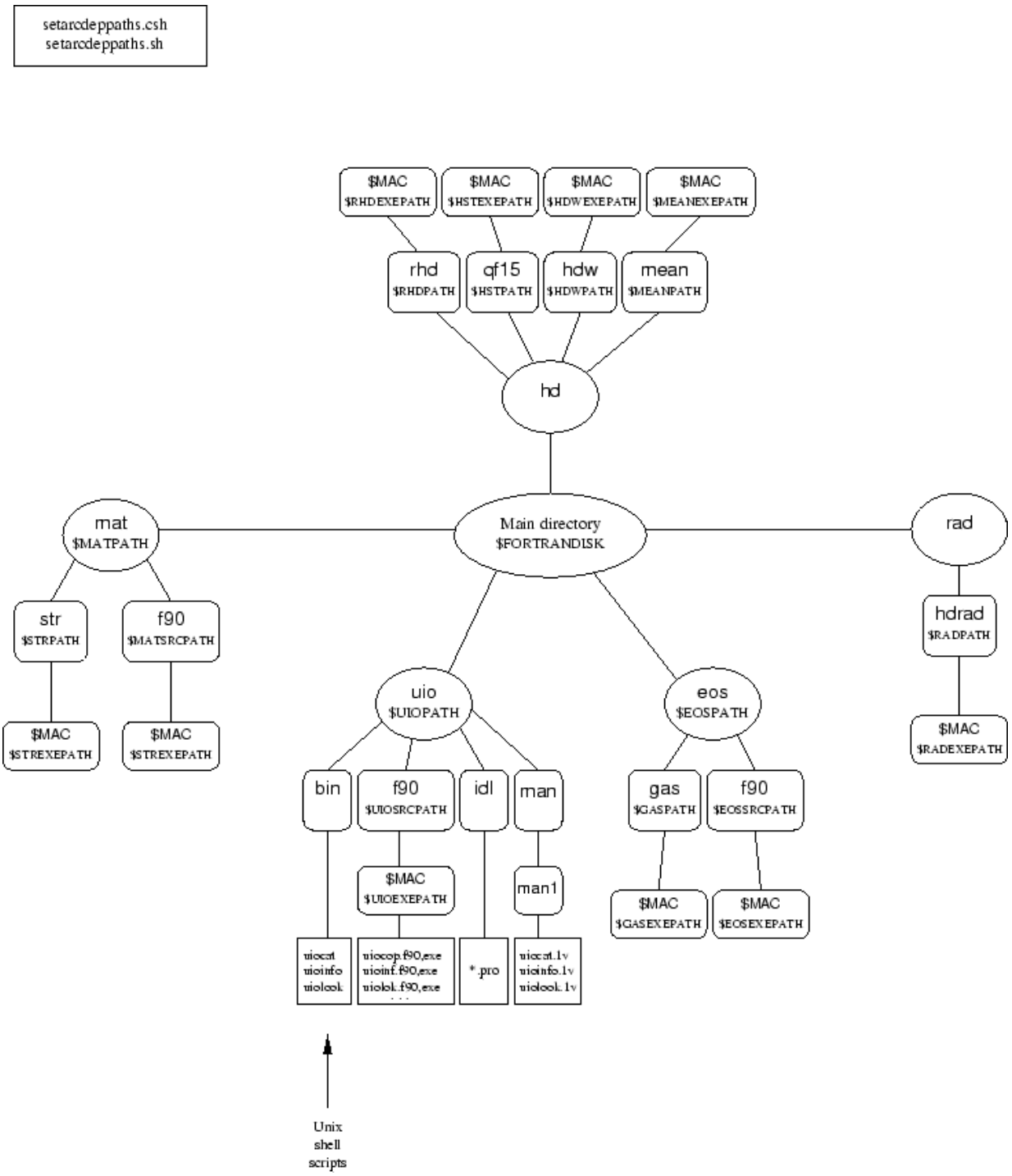


Figure 1: Old directory scheme

Paths	Abb.	Description
`${HOME}/for/con/f90/`	CON	constants and units
`${HOME}/for/dust/f90/`	DUST	source terms due to dust or molecules
`${HOME}/for/hion/f90/`	HION	time-dependent hydrogen ionization
`${HOME}/for/chem/`	CHEM	chemical reaction network
`${HOME}/for/eos/f90/`	EOS	equation of state
`${HOME}/for/hd/mhd/`	MHD	MHD routines
`${HOME}/for/hd/rhd/`	RHD	main rhd routines (hydro, Bernd's radiation transport)
`${HOME}/for/hd/rhdb/`	RHDB	basic rhd routines
`${HOME}/for/mat/str/`	STR	string handling
`${HOME}/for/opa/opta/`	OPTA	opacities
`${HOME}/for/rad/hdrad/`	RAD	Matthias' radiation transport
`${HOME}/for/uio/f90/`	UIO	I/O routines
`${HOME}/for/time/f90/`	TIME	timing routines

Table 1: List of source directories with path and file name, abbreviation, and a short description.

3.4 Fortran Files

Tables 2 and 3 show a list of all source files necessary to compile the complete version of CO5BOLD.

3.5 Configure Script

The configure script produces a Makefile.

It is controlled by environment variables (see below). It tries to use reasonable default values if they are not set (properly). In the script the machine type is determined with 'uname -m'. According to the control variables and the machine architecture the compiler name and its compiler flags are composed. These are written into the header of a Makefile which is produced in the end. An existing Makefile is appended to

```
Makefile_old.
```

Additionally the compilation command is written into the file

```
'compiler_flags.info'
```

in a form ready to be included in a Fortran program.

The environment variables that control the script are

- `F90_COMPILER`:
  Fortran compiler:
  - `''`: a machine dependent default is chosen individually for each architecture
  - `f90`: general default
- `F90_PREFLAGS`:
  Compiler flags to be put at the beginning of the list. Usually, the list of compiler flags produced by the configure script should be pretty complete. But you might want to add special switches like '-Bstatic' to enforce static linking of libraries.
  - `''`: No extra flags
- `F90_POSTFLAGS`:
  Compiler flags to be put at the end of the list. Usually, the list of compiler flags produced by the configure script should be pretty complete. However, you might want to overwrite some settings. This can be done by setting this variable to a none-empty value because typically a compiler should interpret the flags from left to right.

File and path	Abb.	Description
hd/rhd/rhd.F90	RHD	main program
hd/rhd/rhd_hyd_module.F90	RHD	hydrodynamics routines
hd/rhd/rhd_lhdrad_module.F90	RHD	radiative transfer routines, long characteristics, supergiant case
hd/rhd/rhd_shortrad_module.F90	RHD	radiative transfer routines, short characteristics, supergiant case
hd/rhd/rhd_shortrad_dtauop01.f90	RHD	short characteristics tau-coupling
hd/rhd/rhd_shortrad_dtauop02.f90	RHD	short characteristics tau-coupling
hd/rhd/rhd_shortrad_operator00.f90	RHD	short characteristics operator
...		
hd/rhd/rhd_shortrad_operator08.f90	RHD	short characteristics operator
hd/rhd/rhd_vis_module.F90	RHD	tensor viscosity routines
hd/mhd/rhd_mhd_module.F90	MHD	magnetic fields (first version)
rad/hdrad/rhd_rad_module.f90	RAD	interface for Matthias' radiation routine
rad/hdrad/MSrad3D.F90	RAD	Matthias' radiation transport routines, long characteristics, periodic sides
eos/f90/gasinter_routines.f90	EOS	equation of state
opa/opta/cubit_module.f	OPTA	cubic interpolation
opa/opta/opta_par_module.f90	OPTA	parameters for opacity routines
opa/opta/opta_routines.f	OPTA	opacity
hd/dust/rhd_dust_module.F90	DUST	dust/molecule formation
hd/dust/dust_k3mon_module.f	DUST	1 or 2 component dust model
hd/dust/dust_bins_module.f90	DUST	multi-bin dust model
dust_momentc2_module.f	DUST	4 moment dust model
C2.INC	DUST	dust include file: C_2 molecule
C2H.INC	DUST	dust include file: C_2H molecule
C2H2.INC	DUST	dust include file: C_2H_2 molecule
CHPAR_CT.INC	DUST	dust include file
DINDEX.INC	DUST	dust include file
DKSPLINT.INC	DUST	dust include file
H2.INC	DUST	dust include file: H_2 molecule
chem_rn_module.F90	CHEM	chemical reaction network
chem_rn_dvode.F90	CHEM	chemical reaction network: solver
hion_main_module.f90	HION	hydrogen ionization
hion_io_module.f90	HION	hydrogen ionization: I/O
hion_def_module.f90	HION	hydrogen ionization: definitions
hion_dvode_module.f90	HION	hydrogen ionization: solver
hion_lineq_module.f90	HION	hydrogen ionization: linear algebra
hion_util_module.f90	HION	hydrogen ionization: utility package
hion_devel_module.f90	HION	hydrogen ionization: developer kit
edens_module.f90	HION	electron densities

Table 2: List of all high-level modules: the table shows the file name with part of its path, the shortcut for the directory, and its description.

File and path	Abb.	Description
hd/rhdb/rhd_action_module.f90	RHDB	routines for control parameter passing
hd/rhdb/rhd_box_module.f90	RHDB	box handling routines
hd/rhdb/rhd_dat_module.f90	RHDB	handling of additional data (averages)
hd/rhdb/rhd_gl_module.f90	RHDB	global parameters
hd/rhdb/rhd_io_module.f90	RHDB	input/output routines
hd/rhdb/rhd_mac_cray_module.f90	RHDB	machine dependent routines (CRAY)
hd/rhdb/rhd_mac_default_module.f90	RHDB	machine dependent routines (default)
hd/rhdb/rhd_mac_hitachi_module.f90	RHDB	machine dependent routines (Hitachi)
hd/rhdb/rhd_mac_sun_module.f90	RHDB	mac-dependent routines (Sun, others)
hd/rhdb/rhd_mean_module.f90	RHDB	averaging routines
hd/rhdb/rhd_prop_module.f90	RHDB	box properties
hd/rhdb/rhd_sub_module.f90	RHDB	additional routines
con/f90/const_module.f90	CON	physical and mathematical constants
mat/str/str_module.f90	STR	string handling
time/f90/timing_module.f90	TIME	timing routines
uio/f90/uio_base_module.f90	UIO	I/O routines
uio/f90/uio_bulk_module.f90	UIO	I/O routines
uio/f90/uio_filedef_module.f90	UIO	I/O routines
uio/f90/uio_mac_crayts_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_crayxmp_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_decalpha_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_hitachi_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_ieee_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_intel_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_module.f90	UIO	I/O routines, m.-d., minimal version
uio/f90/uio_mac_nec_module.f90	UIO	I/O routines, machine dependent part
uio/f90/uio_mac_sun_module.f90	UIO	I/O, m.-d., works in most cases

Table 3: List of all low-level modules: the table shows the file name with part of its path, the shortcut for the directory, and its description.

- '': No extra flags

- F90_PARALLEL:
  Parallelization scheme:
  - scalar: no parallelization (default)
  - openmp: OpenMP (appropriate for CO5BOLD)
  - auto: auto-parallelization (not implemented for all machines)

- F90_DEBUG:
  Debugging level:
  - 0: No extra debugging information produced, full optimization is chosen (default)
  - 1: standard debugging mode (typically switch '-g' instead of '-fast')
  - 2: other debugging (or array checking) modes possible if implemented for the requested machine

- F90_LHDRAD:
  LHDrad radiation transport:
  - 0: do not activate (compile and link) this module (default)
  - 1: activate this radiation transport module

- F90_MSRAD:
  MSrad radiation transport:
  - 0: do not activate (compile and link) this module (default)
  - 1: activate this radiation transport module

- F90_SHORTRAD:
  SHORTrad radiation transport:
  - 0: do not activate (compile and link) this module (default)
  - 1: activate this radiation transport module

- F90_CHEM:
  CHEM module (chemical reaction networks):
  - 0: do not activate (compile and link) this module (default)
  - 1: activate this source step module

  Setting this variable to 1 will set F90_DUST=1. The compiler is then called with -Drhd_chem01.

- F90_HION:
  HION module (time-dependent hydrogen ionization):
  - 0: do not activate (compile and link) this module (default)
  - 1: activate this source step module

  Setting this variable to 1 will set F90_DUST=1. The compiler is then called with -Drhd_hion01.

- F90_DUST:
  DUST module:
  - 0: do not activate (compile and link) this module (default)
  - 1: activate this source step module

If this variable is set to 1 the compiler is called with `-Drhd_box_quc01=1`, see Sect. 3.6.

- `F90_MHD`:
  MHD module:
  - `0`: do not activate (compile and link) this module (default)
  - `1`: activate this magnetohydrodynamics module (MHD HLL solver)

  If CO5BOLD is compiled with the MHD module, your start model must include magnetic fields, otherwise you will get an error message!

- `F90_MACHINE`:
  Explicit machine specification. This is usually not necessary, use 'local' or " instead.
  - `''`: local machine
  - `sun4u`: Sun
  - `...`: See the header of the configure script for an up to date list
  - `local`: local machine (default)
  - `dummy`: Do not use any machine dependent flags but use module selections
  - `empty`: Compiler flags are composed from `F90_PREFLAGS` and `F90_POSTFLAGS` only

- `F90_BASEPATH`:
  Path for CO5BOLD base directory.
  - `''`: The configure script tries to determine the base directory name automatically (default). This should work if the local directory is located somewhere below `.../hd/rhd/`
  - otherwise: This string is used as base directory name (e.g. `/home/user/for`)

Some examples can be found in Sect. 3.2.

3.6 Compiler Macros

Some of the modules of the CO5BOLD code (with suffix ".F90") employ compiler macros to switch between code versions during compile time. Typically you define at least one of the three switches `rhd_r01`, `rhd_r02`, or `rhd_r03` to choose a radiation transport module. The others have reasonable default values. To find the combination with the optimal performance, you should look into Sect. 3.7

The macros are sorted into different categories:

Some *activate a certain feature* (like a radiation transport module or the dust module). They have to be selected by the user (typically via environment variables and the configure script, see Sect. 3.5) each time the code is compiled for a certain purpose.

Other macros are meant to *improve the performance* by offering the choice between e.g. different loop structures or case distinctions. These macros are set by the configure script to the best knowledge of the author(s). Ideally, they should be checked and modified if necessary each time CO5BOLD is compiled on a new machine. It should be save to modify these settings: the results between runs with different settings should only differ slightly due to round-off errors.

Some macros *select between different numerical approximations*. A change here should be visible in a (more or less drastic) change of the results of a simulation. Usually, the default values should be accepted. Other settings typically only exist to allow the comparison with older versions of CO5BOLD or because there are new developments going on which have not yet managed to become the default.

A couple of macros only activate timing measurements and result in *additional output*. Some of them are not thread-save und should only be activated for runs on one thread (as done by the configure script). It is always save to switch any of them off (by removing or undefining them).

The macros in the category *test* mark parts of code under development. The default values should only be changed with great care (typically by the author of that code segment). The configure script does not touch these settings.
General:

- `timing_c_factor`:
  in `timing_module.F90`, ("timing count factor").
  Category: account for property of machine.
  To produce the timing statistics printed at the end of a simulation run the standard Fortran routine `SYSTEM_CLOCK` is used. The macro `timing_c_factor` specifies by how much the count rate of this routine is reduced when storing its count value. This does not prevent all overflows but can make the output much more useful. Values:
  - `1`: (default) count rate of `SYSTEM_CLOCK` is used directly.
  - otherwise: e.g. 1000, count rate of `SYSTEM_CLOCK` is reduced by this factor.

  By a proper choice of this factor the timing measurements of individual routines can be made meaningful: the reduction of the count rate prevents overflows due to the addition of several measurements. An overflow during an individual measurement can not be prevented. Therefore, the count rate for the entire program still tends to produce overflows.

- `gasinter_l01`:
  in `gasinter_routines.F90`, ("gas interpolation l01").
  Category: performance enhancement.
  This switch determines how temporary arrays are handled to improve performance Values:
  - `0`: (default) Temporary coefficient arrays are actually copied.
  - `1`: Temporary coefficient arrays just get a pointer link into the big arrays.

- `rhd_box_grav01`:
  in `rhd_box_module.F90`, ("rhd box gravitation 01").
  Category: feature activation.
  Switch to activate the array for the gravitational potential in the box structure. If the switch is set to 1, a 3D array for the potential is created, copied, removed, ... There is no module to compute the gravitational potential, yet. Therefore the entire thing has no practical value, yet. Values:
  - `0`: (default) no handling of array.
  - `1`: array handling activated.

- `rhd_box_quc01`:
  in `rhd_box_module.F90` and `rhd.F90`, ("rhd box quantity centered 01").
  Category: feature activation.
  CO5BOLD is able to handle a number of further quantities (`quc`: "quantity centered") in addition to the basic hydrodynamics quantities (ρ, ei, ...) if this compiler switch is activated. These additional quantities can be e.g. densities of dust distribution moments or densities of molecules. They are required for the treatment of chemical reaction networks and time-dependent hydrogen ionization. For the latter the `quc` arrays contain the number densities of the atomic level populations. For the chemical reaction network, the arrays contain the species number densities in cm^{-3} and with headers following this example: "Number density of H2".

  Values:
  - `0`: (default) no handling of additional quantities (density arrays).
  - `1`: handling of additional density arrays is activated.

To actually include dust formation in a simulation, it is necessary to

1. set the switch `-Drhd_box_quc01=1` during compilation (this is done by the configure script if the environment variable `F90_DUST` is set to 1, see the description of the variable in Sect. 3.5),
2. put arrays specifying the initial conditions of the additional density into the start model (as `real quc001`, `real quc002`, ...),
3. select a proper model describing dust (or molecule) formation in the parameter file (with `character dustscheme`).

- `rhd_box_bmag01`:
  in `rhd_box_module.F90` and `rhd.F90`, ("rhd box b magnetic 01").
  Category: feature activation.
  CO5BOLD can handle magnetic field arrays if this compiler switch is set. Values:
  - : (default) no handling of magnetic field arrays.
  - : handling of magnetic field arrays is activated.

  To actually account for magnetic fields in a simulation, it is necessary to
  1. set the switch `-Drhd_box_bmag01=1` during compilation (this is done by the configure script if the environment variable `F90_MHD` is set to 1, see Sect. 3.5),
  2. put arrays specifying the initial conditions of the boundary centered magnetic field arrays into the start model (as `real bb1`, `real bb2`, `real bb3`),
  3. select an hydrodynamics scheme that is able to handle magnetic fields in the parameter file (with `character hdscheme`).

Hydrodynamics (Roe solver):

- `rhd_roe1d_slope_l01`:
  in `rhd_hyd_module.F90`, ("rhd roe 1 dimension slope loop 01").
  Category: feature activation.
  When this compiler switch is set, a new extra stabilization mechanism can be activated: If one of the reconstruction methods `VanLeer`, `Superbee`, or `PP` (see Sect. 5.3.7) is activated, the slope can be reduced (by averaging with the results from a `MinMod` reconstruction) by setting `c_slopered` (see Sect. 5.3.7) to a positive non-zero value. This can improve the stability without significantly reducing the effective numerical resolution. Switch values:
  - `0`: (default) no slope reduction.
  - `1`: slope reduction in case of expansion wave.
  - `2`: slope reduction in case of strong density contrast.

- `IDF`:
  in `rhd_hyd_module.F90`, ("Integer Delta Flux").
  Category: performance enhancement.
  Number of padding cells for flux-like variables. This number was introduced to check whether the increase of the size of vectors for flux-like quantities (defined at cell boundaries) can improve the performance (especially on a CRAY machine). The gain is marginal (if present at all). The parameter is usually set to zero or left undefined. Values:
  - `0`: (default) no padding cells
  - `1,2,3,...`: extra padding cells

- `rhd_hyd_gravcorr_p01`:
  in `rhd_hyd_module.F90`, ("rhd hydrodynamics gravitation correction parameter 01").
  Category: selection of approximation.
  This parameter controls the way the Roe solver handles the source terms due to gravity. A different choice results in different simulation results and not just in slightly faster (or slower) code. The problem is that the original Roe solver interpretes the pressure gradient in a hydrostatic stratification a fluctuation due to shock waves. In case of strong stratification this can lead to weird effects. With activated correction the Roe solver treats only the deviations from a hydrostatic stratification as due to waves (or shocks). Several correction formulas have been tried. The latest is the recommended default. Values:
  - `0`: No pressure correction terms in Roe solver.
  - `1`: Simple correction with rhomean, no new average pressure.
  - `2`: Simple correction with rhomean, new average pressure.
  - `3`: Correction with local rho, limited, new average pressure.
  - `4`: Correction with local rho, new (different formula) average pressure.
  - `5`: (default) Correction with local rho, new limit, new average pressure.
  - `6`: Modification of `5` with different geometry factors in case of non-equidistant grid.
- `rhd_hyd_entropyfix_p01`:
  in `rhd_hyd_module.F90`, ("rhd hydrodynamics entropy fix parameter 01").
  Category: performance enhancement.
  The entropy fix can be done in one of two ways to get optimum performance (with essentially the same results). Values:
  - `0`: (default) "if... then... else" construction
  - `1`: use a mask and the signum function
- `rhd_hyd_upwind_p01`:
  in `rhd_hyd_module.F90`, ("rhd hydrodynamics upwind parameter 01").
  Category: performance enhancement.
  The determination of the upwind direction can be done in one of two ways to get optimum performance (with essentially the same results). Values:
  - `0`: (default) "if... then... else" construction
  - `1`: use a mask and the signum function
- `rhd_hyd_roe1d_l01`:
  in `rhd_hyd_module.F90`, ("rhd hydrodynamics roe 1 dimension loop 01").
  Category: performance enhancement.
  The computation of the Roe fluxes can be done by either of two sets of routines to find the set which gives optimum performance (with essentially the same results). Values:
  - `0`: (default) lots of small routines acting on scalars, inlining needed, cache reuse is optimized
  - `1`: routines acting on arrays, more temporary arrays necessary, vectorization is easier
- `rhd_roe1d_flux_l01`:
  in `rhd_hyd_module.F90`, ("rhd roe 1 dimension flux loop 01").
  Category: test.
  By setting this switch an alternative way of computing the upwind centered Roe states is activated (only for 'constant' reconstruction, for performance test purposes only: do not activate!). Values:
  - `undefined`: (default) Use standard method to compute the Roe states.

- `defined`: Use non-standard method to compute the Roe states.

- `rhd_bound_t01`:
  in `rhd_hyd_module.F90`, ("rhd bound timing 01").
  Category: additional output.
  Produce timing information for "inner boundary" routine (central potential) or lower and upper boundary routines (constant gravitation). It can be used together with OpenMP. Values:
  - `undefined`: (default) no timing information.
  - `defined`: call subroutines to measure elapsed time.

- `rhd_roe1d_flux_t01`:
  in `rhd_hyd_module.F90`, ("rhd roe 1 dimension flux timing 01").
  Category: additional output.
  Produce timing information for the routine which computes the Roe fluxes. It should not be used in conjunction with OpenMP. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time

- `rhd_roe1d_step_t01`:
  in `rhd_hyd_module.F90`, ("rhd roe 1 dimension step timing 01").
  Category: additional output.
  Produce timing information for the routine which performs the Roe step. It should not be used in conjunction with OpenMP. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time

Hydrodynamics (tensor viscosity):

- `rhd_vis_density_p01`:
  in `rhd_vis_module.F90`, ("rhd viscosity density parameter 01").
  Category: selection of approximation.
  Choose formula for density average at cell boundary in tensor viscosity routines. Values:
  - `0`: rhomean=min(rholeft,rhoright)
  - `1`: (default) rhomean=0.5 * (rholeft + rhoright)

- `rhd_vis_t01`:
  in `rhd_vis_module.F90`, ("rhd viscosity timing 01").
  Category: additional output.
  Produce timing information for 2D/3D tensor viscosity routines. It should not be used in conjunction with OpenMP. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time

Radiation transport:

- `rhd_r01`:
  in `rhd.F90`, ("rhd radiation 01").
  Category: feature activation.
  Switch to include LHDrad radiation transport module. It uses long characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (old "supergiant module"). Values:

- undefined: (default) LHDrad routines are deactivated.
- 1: LHDrad routines are recognized by the compiler.

- rhd_r02:
  in rhd.F90, ("rhd radiation 02").
  Category: feature activation.
  Switch to include MSrad radiation transport module. It uses long characteristics. The lateral boundaries have to be periodic. Top and bottom can be closed or open ("solar module"). Values:
  - undefined: (default) MSrad routines are deactivated.
  - 1: MSrad routines are recognized by the compiler.

- rhd_r03:
  in rhd.F90, ("rhd radiation 03").
  Category: feature activation.
  Switch to include SHORTrad radiation transport module. It uses short characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (new "supergiant module"). Values:
  - undefined: (default) SHORTrad routines are deactivated.
  - 1: SHORTrad routines are recognized by the compiler.

- rhd_rad3d_toray_l01:
  in rhd_lhdrad_module.F90, ("rhd radiation 3 dimensions to ray loop 01").
  Category: performance enhancement.
  There might be a performance gain by splitting the main loop in routine rhd_rad3d_toray into three separate loops. Typically, one big loop is to be preferred. Values:
  - undefined: (default) One big loop
  - defined: Three smaller loops

- rhd_rad3d_fromray_l01:
  in rhd_lhdrad_module.F90, ("rhd radiation 3 dimensions from ray loop 01").
  Category: performance enhancement.
  There might be a performance gain by splitting a big loop in routine rhd_rad3d_fromray into two separate loops. Typically, one big loop is to be preferred. Values:
  - undefined: (default) One big loop
  - defined: Two smaller loops

- rhd_rad3d_r02:
  in rhd_lhdrad_module.F90, ("rhd radiation 3 dimensions radiation 02").
  Category: test.
  Module rhd_lhdrad_module contains a routine for the handling of periodic boundaries. It is in an experimental state and is deactivated by default. Values:
  - undefined: (default) Skip routine rhd_rad3d_dirper during compilation
  - defined: Compile routine rhd_rad3d_dirper

- rhd_rad3d_solve_t01:
  in rhd_lhdrad_module.F90, ("rhd radiation 3 dimensions solve timing 01").
  Category: additional output.
  Produce timing information for the routines which solves the 1D radiation transport equation along single ray. This routine is called very frequently. The timing measurement might slow it down somewhat. It should not be used in conjunction with OpenMP. Values:

- `undefined`: (default) no timing information
- `defined`: call subroutines to measure elapsed time

- `rhd_rad3d_dir_t01`:
  in `rhd_lhdrad_module.F90`, ("rhd radiation 3 dimensions direction timing 01").
  Category: additional output.
  Produce timing information for the routines which solves the radiation transport equation for one direction field. The timing measurement are called very frequently and might slow down the code. It should not be used in conjunction with OpenMP. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time

- `rhd_rad3d_step_t01`:
  in `rhd_lhdrad_module.F90`, ("rhd radiation 3 dimensions step timing 01").
  Category: additional output.
  Produce timing information with main 3D radiation transport routine. It can be used together with OpenMP and should cause no noticeable performance loss. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time

- `rhd_shortrad_operator_l01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation operator loop 01").
  Category: performance enhancement, selection of approximation.
  Choose type of short characteristics operator. The operators usually come in pairs (1/2, 3/4, 5/6). There is a development from 1/2 over 3/4 to 5/6 towards higher stability. Both members of each pair should do the same operation but use different ways to do a case distinction. The 'even' operator has in some cases the better performance. But the 'odd' operator might be saver to use. Values:
  - `0`: simple test operator, fast but results are utterly useless!
  - `1`: case distinction with "if..then..else" construct.
  - `2`: case distinction with masks (weights 0.0 or 1.0).
  - `3`: case distinction with "if..then..else" construct, slope reduction of source function.
  - `4`: case distinction with masks (weights 0.0 or 1.0), slope reduction of source function.
  - `5`: case distinction with "if..then..else" construct, modified slope reduction of source function.
  - `6`: (default) case distinction with masks (weights 0.0 or 1.0), modified slope reduction of source function.
  - `8`: test version.

- `rhd_shortrad_operator_l02`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation operator loop 02").
  Category: performance enhancement.
  Select the way the short characteristics operator is accessed. Values:
  - `0`: (default) The routine with the short characteristics operator is called within a loop and should be inlined.
  - `1`: The program fragment with the short characteristics operator is included. No inlining necessary.

- `rhd_shortrad_dtauop_l01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation delta tau operator loop 01").
  Category: performance enhancement.
  Choose type of short characteristics tau coupling operator. Values:
  - `1`: case distinction with "if..then..else" construct, default if `rhd_shortrad_operator_l01`=1,3,5.
  - `2`: case distinction with masks (weights 0.0 or 1.0), default if `rhd_shortrad_operator_l01`=2,4,6.

- `rhd_shortrad_dtauop_l02`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation delta tau operator loop 02").
  Category: performance enhancement.
  Select the way the operator for the tau coupling (short characteristics module) is accessed. Values:
  - `0`: (default) The routine with the tau coupling operator is called within a loop and should be inlined.
  - `1`: The program fragment with the tau coupling operator is included. No inlining necessary.

- `rhd_shortrad_formal_l01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation formal loop 01").
  Category: performance enhancement.
  Select version of loop splitting for exp(-dtau) computation. Values:
  - `0`: (default) `dtauhalf`, `exp_mdtauhalf`, `expl2t_mdtauhalf` are computed in a single loop
  - `1`: (`dtauhalf`, `exp_mdtauhalf`), (`expl2t_mdtauhalf`) are computed in separate loops. This prevents the SUN1 machine (Sunfire, Solaris, Forte 6.2) from doing some performance degrading optimization

- `rhd_shortrad_dir1_l01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation direction 1 loop 01").
  Category: performance enhancement.
  Choose routine version for rays in x1 direction. Values:
  - `0`: (default) Use routine with permuted indices for rays in x1 direction. In this case the innermost loop index is the third array index. The transposition of arrays is not needed but some machines (e.g. SUN1) do not like this index arrangement.
  - `1`: Transpose arrays and use routine `rhd_shortrad_dir3` for rays in x1 direction. The extra step for the transposition of some arrays (and the reverse procedure) needs some time. But now the routine with the optimum index ordering can be used.

- `rhd_shortrad_dir_l02`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation direction loop 02").
  Category: performance enhancement, OpenMP.
  Determine position of PARALLEL statement relative to outer loop in `rhd_shortrad_dirX`. Both settings give the same results but might show a different performance on a specific machine. Values:
  - `0`: (default) PARALLEL statement inside of outer loop
  - `1`: PARALLEL statement outside of outer loop

- `rhd_shortrad_lambda_l01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation lambda loop 01").
  Category: feature activation.
  Handling of extra arrays to allow partially implicit Lambda* iteration Values:
  - `0`: (default) Only fully implicit Lambda* iteration allowed (or fully explicit treatment).
  - `1`: Also partially implicit Lambda* iteration allowed.
- `rhd_shortrad_formal_t01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation formal timing 01").
  Category: additional output.
  Produce timing information for routine which gives the formal solution of the radiation transport equation with the help of short characteristics. It can be used together with OpenMP and should cause no noticeable performance loss. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time
- `rhd_shortrad_step_t01`:
  in `rhd_shortrad_module.F90`, ("rhd short-characteristics radiation step timing 01").
  Category: additional output.
  Produce timing information for main short characteristics routine. It can be used together with OpenMP and should cause no noticeable performance loss. Values:
  - `undefined`: (default) no timing information
  - `defined`: call subroutines to measure elapsed time
- `MSrad_raytas`:
  in `MSrad3D.F90`, ("Matthias Steffen radiation ray tau s").
  Category: performance enhancement.
  Values:
  - `0`: (default) Loop with IF..THEN..ELSE
  - `1`: Loop with ABS,SIGN
  - `2`: Loop with MIN,MAX

3.7 Optimization, Compiler Switches

In this section some mandatory or useful compiler flags are described. These have different functions:

- Enable necessary macro processing/expansion for the `F90` files.
- Force proper handling of binary I/O.
- Choose module for radiative transfer.
- Activate module for dust formation and/or magnetic field transport.
- Enable parallelization with OpenMP directives.
- Choose a version of a subroutine or loop which is optimized for a specific architecture.
- Tell the compiler if and what to inline.
- Improve the general performance.

3.7.1 General: OpenMP settings

To activate OpenMP you have to set the corresponding environment variable (see 3.5) before calling the configure script like

```
export F90_PARALLEL=openmp
./configure
make
```

This will insert the corresponding compiler switch (e.g. `-openmp`, `-omp`, `-mp`,... confer the following sections) into the compiler calls in the makefile (see Sect. 3.5).

The calls to the timing routines that would be executed in parallel are removed by (not) setting the appropriate compiler macros (see Sect. 3.6).

In addition, the switch `rhd_shortrad_dir_l02` (see 3.6) might be set, according to experience about performance enhancements.

The user has to find optimum values for the parameters `n_hydcellsperchunk` (for the Roe solver module, see Sect. 5.3.7) and `n_viscellsperchunk` (for the tensor viscosity module, see Sect. 5.3.8) to optimize the size of the chunk given to one thread per time.

So far, only for the SHORTrad module the environment variable `OMP_SCHEDULE` can be set (before running CO5BOLD) to control its OpenMP scheduling behavior. Important parallel loops in the SHORTrad module have a `SCHEDULE(RUNTIME)` modifier that allows this external control. The old default is achieved by not defining the variable or by setting

```
export OMP_SCHEDULE="STATIC,1"
```

On some machines (e.g. Intel Xeon with Linux and PGI compiler) a dynamic scheduling activated with

```
export OMP_SCHEDULE="DYNAMIC,1"
```

is advantageous. The size of the individual chunks might be set to larger values than 1 (in the examples above). The optimal value has to be found empirically. A good starting point is `number_of_grid_points_in_1D/Number_of_treads`, which gives for a model with 171^3 grid points on a 4-processor machine

```
export OMP_NUM_THREADS=4
export OMP_SCHEDULE="STATIC,43"
```

The behavior of the other modules is not affected.

The number of threads should equal the number of available processors and has to be set at run-time with the environment variable `OMP_NUM_THREADS`, e.g. with

```
export OMP_NUM_THREADS=16
```

3.7.2 General: Inlining

Candidate routines for inlining are (i.e. they should be inlined if anyhow possible):

- file `rhd_hyd_module.F90`:
  `rhd_hyd_avg`, `rhd_hyd_upwind`, `rhd_hyd_pred0`, `rhd_hyd_predm`, `rhd_hyd_predp`, `rhd_hyd_alpha`, `rhd_hyd_constanteq`, `rhd_hyd_minmodeq`, `rhd_hyd_minmod`, `rhd_hyd_vanleereq`, `rhd_hyd_vanleer`, `rhd_hyd_superbeeeq`, `rhd_hyd_superbee`, `rhd_hyd_ppeq`, `rhd_hyd_pp`, `rhd_hyd_hdflux`
- file `rhd_lhdrad_module.F90`:
  `rhd_rad3d_raylhd`, `rhd_rad3d_solve`, `rhd_rad3d_solveeq`

- file `rhd_shortrad_module.F90`:
  `rhd_shortrad_operator`, `rhd_shortrad_dtauop`.

On some machines the makefile generated by the configure script contains this list explicitely. On others, one has to rely on automatic inlining (see the following sections).

All routines that should be inlined are contained in the same modules as the calling routines. Therefore, no "inter-procedure-inlining" is needed.

3.7.3 General: Single versus double precision

Usually, the files containing the hydrodynamics and EOS data use 4 byte to represent a single number and most of the computations within CO5BOLD are performed in single precision – except for certain routines in e.g. MSrad or some dust modules.

To switch to double precision everywhere one has to deal with the binary files and force the transformation of single precision variables to double precision during the compilation. Compiling all CO5BOLD files with such a switch produces problems with the UIO modules: there would be a name conflict between the routines that usually deal with double precision reals and those that are written to deal with single precision reals and are now forced to pretend to be also a double precision version.

Therefore, one should compile the UIO routines and the rest with separate settings, e.g. for the Intel compiler:

```
./configure
make UIO

export F90_PREFLAGS="-r8 -fpconstant"

./configure
make
```

Code compiled in this way cannot read anymore single precision binary UIO files. However, there are no problems with the opacity tables (ASCII files) and *formatted* UIO files. To make existing single precision binary UIO files readable one could transform them to the formatted version with `uiocat` (see 4.6.3), e.g. like:

```
uiocat -f formatted -o rhd_ascii.sta rhd_binary.sta
```

New start models could be written in double precision binary UIO format directly using the `double_flag` in the IDL routine `rhd_wrboxdata.pro`.

For the EOS table `eos_mm00_l5.eos` there exists a double precision binary version.

3.7.4 Cray: SV1

On craSHi in Kiel (a "CRAY SV1 20-32768 SN9542", now out of service) CO5BOLD could use all 4 processors per board. Documentation about the system and the compiler can be found with the CRAYdoc[1] system. The new configure script still includes a branch for this system even if has never been tested on that machine.

In some cases the non-default versions of loops in the CO5BOLD code vectorize better and are preferred over the standard ones:

- `-F`: Enable macro expansion
- `-Otask1`: Parallelization: Enable tasking (in this case OpenMP).
- `-Oinline3`: Optimization: enable (high level) of inlining.
- `-Ovector3 -Oscalar3`: General optimization

[1] http://www.cray.com/craydoc/

- `-Drhd_hyd_roe1d_l01=1`: Optimization: Choose non-standard set of routines for Roe solver. See Sect. 3.6.
- `-Drhd_hyd_entropyfix_p01=1`: Optimization: version with masks (weights). See Sect. 3.6
- `-Drhd_hyd_upwind_p01=1`: Optimization: version with masks (weights).
- `-Drhd_shortrad_operator_l01=2`: Optimization: short characteristics operator with masks (weights).
- `-Drhd_shortrad_dir_l02=1`: Optimization: `OMP PARALLEL` statement outside of outer loop in `rhd_shortrad_dirX`.

3.7.5 Compaq: alpha

The appropriate machine dependent UIO module is `uio_mac_decalpha_module.f90`. It allows the reading and writing of files in `little_endian` and `big_endian` format.

- `-assume byterecl`: Necessary for the UIO routines: specify that the length of a record is measured in bytes (and not in words).
- `-cpp`: invoke the preprocessor on all source files.
- `-inline speed -V`: Force automatic inlining, optimized for speed.
- `-O4`: General optimization.
- `-Drhd_hyd_roe1d_l01=0`: Optimization: Choose standard set of routines for Roe solver. See Sect. 3.6.
- `-DMSrad_raytas=0`: Optimization: choose default version of loop in `SUBROUTINE raytas` in file `MSrad3D.F90`. See Sect. 3.6.

3.7.6 Hewlett-Packard: V2500

The 12-processor machine "zeipel" from Hewlett-Packard[2] is a "V2500 PA 2.0" system. Now, there is a first success to force the compiler to accept the OpenMP directives in CO5BOLD. Yet, when running on several processors, only some routines (e.g. `rhd_shortrad_dirsimple1`) in CO5BOLD can benefit while others (`rhd_shortrad_dirsimple2`, `rhd_shortrad_dirsimple3`) are significantly slower than on one processor. In addition, the single-processor performance is not very good, partly because the achievable optimization level is not very high.

Some macros, which seem to be necessary:

- `+U77`: Link proper library to make the machine understand e.g. `call flush(6)`.
- `+cpp=yes`: Switch on the C preprocessor. Note that all Fortran90 files have to end with ".f90". The ".F90" suffix does not seem to work.
- `+Oparallel +Oopenmp +Onoautopar`: Try to enable parallelization with OpenMP directives, disable auto-parallelization.
- `+Onoinline`: Disables inlining. This can simplify things. With a proper choice of routine versions inlining is not really necessary anymore.
- `+O3 +Olimit`: General optimization with limited resource usage during compilation. Some modules should only be compiled with `+O2`, others compile even with `+O3 +Onolimit`.

The UIO modules and the string handling module should be compiled in debug mode. A proposed compiling sequence is (MSrad does not compile; all other modules are activated):

[2] http://h21007.www2.hp.com/dspp/tech/tech_TechDocumentDetailPage_IDX/1,1701,1845,00.html

```
export F90_LHDRAD=1
export F90_MSRAD=0
export F90_SHORTRAD=1
export F90_DUST=1
export F90_MHD=1
export F90_PARALLEL=openmp

export F90_DEBUG=1
./configure
make UIO STR

export F90_DEBUG=0
./configure
make
```

3.7.7 Hewlett-Packard: Itanium 2

The 2-processor system "gunnar" from Hewlett-Packard is a dual Itanium 2 machine with two 900MHz ia64 CPU modules, 4GB of RAM and 70GB user disk space.

The single-processor performance of CO5BOLD is very good. On two processor the code runs even faster but just stops after a few time steps. The number of time steps varies even for simulations with the very same start model and parameter file. Therefore, OpenMP should not be activated currently.

The compiler settings are somewhat similar to the settings of the HP V2500 system in Section 3.7.6:

- `+U77`: Link proper library to make the machine understand e.g. `call flush(6)`.
- `+cpp=yes`: Switch on the C preprocessor. Note that all Fortran90 files have to end with ".f90". The ".F90" suffix does not seem to work.
- `+Ofast`: High optimization level. And `+Ofaster` is even higher.
- `+Oopenmp +Onoautopar`: Try to enable parallelization with OpenMP directives, disable auto-parallelization. The code compiles and runs fast but crashes after a few time steps.

A proposed compiling sequence is (LHDrad, DUST, MHD do not compile):

```
export F90_MSRAD=1
export F90_SHORTRAD=1
./configure
make
```

3.7.8 Hitachi SR8000

Some information about the Hitachi compiler is here[3].

The appropriate machine dependent UIO module is `uio_mac_hitachi_module.f90`. The appropriate machine dependent RHD module is `rhd_mac_hitachi_module.f90`.

- `-conti199`: Up to 199 continuation lines can be interpreted (otherwise not more than 39 continuation lines are accepted).
- `-limit`: Limits the amount of time and memory for compilation.

[3] http://www.hitachi.co.jp/Prod/comp/hpc/foruser/sr8000/tebiki-e/fort_opt.html

- `-opt=ss`: use highest possible optimization level.
- `-nopredicate`: this option switches off a sub-option activated by opt=ss. It is necessary to disable the -predicate option because the code crashes otherwise (segmentation violation). The switch must appear *after* setting `-opt=ss`.
- `-pvfunc=2`: References the pseudo-vectorizing mathematical function and applies the temporary array to reference the pseudo-vectorizing mathematical function.
- `-omp -parallel=1`: parallelize based on OpenMP directives only.
- `-procnum=8`: generated code for 8 processors on one node
- `-orphaned=1`: Checks if the regions sequentially executed contain orphaned directives during run-time when PROCNUM=8 is specified. If a sequentially executed region contains an orphaned directive, the system outputs a message and terminates the program.
- `-nestcheck=1`: Checks for nesting errors in parallel regions. If a parallel region is nested, the system returns an error and terminates the program. *Without this option, the code aborts with an error message, indicating illegal nesting. Compiler bug?*
- `-pmpar`: Collects the performance monitor information for each parallelization unit.
- `-pmfunc`: Collects the performance monitor information for each procedure.
- `-Drhd_hyd_roe1d_l01=1`: Optimization: Choose non-standard set of routines for Roe solver. See Sect. 3.6.
- `-DMSrad_raytas=0`: Optimization: choose default version of loop in `SUBROUTINE raytas` in file `MSrad3D.F90`. See Sect. 3.6.
- **Important note:** The UIO routines need in addition the compiler option `-subchk`: Array bound checking. Without this checking option, some UIO routines are not working properly (compiler bug?).

A proposed compiling sequence is (only default modules activated):

```
export F90_PREFLAGS="-subchk"
./configure
make UIO

export F90_PREFLAGS=
./configure
make
```

Performance tests on hwwsr8k

Some tests have been performed on the machine hwwsr8k at HLR Stuttgart in order to determine the optimum chunk sizes which are set by the parameters `n_hydcellsperchunk` and `n_viscellsperchunk` (see Sect. 5.3.7 and Sect. 5.3.8). Two different models have been used, one consisting of 128x128x192 grid cells, the other of 252x252x188, respectively. Grey radiative transfer has been performed with the MSrad module. Different values for the chunk size(s) have been assumed where the hydrodynamics and the viscosity parameter were set equal. In all cases three time steps have been computed. The results are shown in Fig. 2. The number of resulting chunks for step HYD1 (the values for HYD2, HYD3, and VIS are very similar), total memory, performance, and the wall clock duration of the hydrodynamics and the viscosity routines are shown as functions of the chunk size parameter(s). Clearly, the number of chunks decreases towards larger chunk sizes whereas the required memory increases – in particular for very large chunk size values.

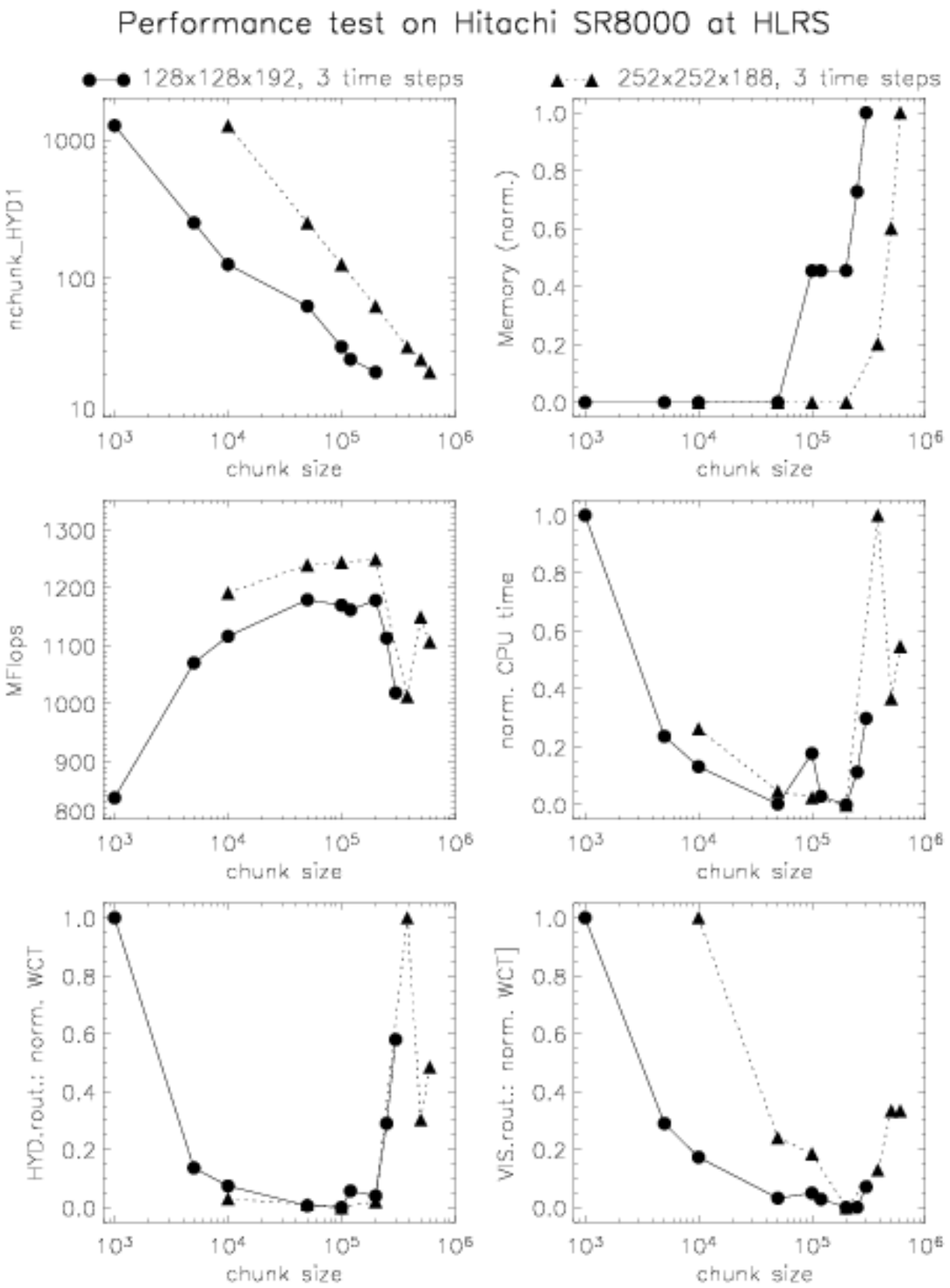


Figure 2: Performance tests on Hitachi SR8000 at HLR Stuttgart. For models with 128x128x192 and 252x252x188 grid cells different values for the hydrodynamics and viscosity chunk size parameters were used. See text for more details.

Moreover, performance and CPU time can be optimized by choosing the right parameter values. Interestingly, the optimum chunk size is different for hydrodynamics and viscosity. Based on these tests, a larger value seems to be preferable for the viscosity (`n_viscellsperchunk`). In the case of the smaller model, 50000 seems to be fine for the hydrodynamics whereas the optimum viscosity chunk size is 200000. This difference explains the double-peaked structure of performance and CPU time. Note that the optimum values do not only depend on the architecture used but also on the dimensions of the model. We recommend to test some chunk size values since it might lead to a higher performance.

3.7.9 IBM

Useful links:
IBM compiler documentation: "IBM: XL Fortran"[4], especially "IBM AIX compiler information center"[5]. Another source of the compiler documentation: "Documentation for AIX Systems"[6], especially "IBM XL Fortran for AIX Version 8.1.1 Library"[7]. Particularly useful hints: "Porting Programs from the Crays to the SP"[8].

The compiler to be used for OpenMP runs is called with `xlf90_r` which "binds the object files to the thread-safe components" (IBM documentation). For scalar code `xlf90` might be sufficient.

Important switches are:

- `-qsuffix=f=f90 -qsuffix=cpp=F90`: To tell the compiler about the existence of Fortran90 and to enable the preprocessing for files with suffix "F90".
- `-qextname=flush:etime`: Append underscore to both routine names. The non-standard routine `call_system` used by the `uio_mac_sun_module` is recognized automatically.
- `-WF,-Drhd_r03`: The compiler does not send switches starting with `-D` to the preprocessor but tries to interpret it itself – unlike all other compilers. Therefore, each switch (e.g. `-Drhd_r03`) has to "escaped" with `-WF,` (as e.g. `-WF,-Drhd_r03`).
- `-q64`: Activate the 64-bit mode. In the default 32-bit mode a very small model (with total memory requirements far below the 2 GByte limit) might run. However, experienced IBM users might experiment instead with the compiler switches `-bmaxstack`, `-bmaxdata`, and `-qsmallstack`, with the UNIX commands `limit` or `ulimit`, or with the settings in the header of the batch script...
- `-O3`: Choose optimization level. Higher levels that involve interprocedural analysis cause the compiler to stop with an error message.
- `-qarch=auto -qtune=auto -qcache=auto`: To allow optimization specific for the local machine (default in the configure script). "Cross compilation" can be activated e.g. with `-qarch=pwr3 -qtune=pwr3` or `-qarch=pwr4 -qtune=pwr4` (by setting an environment variable, e.g. `F90_MACHINE="(pwr3)"` before calling `configure`).
- `-Q -Q+...`: To activate inlining and to specify the list of routines that should be inlined (see Sect. 3.7.2).
- `-qsmp=noauto:omp`: Parallelization: OpenMP directives are activated.

A job script `rhd.job` on the Loadleveler batch system on `io.cines.fr` can be submitted with

```
llsubmit rhd.job
```

[4] http://www-306.ibm.com/software/awdtools/fortran/xlfortran/library/
[5] http://publib.boulder.ibm.com/infocenter/comphelp/index.jsp
[6] http://os.cc.biu.ac.il/documentation/
[7] http://os.cc.biu.ac.il/documentation/xlf_8.1.1/html/
[8] http://hpcf.nersc.gov/computers/SP/craytoSP.html/

The jobs in the queue for user `testuser` can be checked with

```
llq -u testuser
```

A job with ID `n34.56789.0` can be canceled with

```
llcancel n34.56789.0
```

3.7.10 Linux: PGI Compiler

Under Linux the compiler of the Portland Group[9] was first used to compile CO5BOLD. It is called with `pgf90`.

Important switches are:

- `-byteswapio`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa.
- `-fast`: General optimization flag to choose (close to) optimum optimization for local machine.
- `-Mvect=sse`: Optimization: Allow Pentium III vector commands.
- `-Mcache_align`: Optimization: Align some data object on cache-line boundaries.
- `-fastsse`: From compiler version 4.0 on, this option can be used instead of the three previous ones. It contains and supersedes them.
- `-Minline=...`: Optimization: the routines that should be inlined are listed in Sect. 3.7.2.
- `-DMSrad_raytas=2`: Optimization: choose non-default version of loop in `SUBROUTINE raytas` in file `MSrad3D.F90`. See Sect. 3.6.
- `-Drhd_hyd_roe1d_l01=0`: Optimization: choose standard set of routines for Roe solver. See Sect. 3.6.
- `-Drhd_shortrad_operator_l02=1`: Optimization: use the "manually inlined version" of the short characteristics operator.
- `-Drhd_shortrad_dtauop_l02=1`: Optimization: use the "manually inlined version" of the optical coupling operator.

3.7.11 Linux: Intel Compiler

With Version 7.0 and 7.1 of the Intel compiler[10] CO5BOLD compiled (with tricks, see below). Version 8.0 still caused trouble. With version 9.1 everything compiles smoothly.

The native format on Intel machines is `little_endian`. With

```
export F_UFMTENDIAN=big
```

(to be set at runtime after compilation before running CO5BOLD) the default can be changed to `big_endian`. The appropriate UIO modules are `uio_mac_intel_module.f90` in the `little_endian` case and `uio_mac_sun_module.f90` in the `big_endian` case. The compiler is called with `ifc`.

Important switches are:

- `-Vaxlib`: Link proper library to make the machine understand e.g. `call flush(6)`.

[9] http://www.pgroup.com/

[10] http://www.intel.com/software/products/compilers/flin/index.htm

- `fpp`: Activate the preprocessor (silently).
- `-O3`: General optimization flag.
- `-tpp6 -xK`: Optimization especially for Pentium III (and Athlon, includes SSE vector commands).
- `-tpp7 -xW`: Optimization especially for Pentium IV (includes SSE2 vector commands).
- `-xP`: Optimization especially for Core 2 Duo and simular architectures.
- `-ip`: Optimization: activate interprocedural optimization within each source file. This enables inlining.
- `-DMSrad_raytas=2`: Optimization: choose non-default version of loop in `SUBROUTINE raytas` in file `MSrad3D.F90`. See Sect. 3.6.
- `-Drhd_shortrad_dir1_l01=1`: Optimization: Transpose arrays and use routine `rhd_shortrad_dir3` for rays in x1 direction. See Sect. 3.6.
- `-openmp`: Parallelization: OpenMP directives are activated. Note that the for compiler versions before 9.0 the UIO routines should be compiled without OpenMP support (even if they do not contain any OpenMP directives themselves).
- `-i_dynamic`: Helpful against "undefined reference to '`__ctype_b`'" errors.
- `-r8 -fpconstant`: Useful to force compilation in double precision (see 3.7.3).

On Macintosh machines the typical optimization flags are `-O3 -no-prec-div -fno-alias -ip`. A big problem is the tiny stack size on those machines: large arrays taken from the stack should be avoided. For the SHORTrad module, this can be achieved by setting `-Drhd_shortrad_arrays_l01=2` during compilation. In addition, relatively small chunk sizes should be specified in `rhd.par`, see Sect. 5.3.7 and Sect. 5.3.8.

Using the Intel compiler (before version 9.1) there was a problem with the UIO modules when OpenMP is activated. This was a bit weird because the UIO modules do not contain any OpenMP directives. However, this means that OpenMP can be safely deactivated for these modules. A proposed compiling sequence is (all modules activated):

```
export F90_LHDRAD=1
export F90_MSRAD=1
export F90_SHORTRAD=1
export F90_DUST=1
export F90_MHD=1

export F90_PARALLEL=scalar
./configure
make UIO

export F90_PARALLEL=openmp
./configure
make
```

In some cases it might be helpful to set

```
export LD_ASSUME_KERNEL=2.4.19
```

when encountering problems with OpenMP.

3.7.12 Linux: PathScale Compiler

Some experiments with the PathScale compiler[11] have been made. It is called with `pathf90`. The result is not entirely satisfying, yet.

Important switches are:

- `-byteswapio`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa.
- `-O3`: General optimization flag. More aggressive optimization can be activated with `-Ofast` or `-Ofast -ipa`.
- `-mp`: Parallelization: OpenMP directives are activated.

3.7.13 Linux: GNU g95 Compiler

One of the available GNU Fortran compilers is the g95 compiler[12] with the g95 home page[13]. It is called with `g95`.

Important switches are:

- `-fendian=big`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa.
- `-O3`: General optimization flag.

The appropriate UIO module is `uio_mac_ieee_module.f90`.

OpenMP is not there yet. The binary I/O format ("unformatted") is incompatible with the one used before in CO5BOLD: no existing UIO files can be read.

3.7.14 Linux: GNU gfortran Compiler

The Fortran compiler[14] of the GNU project[15] is called with `gfortran`.

Important switches are:

- `-fconvert=big-endian -frecord-marker=4`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa. In addition, the old 32-bit record marker convention is maintained and existing UIO files can be read.
- `-O3`: General optimization flag.
- `-fopenmp`: Activates the OpenMP directives, but causes CO5BOLD to crash – currently.

The appropriate UIO module is `uio_mac_ieee_module.f90`. And use `rhd_mac_default_module`. I haven't found out how to use the standard modules, yet.

OpenMP does not work, yet. And the scalar code is significantly slower than code compiled e.g. with the Intel compiler (see Sect. 3.7.11. However, the factor is not prohibitive. For not too demanding test runs the `gfortran` compiler can already be useful.

[11] http://www.pathscale.com/docs.html
[12] http://g95.sourceforge.net/
[13] http://www.g95.org/
[14] http://gcc.gnu.org/fortran/
[15] http://www.gnu.org/

3.7.15 NEC SX-5, SX-6, SX-8

First attempts to compile CO5BOLD on neSH at the Rechenzentrum Kiel and on hwwsx5 at HLR Stuttgart:

An environment variable has to be set to `F_RECLUNIT=BYTE` (before execution of a program) to enable UIO to compute proper record lengths. The cross compiler (on sunsrv or crossi) is called with `sxf90`. Thus, the environment variable `F90_COMPILER=sx90` has to be set before running the configure script.

No optimized version of CO5BOLD has been achieved yet.

Some maybe useful switches are

- `sx5`: generate instructions for SX-5. Use `sx6` or `sx8` when appropriate.
- `C vopt`: normal optimization in vector mode
- `-Wf'-M noflunf -M noinv -M noinexact -M setall'`: suppress some exceptions
- `-P openmp`: parallelization with OpenMP
- `-Ep`: call cpp preprocessor
- `-pi exp=...`: inlining of a list of routines (see Sect. 3.7.2)
- `-dw -float0` (no special environment variable): use internally and in files the 4 Byte `big_endian` format

For the SX-5 the compiler flags in the configure script are

```
F90FLAGS="-C hopt -sx5 -dw -float0
-Wf'-L nostdout -L fmtlist -L inclist -L mrgmsg -L transform -M noflunf
    -M noinv -M noinexact -M setall'
-pi exp=rhd_shortrad_operator exp=rhd_shortrad_dtauop $F90MODULES
$F90TIME -DMSrad_raytas=1"
```

For the SX-8 the configure scripts gives the output

```
sxf90 -EP -P openmp -Chopt -sx8 -Wl'-Z 8G -m' -dw -float0
  -Wf'-L nostdout -L fmtlist map summary transform -L inclist -L mrgmsg -M noflunf -M noinv
  -Drhd_r03 -Drhd_shortrad_step_t01 -Drhd_shortrad_formal_t01 -DMSrad_raytas=1
  -Drhd_hyd_entropyfix_p01=1 -Drhd_hyd_upwind_p01=1 -Drhd_hyd_roe1d_l01=1 -Dgasinter_l01=2
```

3.7.16 SGI: Origin

CO5BOLD has been compiled and tested on up to 8 processors on the SGI 2000 machine at TAC in Copenhagen and the SGI 3800 machine at the NSC[16] in Linköping. More recently, the code was used on the UKAFF machines (see Sect. 3.7.17) and the computers at CINES.

See e.g. the excellent SGI Fortran90 manual[17] .

Information about the CINES machines can be found under CINES, or CINES : Introduction au calcul scientifique.

Important switches are:

- `-macro_expand`: Enable macro expansion
- `-mp`: Enable parallelization with OpenMP directives
- `-INLINE:aggressive=ON -INLINE:list -INLINE:preempt=ON`: General keywords for inlining

[16] http://www.nsc.liu.se/systems/sgi3k/

[17] http://techpubs.sgi.com/library/tpl/cgi-bin/init.cgi

- `-INLINE:must=...`: Optimization: routines that should be inlined (see Sect. 3.7.2).
- `-Ofast -OPT:Olimit=0`: General optimization. On older compiler versions `-O3` was the achievable optimum.
- `-IPA:plimit=5500`: Even more optimization. This option requires lots of memory (¿ 1 GByte). To get it it might be necessary to ask for more than one processor for the compilation (especially on the CINES machines).
- `-CG:longbranch_limit=60000`: This switch limits needed compiler resources. It is suggested by the compiler (on the CINES machines) itself.
- `-Drhd_roe1d_step_l01=1`: Slight performance improvement

3.7.17 SGI: Origin 2000/3800 at UKAFF

CO5BOLD has been also compiled and tested on up to 22 processors on the machines of the UK Astrophysical Fluids Facility (UKAFF)[18] in Leicester, England. UKAFF operates two machines: an SGI Origin 3800 with 128 processors (named "ukaff"), and an older SGI Origin 2000 with 22 processors (named "grand") which is mainly used for development and test purposes. Both machines are binary compatible. At the time of testing (April 2003) the SGI MIPSpro Compilers (Version 7.4) was installed.

Most of the compiler switches given in the previous section were used, except for the following modifications which either gave empirically a better performance or were recommended by the UKAFF *Hints for users*:

- `-Ofast`: Replaces `-O3`, gave better performance
- `-LNO:cs1=32k:ls1=32:cs2=8M:ls2=128`: Explicit cache architecture added

The option `-Ofast` is now the default selected by the configure script for all SGIs with IP35 architecture. The cache architecture settings are activated for the UKAFF machines only.

A glitch in the system libraries made it necessary to add a work-around to the source code (file `rhd.F90`). A "bus error" occurred whenever the system routine "flush" was trying to flush an empty file buffer. The temporary work-around was simply to add a write statement before every call of "flush". This made the log-file look less nice but did the job. Now, the few "flush" statements that are not necessarily preceded by a write statement are removed.

The main goal was to investigate the scaling of the performance of CO5BOLD with the number of processors. This was done only for the MSrad module, considering local surface convection models. Two model sizes were tested: a small one with 125x125x81 grid points employing non-grey radiative transfer (4 frequency bands), and a large one with 315x315x81 grid points employing grey radiative transfer. Rather short runs of 10 (small model) and 3 (large model) time steps were performed. Even for the large model the memory demand was ca. 800Mb, which is very modest considering that every sub-node of the machine — consisting of 4 processors — has 2Gb of memory.

The results are summarized in the following three figures. The black lines give the scaling of the total time, the green lines the scaling of the time needed by the hydrodynamics routines, and the red lines the scaling of the radiative transfer routines. The scaling is presented as the increase of processing time per processors as the problem is distributed among more and more processors. The times are normalized to the time that is used in a scalar, i.e. single processor setup. Ideally, one would like a constant behavior which stays close to one.

The perhaps most interesting result is that the speedup on "ukaff" is about 11 for the large model on 16 processors. Perhaps not ideal, but within the range of practical interest. In general, the hydrodynamics routines scale more favorably than the radiation routines. This is perhaps simply related to the fact that in explicit hydrodynamics communication is restricted to neighboring grid cells.

[18] http://www.ukaff.ac.uk/

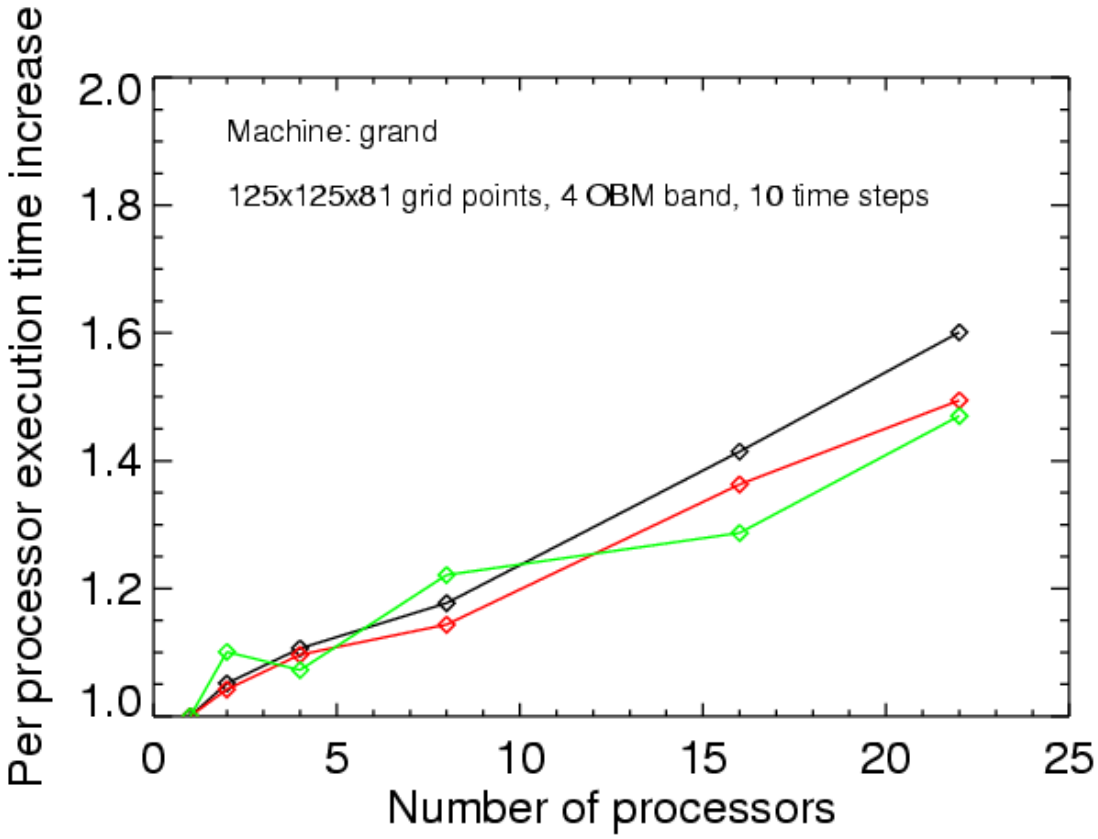


Figure 3: UKAFF: machine: grand; small model

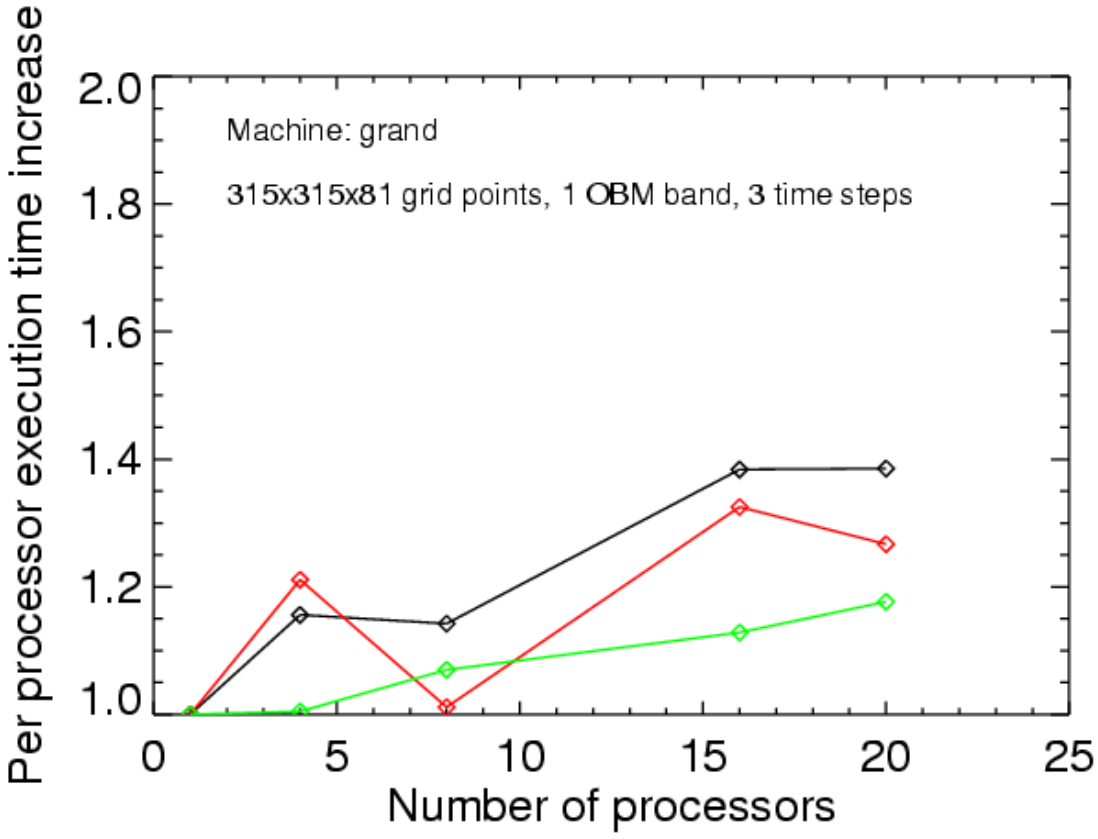


Figure 4: UKAFF: machine: grand; large model

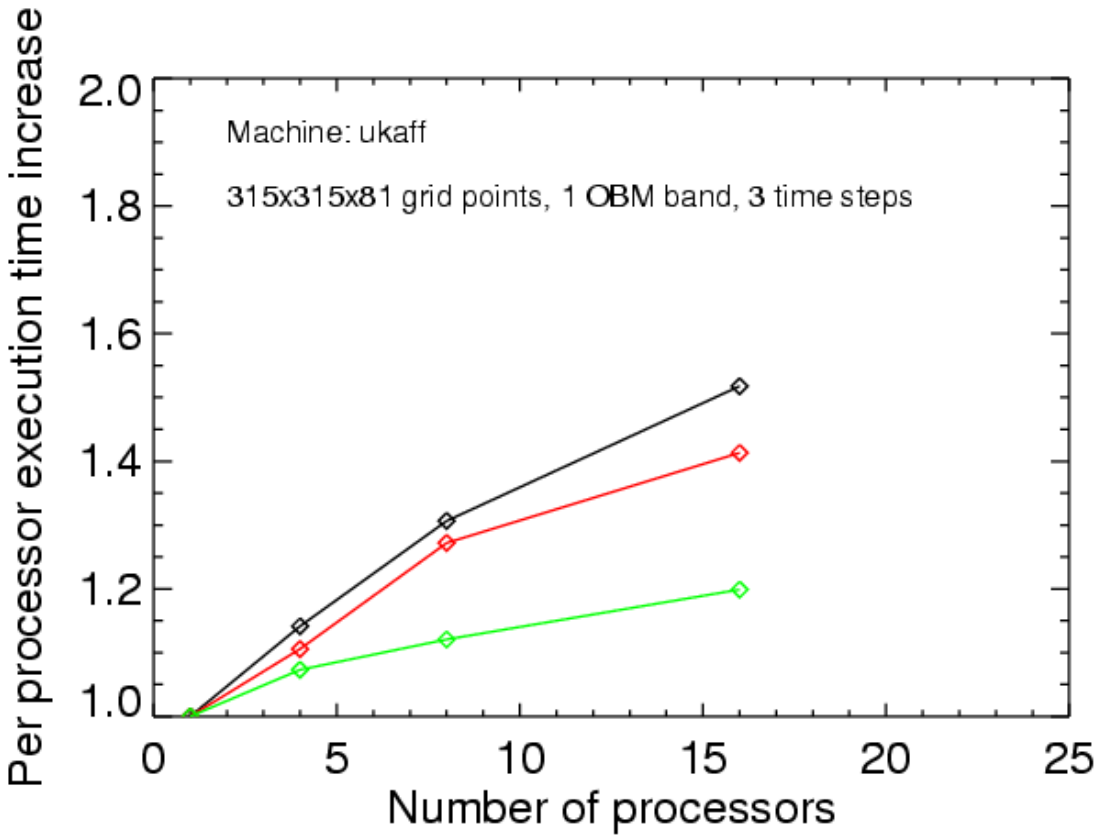


Figure 5: UKAFF: machine: ukaff; large model

For those wondering: the black curves do not lie between the red and green curve since more components than just radiation and hydrodynamics add up to the total time. Furthermore, the normalization of the execution times given by CO5BOLD is not exact.

3.7.18 Sun: SunFire

CO5BOLD has been used on the SunFire machines"fire1", "fire2", and "fire3" in Uppsala with compiler version "Sun WorkShop 6 update 2 Fortran 95 6.2 2001/05/15" and later. An older version was not able to compile CO5BOLD properly. Information about Fortran and the Sun compiler can be found on the Sun Fortran data sheet page[19] under "Documentation". Ångström Sun cluster[20]

Important switches are:

- `-openmp`: Enable OpenMP.
- `-fast -xvector=yes/no`: General optimization. On the Sun the `-fast` option switches on more or less all optimization features of the compiler. That works reasonable well. However, during the compilation of `gasinter_routines.f90` (and only there) the switch `-xvector=no` is required! This is done automatically in the Makefile.
- `-inline=...`: Optimization: routines that should be inlined: see Sect. 3.7.2.
- `-DMSrad_raytas=2`: Optimization: choose non-default version of loop in `SUBROUTINE raytas` in file `MSrad3D.F90`. See Sect. 3.6.
- `-Drhd_shortrad_formal_l01=1`: Optimization: split loop for exp(-dtau) computation into two loops. See Sect. 3.6.

[19] http://developers.sun.com/sunstudio/products/previous/fortran/datasheet.html
[20] http://www.uppmax.uu.se/ComputerSystems/AngstromSunCluster/SunCluster.html

- `-Drhd_shortrad_dir1_l01=1`: Optimization: Transpose arrays and use routine `rhd_shortrad_dir3` for rays in x1 direction. See Sect. 3.6.
- `-Drhd_hyd_entropyfix_p01=1`: Optimization: version with masks (weights). See Sect. 3.6.
- `-xarch=native64`: Produces 64-bit code optimized for local machine.

4 UIO Data Format

4.1 Quickstart: Introduction to UIO

The UIO ("Universal Input Output") routines are a set of routines in Fortran90 and IDL to manage I/O of scalars, arrays and a certain table type. Files can be formatted or unformatted. The formatted (ASCII text) data representation is machine-independent and appropriate for human reading (for short files).

The binary representation uses the Fortran "unformatted" read and write routines, provides much faster I/O, gives smaller files, and the IEEE format is a quasi-standard among many platforms/compilers. On all machines the native binary representation can be chosen. On some platforms additional conversion types are offered (IEEE on most machines, CRAY format an CRAYs).

The Fortran standard does not guarantee that unformatted (i.e. also UIO) files are readable on all machines. But it is always possible to produce (formatted) UIO files on a machine which are readable on all others. And with some fiddling with compile options or the call of machine-specific subroutines provided by the compiler vendor it was up to now always possible to enable the access to binary UIO files (of one common format: IEEE `big_endian`) on all machines and compilers tested: Compaq alpha, Cray, Hitachi, HP V2500, HP Itanium2, IBM, Intel/AMD (with Linux OS and PGI, Intel, or Pathscale compiler), NEC SX-5, SGI, and Sun. Problems might arise with the transition to records larger than 2 GByte which require an extension of the current standard. The GNU Fortran compilers (particularly g95) might introduce a 64-bit system that does not allow to read older 32-bit files (even small ones).

Each file entry is a header-data-unit. The header contains information to identify the entry and to specify the format and size of the following data block. This block usually consists of a scalar or an array. In some cases it is empty (e.g. for labels) or it contains more complex information (for tables).

The first version of UIO routines was written in FORTRAN77. It still exists. However, further development was done with the Fortran90 versions. Therefore, the use of the FORTRAN77 routines is not recommended anymore. The current Fortran version of the UIO routines is a set of Fortran90 modules.

To allow a communication between Fortran and IDL programs, an IDL version of the UIO routines has been written. The correspondence between Fortran and IDL routines is rather close. But in detail, there are differences. Currently, IDL Version 6.0 is used. Amazingly, the UIO routines also used to work under *PV-WAVE* (Version 6.01, sun4 solaris sparc).

So far, there exist three UNIX shell scripts (calling Fortran routines) useful to quickly examine data sets or to change the format or conversion type of files. The installation of these scripts with a "configure-make-make install" sequence is described in Sect. 4.6.1.

Without these scripts an UIO file in ASCII format can be examined with any text editor or with `more`. To get an overview about the contents of a binary file the command

```
strings -30 uio_example_file.dat
```

can be useful.

4.2 Example of UIO Data File

To give a first impression about the data structure, here follows a simple test file, which contains the header, a label, a couple of scalars, an array, and a short table:

```
fileform uio form=formatted convert=native version=0.1.1997.11.29 &
date='29.11.1997 21:23:39.835' system=IRIX machine=atlas osrelease=6.3 &
osversion=12161207 hardware=IP32 language=Fortran90 program=uiotst

label testdata n='sample test data field' date='29.11.1997 21:23:39.835'

integer ia f=I3 b=4 n='This is the answer'
```

```
 42
complex ca f='''('',E13.6,'',',E13.6,'')''' b=8 n='This is a complex answer'
( 0.400000E+01, 0.200000E+01)
real da f=E23.15 b=8 n='precise answer'
  0.420000000000000E+02
real answer f=F4.0 b=4 n=answer u=1
 42.

real real2d d=(100:103,200:204) f=E13.6 p=4 b=4
 0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+01
 0.500000E+01 0.600000E+01 0.700000E+01 0.800000E+01
 0.900000E+01 0.100000E+02 0.110000E+02 0.120000E+02
 0.130000E+02 0.140000E+02 0.150000E+02 0.160000E+02
 0.170000E+02 0.180000E+02 0.190000E+02 0.200000E+02

table f77table d=(1:5,1:7) f=1X b=1 n='test table to test the table routines'
integer   int1  f=I5    b=4  n='Integer: 1. column'
real      real1 f=F5.1  b=4  n='Real: 2. column'
character char1 f=A16   b=16 n='Char: 3. column'
real      real2 f=E13.6 b=4  n='Real: 4. column'
integer   int2  f=I5    b=4  n='Integer: 5. column'
 int1 real1            char1         real2  int2
    1   2.0 a                 0.100000E+02     1
    2   4.0 ab                0.200000E+02     2
    3   6.0 abc               0.300000E+02     3
    4   8.0 abcd              0.400000E+02     4
    5  10.0 abcde             0.500000E+02     5
    6  12.0 abcdef            0.600000E+02     6
    7  14.0 abcdefg           0.700000E+02     7
```

4.3 Structure of UIO Files

4.3.1 Data Representation: ASCII or Binary

While opening a file for writing, the file format ("formatted" or "unformatted") and the conversion type ("native", e.g. "ieee_4", ...) have to be specified.

The *formatted* ASCII data representation allows I/O independent of platform or compiler. It is useful for parameter files which can be read and edited by hand, for the direct inspection of data, the transfer between very different systems, or for the import of data which exist e.g. in a table format. From the specified conversion type only the default output format for numbers (e.g. "E13.6" for 4 byte reals) is determined.

The *unformatted* binary I/O is much faster and gives usually more compact files with higher accuracy (ideally exact) in the numerical data representation. But – in principle – the file format is machine dependent. Fortunately, the IEEE format turns out to become a quasi-standard among a variety of machines. Most workstations work internally with this format. Some CRAYS which have a different internal data representation allow the hidden transformation between the internal and IEEE format during the I/O process. The UIO routines support this feature of CRAY FORTRAN compilers by means of a module (`uio_mac_module`) individually designed for (two types of) CRAY machines using certain CRAY specific system calls (CRAY FFIO assign logic). Nevertheless, there is also a machine independent version of this module, written completely in standard Fortran90 but providing less features than the machine-dependent versions.

Besides the format, the conversion type (see table 4) has to be specified. The "native" conversion type is the internal binary data representation, which is also standard for unformatted Fortran output. If this representation happens to be conformal with the IEEE standard the conversion type "ieee_4" should be used. It gives the same data format, but in the header of the file the term "convert=ieee_4" instead of "convert=native" describes the data format precisely – in a way also understandable by other machines. On CRAY machines the native format is equal to the conversion type "crayxmp_8", but also the conversion types "ieee_4", "ieee_4_limit", and

"ieee_8" can be chosen. The last three conversion types correspond to the CRAY internal types "ieee_32", "ieee_dp", and "ieee_64", respectively.

On a machine with an internal data representation not within the list in the existing `uio_mac*_module.f90` files one could use the standard file `uio_mac_module.f90` and is restricted to the "native" conversion type. But it is better to invent an appropriate name for the new data format and to build a proper machine dependent UIO file, e.g. from `uio_mac_ieee_module.f90`.

conversion type	I	R	D	description
`native`	?	?	?	internal data format on all machines (sometimes useful but not recommended)
`ieee_4`	4	4	8	standard IEEE `big_endian` format (recommended)
`ieeele_4`	4	4	8	IEEE `little_endian` format
`ieee_8`	8	8	16	double precision IEEE `big_endian` format (on some machines possible)
`crayxmp_8`	8	8	16	CRAY internal data format
`idl`	4	4	8	IDL format (but IDL also supports `ieee_4`)
`xdr`	4	4	8	format possible with IDL
`ieee_4_limit`	4	8	8	standard IEEE format → `ieee_4`
`ieee`	?	?	?	IEEE format, unknown length (not recommended)

Table 4: UIO conversion types with length of integers, single precision reals, and double precision reals in bytes, and an explanation.

Some attention has to be paid if weird compiler switches (as e.g. `-r16 -i2`) are used to modify the accuracy and standard memory size of variables.

If an existing file is opened for reading, the file format and conversion type are determined automatically from the file if the conversion type of the data in the file is among the conversion types supported by the compiler. If the file has a conversion type "native" but is created on a machine with different internal data representation, the file header might be readable, but an error will probably occur during the reading of a real variable.

4.3.2 Data File Structure

The UIO routines only handle sequential files. Each file consists of a list of entries. The first entry describes the file format, conversion type, and the machine who is responsible for it. The following entries contain data (scalars and 1D ... 4D arrays of type integer, real (single & double precision), complex (single precision), character; tables with columns of type integer, real (single precision), or character), or structuring information (labels).

Each entry consists of the header and the (possibly empty) data block.

Each header is a list of at most 20 terms separated by blanks or linefeeds. The first term is the entry type (e.g. `real`, see table 5), followed by an identifier. This identifier should follow the standard rules for variables (lowercase letters, numbers, underscore; starting with letter). It is a name as e.g. `rho`, `v_1`. The rest of the terms come in the form "keyword=value". See Tab. 6 for some pre-defined keywords.

A header line has a maximum length of 80 characters. A continuation line is indicated by ␣& at the end of the line. A header consists of 20 lines at maximum. It can be preceded by empty lines (except for the file header entry). Example:

```
real time f=F9.2 b=4 n='Time' u=s c0='Simulation time in seconds' &
  c1='Time count starts at 0.0'
    12.34
```

The entry header is followed by the entry data block. This block is empty for labels and the fileform entry but non-empty otherwise.

entry type	entry contents
`fileform`	file description (first entry)
`integer`	scalars, 1D ... 4D arrays
`real`	scalars, 1D ... 4D arrays, single & double precision
`complex`	scalars, 1D ... 4D arrays, single precision
`character`	scalars, 1D ... 4D arrays
`table`	table with integer, real, character columns
`label`	label entry for file structuring

Table 5: UIO entry types

In an *unformatted* file each header line is an individual record containing a string with exactly 80 characters. The following data block (scalar or array) is one single record.

In a *formatted* file each header line is a string of at most 80 characters delimited by a `LINEFEED` of whatever the operating system decided to be appropriate as `EOL` character (sequence). The following data block is written as sequence of lines. The number of items per line is specified by the "p=?" keyword in the header.

4.3.3 Tables

For a table the entry header is followed by a list of headers for the individual table columns, a single table header line consisting of (abbreviations of) the table entry identifiers and the table itself (see the example in section 4.2). The dimension keyword gives the number of columns and rows in the form "d=(1:columns,1:rows)".

The Holweger-Müller-Atmosphere is chosen as the following "real world" example for a file with a table in UIO format:

```
fileform uio form=formatted convert=ieee_4 version=0.0.1996.10.29 &
  date='20-Feb-1997 18:40:45' system=SunOS machine=saturn osrelease=4.1.3 &
  osversion=3 hardware=sun4m language='IDL 4.0' program='by hand'

character description d=(0:3) f=A80 p=1 b=80 d='13-Nov-1996 18:29:48'
Holweger-Mueller-Atmosphere,
Hartmut Holweger & Edith Mueller (1974) Solar Physics 39, 19-30, table II,
empirical solar temperature stratification to fit solar spectral lines and
limb darkening

character history d=(0:3) f=A80 p=1 b=80 d='13-Nov-1996 18:29:52'
Holweger-Mueller-Atmosphere, from 1974
uio-form:              13-Nov-1996 18:29:52
conversion type added: 20-Feb-1997 18:21:01
xi -> vmicro:          20-Feb-1997 18:23:43

real teff f=F6.1 b=4 n='effective temperature' u=K texa='T_ eff'
5780.0

table atmosphere d=(1:7,1:29) f=X b=1 n=Holweger-Mueller-Atmosphere &
c0='Hartmut Holweger & Edith Mueller (1974) Solar Physics 39, 19-30, table II' &
  c1=Teff(Sun)=5780K
real tauross f=E9.2 b=4 n='optical depth (Rosseland)' u=1
real tau5000 f=F7.3 b=4 n='optical depth (lambda5000)' u=1 t=log10
real t       f=F7.0 b=4 n=temperature u=K
real pgas    f=F6.3 b=4 n='gas pressure' u=dyn/cm^2
real pel     f=F6.3 b=4 n='electron pressure' u=dyn/cm^2
real vmicro  f=F4.2 b=4 n=microturbulence u=km/s
real q       f=F8.5 b=4 n='Hopf function' u=1 c0='q=((T(tau)/Teff)^4)/0.75)-tau'
  tauross tau5000       t   pgas    pel vmic        q
 2.00E-07  -6.539   3900.  0.769 -3.140 0.00  0.27637
```

keyword	description	example	descriptor	info.	necessary
b	byte number	4	format		yes
d	dimension	(0:9)	format		yes (arrays)
ds	dimension shift	(1:1)		yes	
f	Fortran format	E13.6	format		yes
p	values per line	4	format		yes (arrays)
t	transformation	log10	format		
n	name	density		yes	
u	unit	g/cm^3		yes	
date	date	1.1.98		yes	
c0...9	comment	Dichte		yes	
form	file format	formatted	file		yes (file header)
convert	conversion	ieee_4	file		yes (file header)
version	version	0.1.1997.11.29		yes	
system	system	IRIX		yes	
machine	machine name	atlas		yes	
osrelease	OS release	6.3		yes	
osversion	OS version	12161207		yes	
hardware	machine hardware	IP32		yes	
language	program. language	Fortran90		yes	
program	program	uiotst		yes	
xyz...	user defined	source		yes	

Table 6: Standard UIO entry header keywords: The keyword is given with a short description and an example. The fourth, fifth, and sixth column indicate if the keyword is a mandatory descriptor (in the file header or for the format of an entry) or if it gives only additional information and is optional and therefore not necessary to specify.

```
2.50E-07  -6.279   3920.  1.171 -2.752 0.00  0.28208
5.00E-07  -5.868   3970.  1.598 -2.342 0.00  0.29675
1.00E-06  -5.588   4030.  1.842 -2.105 0.00  0.31510
2.00E-06  -5.334   4080.  2.042 -1.910 0.00  0.33103
5.00E-06  -5.001   4160.  2.279 -1.674 0.00  0.35776
1.00E-05  -4.747   4210.  2.450 -1.508 0.00  0.37527
2.00E-05  -4.486   4270.  2.618 -1.341 0.00  0.39712
5.00E-05  -4.131   4340.  2.835 -1.128 0.00  0.42377
1.00E-04  -3.856   4400.  2.999 -0.967 0.50  0.44765
2.00E-04  -3.577   4460.  3.162 -0.804 0.50  0.47248
5.00E-04  -3.200   4530.  3.377 -0.596 0.50  0.50256
1.00E-03  -2.912   4590.  3.541 -0.437 0.50  0.52925
2.00E-03  -2.621   4640.  3.704 -0.279 0.50  0.55173
5.00E-03  -2.233   4720.  3.919 -0.070 0.50  0.58792
1.00E-02  -1.939   4800.  4.083  0.094 0.50  0.62415
2.00E-02  -1.645   4900.  4.245  0.266 0.65  0.66867
5.00E-02  -1.256   5080.  4.460  0.504 0.85  0.74558
1.00E-01  -0.961   5260.  4.622  0.705 1.00  0.81447
2.50E-01  -0.571   5560.  4.830  1.002 1.25  0.89163
4.00E-01  -0.371   5850.  4.926  1.251 1.40  0.99911
7.00E-01  -0.133   6260.  5.022  1.613 1.50  1.13453
1.00E+00   0.019   6570.  5.070  1.879 1.60  1.22581
1.50E+00   0.191   6880.  5.114  2.140 1.70  1.17659
2.00E+00   0.312   7160.  5.140  2.363 1.80  1.13964
4.00E+00   0.597   7920.  5.191  2.889 1.80  0.70033
6.00E+00   0.761   8250.  5.213  3.092 1.80 -0.46595
8.00E+00   0.877   8420.  5.229  3.196 1.80 -1.99552
1.00E+01   0.967   8500.  5.242  3.245 1.80 -3.76404
```

4.3.4 Recommendations for Standard File Structure

The very first entry in an UIO file is always the `fileform uio` entry, containing information about the file format and conversion type. Afterwards, entries can follow in any order. But it is perhaps a good idea to start the file with three special entries (`file_id`, `description`, `history`) as in

```
fileform uio form=formatted convert=ieee_4 ...

character file_id f=A80 b=80 n='File identification'
uio-demofile

character description d=(1:2) f=A80 p=1 b=80 n='File description'
This is a file to demonstrate the recommended start entries for all
UIO files.

character history d=(1:1) f=A80 p=1 b=80 n='File history'
UIO demo file: 22-Dec-1997 14:15:15
```

A recommended format for sets of multi-dimensional arrays (e.g. hydrodynamics: x-axis, y-axis, z-axis, density, velocities, energy, ...) is shown in Sect. 5.1.

4.4 Files & Directories & Paths

All UIO-routines are located in sub-directories of a common directory (called e.g. `uio`), which also contains a old Readme file. The subdirectories and their contents are

`bin` : shell scripts: `uiolook`, `uiocat`, `uioinfo`
`f90` : Fortran90 source codes, object files, executables
`idl` : IDL routines
`man/man1`: manual pages for shell scripts: `uiolook`, `uiocat`, `uioinfo`
`tex` : old description files in LaTeX, the most recent version is part of this document

To use the UNIX scripts and the makefile you need a global system variable **UIOPATH** pointing to this directory. The path to the shell scripts and to the man-pages should be added to your shell path variables e.g. in one of the login scripts:

C-shell (`.cshrc`):

```
# --- uio ---
setenv UIOPATH "$HOME/uio"
setenv PATH "$PATH:$UIOPATH/bin"
setenv MANPATH "$MANPATH:$UIOPATH/man"
# --- *** ---
```

Korn-shell (`.kshrc`):

```
# --- uio ---
UIOPATH=$HOME/uio
export UIOPATH
PATH=$PATH:$UIOPATH/bin
export PATH
MANPATH=$MANPATH:$UIOPATH/man
export MANPATH
# --- *** ---
```

File	contents
`uio_base_module.f90`	Collection of basic modules
`uio_mac_module.f90`	(Possibly) machine dependent routines Standard version (all machines)
`uio_mac_ieee_module.f90`	Machine dependent routines: IEEE format
`uio_mac_sun_module.f90`	Machine dependent routines: Sun, SGI, Linux, HP
`uio_mac_intel_module.f90`	Machine dependent routines: Linux Intel (`little_endian`)
`uio_mac_crayts_module.f90`	Machine dependent routines: CRAY
`uio_mac_crayxmp_module.f90`	Machine dependent routines: CRAY
`uio_mac_decalpha_module.f90`	Machine dependent routines: alpha
`uio_mac_hitachi_module.f90`	Machine dependent routines: Hitachi
`uio_bulk_module.f90`	Main part of UIO routines
`uio_filedef_module.f90`	Standard file descriptors and labels
`uio_table_module.f90`	Table manipulation routines
`uio_var_module.f90`	definition and handling of UIO flexible variable
`uio_varfile_module.f90`	definition and handling of file structure of UIO flexible variables
`uiocop.f90`	Program to copy and transform UIO files
`uiolok.f90`	Program to look into UIO files
`uioinf.f90`	Program to give information about conversion types
`uiotst.f90`	Program to produce test UIO file

Table 7: UIO Fortran90 files

module	contents
uio_cst_module	channel status information
uio_cvl_module	convert type list of current machine
uio_inf_module	information about environment
uio_nam_module	definition of names
uio_siz_module	string length, table size
uio_base_module	basic set of UIO-routines: string processing, header handling, I/O channel management

Table 8: Contents of uio_base_module.f90

4.5 Fortran90

4.5.1 Files

The Fortran UIO package is a collection of Fortran90 modules and programs described in Table 7.

The file `uio_base_module.f90` contains the basic set of modules (see Table 8).

The files `uio_mac*_module.f90` (Tab. 7) contain machine dependent routines collected in the module uio_mac_module (see Tab. 9).

It comes in various flavors. The machine-independent version is `uio_mac_module.f90` which can be used for first tests but does not provide all possible features. Therefore, it should be discarded afterwards and replaced by a version more suitable for the platform in use. The file `uio_mac_ieee_module.f90` is appropriate for all machines with IEEE `big_endian` binary format. Additionally there exist files containing calls of machine library routines `uio_mac_crayts_module.f90`, `uio_mac_crayxmp_module.f90`, `uio_mac_sun_module.f90`. These make it possible to write information about the platform in use into the file header. The CRAY versions allow unformatted I/O in the CRAY specific format and additionally (via the FFIO ASSIGN logic) in IEEE format. The file `uio_mac_intel_module.f90` is appropriate for all machines with IEEE `little_endian` binary format (and no mechanism for automatic conversion).

routine	purpose
uio_getenv	Get information about environment
uio_mkcvls	Make list with possible conversion types
uio_uopen	Open file with special handling for conversion type
uio_uclose	Close file with special handling for conversion type

Table 9: Contents of uio_mac_module

The main set of routines is contained in `uio_bulk_module.f90` in the module uio_bulk_module.

The three files `uio_base_module.f90`, `uio_mac_module.f90`, and `uio_bulk_module.f90` comprise the standard set of UIO routines.

Additionally there exists a file `uio_table_module.f90` with the single module uio_table_module which permits the I/O and manipulation of a certain table format (see the example in section 4.2).

The latest extension comes within the modules `uio_var_module.f90` and `uio_varfile_module.f90`. The module `uio_var_module.f90` contains a type definition for a variable ("uio flexible variable") of general type (i.e. it may be a scalar integer value or a 1D character array or a 3D real array...) together with some routines for the basic handling of the variables (I/O in UIO format, construction and modification of variables...). The module `uio_varfile_module.f90` contains a type definition for a file built of UIO flexible variables together with routines for the handling of these files.

4.5.2 Use of UIO Modules in Fortran90

To make the UIO routines available in a Fortran program the appropriate modules have to be specified in a `USE` statement.

At maximum five modules play a role: The `uio_bulk_module` contains the main part of the UIO routines (and also uses the relevant sub-modules). Instead of `uio_bulk_module` the module `uio_table_module` is used if the UIO table routines are needed. The modules `uio_siz_module` and `uio_nam_module` contain specifications about the size of some arrays and the length of strings, and the names of types and keywords, respectively. The module `uio_filedef_module` contains some definitions in addition to the basic UIO standard as e.g. the label names which delimit a data set (`label dataset` and `label enddataset`).

A typical case for the use of UIO modules is

```
use uio_bulk_module
use uio_siz_module
use uio_nam_module
```

4.5.3 Compiling and Makefiles

For a certain platform it is necessary to change the name of the module file with the machine dependent routines (`uio_mac*_module.f90`) in a Makefile for the UIO routines. For this purpose the environment variable `UIOMAC` has to be set to the name of the appropriate routine (see Sect. 3.3). For CO5BOLD or the UIO UNIX scripts the respective configure script takes care of this step. Many compilers generate module information files with suffixes like `.M`, `.mod`, or `.kmo`. To clean up information files with other suffixes, they have to be included in the cleaning step.

Calling examples:

```
make
make UIO
make UIO "F90FLAGS=-g"
make clean
```

```
make cleanall
make remove
make removeall
```

A section of a typical makefile using the UIO routines may be

```
...
# --- Compiler options ---
F90C=f90
F90FLAGS=
# --- Libraries ---
UIOMAC=uio_mac_sun_module
...
# --- Dependencies of exe-files on object files and libraries ---
test.exe: test.o
        $(F90C) $(F90FLAGS) -o $@
        $(UIOPATH)/f90/uio_base_module.o $(UIOPATH)/f90/$(UIOMAC).o
        $(UIOPATH)/f90/uio_bulk_module.o

test.o: $(UIOPATH)/f90/UIO test.f90
        $(F90C) -c $(F90FLAGS)          -M$(UIOPATH)/f90          test.f90
...
# --- Dependencies on used modules ---
$(UIOPATH)/f90/UIO:
        cd $UIOPATH/f90 ; make UIO "F90FLAGS=$F90FLAGS"
```

4.5.4 Sample Calls of Fortran UIO Routines

The needed modules have to be declared by a `use` statement like:

```
use uio_bulk_module
```

In the initial phase of the program the UIO routine package has to initialized by exactly one call of the `uio_init` routine with the name of the program as optional parameter:

```
call uio_init(progrm='uiotst')
```

The internal list of logical I/O unit numbers may be changed with calls of `uio_chunit` and `uio_chconv`.

A file can be opened for writing with

```
file='test.txt'
form='formatted'   ! or: 'unformatted'
conv='ieee_4'      ! or: 'native', 'crayxmp_8',...
call uio_openwr(ncout, file, form=form,conv=conv)
```

Header and data block are written together with one command as e.g. in:

```
call uio_wr(ncout, time,       'time', name='time',    unit='s'     )
call uio_wr(ncout, rho(1:10),  'rho',  name='density', unit='g/cm^3')
```

There are two different routines to close a file after reading or writing. A file opened for writing is closed by:

```
call uio_closwr(ncout)
```

To open a file for reading, only the file name has to specified. File form and conversion type are determined automatically:

```
file='test.txt'
call uio_openrd(ncin, file)
```

In contrast to the writing of an entry by one routine call the reading is performed in two separate sub-steps for the header and the data part. After the reading of the header e.g. with

```
use uio_siz_module
use uio_nam_module
...
integer                                 :: ntt
character*(let)                         :: termt(2,nttmx)
...
call uio_rdhd(ncin, termt,ntt)
```

the identifier, type, and dimension (if any) of the entry is contained in the character array `termt` with `ntt` entries and special actions may be taken: The data part may be skipped with

```
uio_skipda(ncin, termt,ntt)
```

or it can be read with:

```
call uio_rd(ncin, termt,ntt, time, ident)
```

If the entry is an array it may be necessary to allocate memory:

```
call uio_exkeyw(termt,ntt,  dimna,dimstr)
call uio_st2dim(dimstr, ilow, iup, ndim=ndim)
allocate(rho(ilow(1):iup(1)))
call uio_rd(ncin, termt,ntt, rho, ident, ilb=ilow(1:1))
```

Alternatively, it is possible to search in the file for a special entry or to search in a specially generated entry list with:

```
call uio_srhd(ncin, termt,ntt, type='real',ident='rho',outstr=outstr,ierr=ierr)
```

Additionally, the module `uio_var_module` makes it possible to read any entry into an UIO flexible variable, and the module `uio_varfile_module` allows the reading of a complete file into a special file structure of UIO flexible variables.

To close a file after reading use

```
uio_closrd(ncin)
```

There are several examples of programs with UIO routines like `uio_var_test.f90`, `uio_varfile_test.f90`, `uiotst.f90`, (`uio_demo.f90`) and – of course – CO5BOLD.

4.6 UNIX Scripts

So far, there exist three UNIX shell scripts useful to quickly examine data sets (`uiolook`), to change the format or conversion type of files (`uiocat`), or to print some information about the conversion types possible on the local machine (`uioinfo`).

4.6.1 Installation of UIO UNIX Scripts

Recently, the installation procedure for the UIO scripts has been updated to make use of its own configure script. Therefore, the procedure should now look like

```
tar -zxvf for.tar.gz
cd for/uio/f90/YOUR_MACHINE
./configure
make
make install
```

or

```
tar -zxvf for.tar.gz
cd for/uio/f90
mkdir YOUR_MACHINE
cd YOUR_MACHINE
ln -s ../conf/configure .
./configure
make
make install
```

Some of the environment variables that control the CO5BOLD configure script are also recognized (see the header of the UIO configure script). The command

```
make install
```

generates a directory `${HOME}/local` and sub-directories. An init script is put into `${HOME}/bin`. And the resource files `.cshrc` and `.bashrc` are modified to call it. Therefore, this installation step is *potentially dangerous*, because its effect is not restricted to the local directory!

4.6.2 Quick Examination of Files: uiolook

The shell script `uiolook` calls the Fortran program `uiolok.f90`. The man-page:

```
UIOLOOK(1V)       Misc. Reference Manual Pages        UIOLOOK(1V)

NAME
     uiolook - print entry headers of file in uio form

SYNOPSIS
     uiolook [ -h ] [ -p ] [ filename ...  ]

AVAILABILITY

DESCRIPTION
     The routine uiolook reads each filename (file in  uio  form)
     in  sequence  and  displays  the  headers  of the entries in
     pretty form.

OPTIONS
     -h    Print usage of uiolook.

     -p    Entry header keywords in (long) pretty form

SunOS 5.5.1       Last change: 27 November 1996                1
```

4.6.3 Transformation of Files: uiocat

The shell script `uiocat` calls the Fortran program `uiocat.f90`. The man-page:

```
UIOCAT(1V)        Misc. Reference Manual Pages         UIOCAT(1V)

NAME
     uiocat - concatenate file(s) in uio form

SYNOPSIS
     uiocat [ -c conversion ] [ -f format ] [ -h ] [ -l  copylist
     ] [ -o outputfilename ] [ filename ...  ]
```

```
DESCRIPTION
     The routine uiocat reads each filename (file in uio form) in
     sequence  and  displays  its  contents formatted on standard
     output or writes it into a file.  In  the  latter  case  the
     format  change  from  'formatted'  to  'unformatted' or vice
     versa is possible.

OPTIONS
     -c    Conversion  type:  'native',  'ieee_4',  ...  (machine
          dependent),  its  specification is only relevant, if an
          output file is specified with the -o option and  output
          format='unformatted'.

     -f    Output  format:  'formatted'  or  'unformatted'.   Its
          specification  is  only  relevant, if an output file is
          specified with the -o option.

     -h    Help: print usage of uiocat.

     -l    List of entries to be copied. E.g.
            uiocat ... -l"real rho"
            uiocat ... -l"real rho,integer i"
            uiocat ... -l"label *,real rho,integer i"
            uiocat ... -l"label *,real rho,* i"
            Here, copylist is a list, separated by ",". Each item
          consists of exactly two items, separated by a blank. No
          additional blanks are allowed.  Use copylist with "" as
          above.

     -o    Output file name. If omitted, standard output is  used
          and "-c" and "-f" are meaningless.

SunOS 5.5.1       Last change: 12 January 1998                1
```

4.6.4 Information about Conversion Types: uioinfo

The shell script `uioinfo` calls the Fortran program `uioinf.f90`. The man-page:

```
uioinfo(1V)       Misc. Reference Manual Pages       uioinfo(1V)

NAME
     uioinfo - print machine dependent information

SYNOPSIS
     uioinfo

DESCRIPTION
     The routine uioinfo prints information about its environment
     and a list of possible conversion types.

OPTIONS

SunOS 5.5.1       Last change: 12 January 1998                1
```

4.7 IDL UIO Routines

The UIO package in IDL comes as a list of routines with names quite similar to the Fortran90 version. Instead of using global variables as in Fortran90 there are now common blocks in Include-files.

```
;*****************************************************************************
; Routines, functions : uio_*.pro:
;               (!: most important, +: user-routine, -: comfortable, .:useful)
; . adkey1:     Add one keyword to term table, keyword-value=' ', no link character
; . adkey2:     Add one keyword to term table with keyword-value
; . adkey3:     Add one keyword to term table with keyword-value or default
; . chconv:     Actualize list of conversion types for all channels
; + chpos:      Give current file position or jump to specified position
; . chunit:     Initialize, store and actualize a list of free and occupied unit
;               numbers
; + closrd:     Close file after reading
; + closwr:     Close file after writing
; - cpentr:     Copy entry from one file to another
; + d:          Read data from uio-file(s) in quasi direct access mode
; + data:       Handle uio-file(s) in quasi direct access mode
; ! dataset_rd: Read uio file and put data into anonymous structure
; ! datasetlist_rd: Read data from list of files and put it into an. structure
;   deform:     Determine the default output format for numbers
;   dim2st:     Compose dimension string
; . exkeyw:     Extract value of keyword from table
;   ex1trm:     Extract one term from the input line
;   exmtrm:     Transform a list of items into its components
; . filcon:     Determine file contents: list of all entries with its positions
;   getenv:     Get information about environment
; ! init:       Initialization procedure for input/output routines
;   me1trm:     Merge the input term: 'keyword', 'value' -> 'keyword=value'
;   memtrm:     Merge a list of terms (keywords and their values) into a line table
;   mkcvls:     Make list with possible conversion types
; . nc2nt:      From column number or entry name find table entry number
; + openrd:     Open file for reading, read header
; + openwr:     Open file for writing, write header
; - pptrmt:     Print term table in pretty form
;   qmaadd:     Transform a string into a string with quotation marks if necessary
;   qmadel:     Parse string "inline" and remove quotation marks if necessary
; + rd:         Reading scalar and array data of all types
; . rdfifo:     Read file header
; + rdhdex:     Read header of variable and extract keywords
;   rdhead:     Read header
; + rdlabl:     Read label
; + rdtab:      Read table of integer, real, and/or character data from file
; + skipda:     Skip data block
; - slhdex:     Search header of variables given by list and extract keywords
; . st2dim:     Parse dimension string
; ! struct_rd:  Read uio file and put data into anonymous structure
; . tab0:       Create empty table structure
; + tabc:       Change and modify table contents: rearrange lines.
; + tabm:       Merge two tables in different ways
; + tabr:       Read 1d array from 2d table array (all types)
; + tabw:       Write 1d array into table (all types)
;   uclose:     Close file with special handling for conversion type
;   uopen:      Open file with special handling for conversion type
;   vnanrm:     Transform a string to give a correct name of a variable
;   wf2rf:      Produce from write format string corresponding read format string
; + wr:         Writing scalar and array data of all types
; . wrfifo:     Write file header
;   wrhdme:     Write header of variable, input: term table.
;   wrhead:     Write header of variable, input: line table.
; + wrlabl:     Write label
; + wrtab:      Write table of integer, real, and/or character data to file
;*****************************************************************************
; Include-Files uio_*.pro:
```

```
;   filedefinc:
;   uiocstinc:  channel status information (common uio_chainf)
;   uiocvlinc:  convert type list of current machine (common uio_cvlist)
;   uionaminc:  names of types, keywords, identifiers; default formats
;               (common uio_defnam)
;   uiosizinc:  length of strings, size of tables (trmtab, lintab)
;   uiotabinc:  empty table structure (common uio_taborg)
;*****************************************************************************
```

Most of the routines are low-level ones and do not have to be worried about because they rarely will be used directly.

For accessing data in UIO format within IDL the initialization routine `uio_init` (see Sect. 4.7.1) and the high-level reading routines (`uio_struct_rd.pro`, `uio_dataset_rd.pro`, and `uio_datasetlist_rd.pro`, see Sect. 4.7.3) might suffice.

4.7.1 Initialization of UIO Routines under IDL

The directory containing the IDL UIO routines should be added to the IDL variable !PATH. This could be done by a program segment in the startup procedure, like:

```
; --- Try to determine language ---
if (n_elements(!X.TICKV) eq 150) then langua='WAVE' else langua='IDL'
;
; --- Add user IDL directory to search path ---
if (langua eq 'IDL') then begin &$
  addpath=expand_path('+$UIOPATH/idl') &$
endif else begin &$
  addpath='/home/supas024/uio/idl' + ':' + '/home/supas024/wave' &$
endelse
if strtrim(addpath,2) ne '' then !path=addpath+':'+!path
delvar, addpath
```

Alternatively, one might want to set the IDL path variable accordingly like

```
export IDL_PATH="+$UIOPATH/idl"
```

for example in the `.bashrc` file. Or one just copies or links the UIO IDL routines to a location in the standard IDL search path.

It is reasonable to include the UIO initialization in the startup procedure as e.g.:

```
; --- Initialize uio-routines ---
uio_init, progrm='by hand'
```

IDL can handle the conversion types `native`, `ieee_4`, `ieeele_4`, `ieee`, `idl`, `xdr` (compare Tab. 4 in Sect 4.3.1). Here, `ieee_4` is the default and should be used as a standard.

Attention: The IDL type "long" corresponds to the standard Fortran type "integer". The IDL types "byte" and "integer" are not known in standard Fortran and are therefore transformed to the IDL type "long" before writing (in the IDL routine `uio_wr`).

Be aware of: The parsing and interpretation of the entry headers can only be done by scalar operations which are comparatively slow in IDL.

4.7.2 Reading Data with uio_data.pro

The IDL routine `uio_data` and the IDL function `uio_d` were the first set of "high-level" routines to read UIO data in IDL. They were useful for the easy reading of not too complex data files. By now, they are replaced by the routines `uio_struct_rd` and `uio_dataset_rd` (see see next Section and Sect 7).
The old routines allow the opening,

```
uio_data, mode='open', filename='model.dat'
uio_data, mode='open', filename='model*.txt'
uio_data, mode='open', filename='model.dat', family='mod1'
uio_data, mode='open', filename='model*.txt', family='mod2'
```

examination,

```
uio_data, mode='content'
uio_data, mode='files'
```

reading,

```
uio_data, mode='read', value=rho, 'rho'
uio_data, value=temp, 'temp'
uio_data, value=p, 'p', filename='model.dat'
uio_data, value=p, 'p', family='mod1'
plot_oi, uio_d('p'), uio_d('t')
```

and closing,

```
uio_data, mode='close', filename='model.dat'
uio_data, mode='close', filename='model*.txt'
uio_data, mode='close', family='mod2'
uio_data, mode='allclose'
```

of UIO files.

4.7.3 Reading Data with uio_dataset_rd.pro or uio_datasetlist_rd.pro

For a detailed description of how to handle UIO files in IDL see Sect 7.

With the new IDL routines `uio_struct_rd.pro`, `uio_dataset_rd.pro`, and `uio_datasetlist_rd.pro` files are not read entry by entry anymore but in larger blocks (or "data sets").

With `uio_struct_rd` all entries in a file are read and put into an IDL structure variable. This is appropriate for the CO5BOLD parameter file or for the UIO table file in Sect. 4.3.3, e.g.

```
par=uio_struct_rd('st35gm04n05_03.par')
atm=uio_struct_rd('holmu.atm')
```

When groups of entries in an UIO file are properly marked with `label dataset` and `label enddataset` delimiters (confer the example in Sect. 5.1) each group can be accessed with `uio_dataset_rd`. The first block can be read with

```
ful=uio_dataset_rd('st35gm04n05_03.full')
```

or

```
ful=uio_dataset_rd('st35gm04n05_03.full', ndataset=0)
```

Dataset number `i+1` (counting starts at zero) can be read with

```
ful=uio_dataset_rd('st35gm04n05_03.full', ndataset=i)
```

If a dataset with that number does not exist, an empty structure is returned. In this case, when called with additional keywords like

```
ful=uio_dataset_rd('st35gm04n05_03.full', ndataset=i, outstr=outstr,ierr=ierr)
```

an error message is returned in `outstr` and `ierr` is set to a value larger than 0.

To read all entries in a list of files in sequence the routine `uio_datasetlist_rd.pro` is convenient, as in the short example

```
ierr=0
delvar, listdata
;
; --- Loop over all datasets ---
while (ierr eq 0) do begin &$
  ; --- Read the next dataset ---
  ful=uio_datasetlist_rd('testmodel_0?.full', listdata=listdata, ierr=ierr) &$
  if (ierr eq 0) then begin &$
    print, '--- ', ful.z.time, format='(A,E15.8)' &$
    ;
    ; --- Now do the data handling (demo) ---
    print, 'Mean density: ', avg(ful.z.rho) &$
  endif &$
endwhile
```

or in the more detailed example

```
model='st33gm06n03' & modelident='_??' & parmodelident='_01'
modeldisk=getenv('HOME') + '/dat/rhd/d' + model + '/'
;
modelfile=modeldisk + model + modelident    + '.full'
parfile  =modeldisk + model + parmodelident + '.par'
;
; --- Read parameter file ---
par=uio_struct_rd(parfile)
;
; --- Open first dataset to get some information about array sizes ---
delvar, listdata
ful=uio_datasetlist_rd(modelfile, listdata=listdata, ierr=ierr)
uio_closrd, listdata.channel
delvar, listdata
;
nxc1=n_elements(ful.z.xc1)
nxc2=n_elements(ful.z.xc2)
nxc3=n_elements(ful.z.xc3)
;
n_timestep=1000  ; --- Some huge value to get everything. Reduce for tests! ---
ierr=0
i=0
;
; --- Loop over all datasets ---
while ((ierr eq 0) and (i lt n_timestep)) do begin &$
  ; --- Read the next dataset ---
  ful=uio_datasetlist_rd(modelfile, listdata=listdata, ierr=ierr) &$
  if (ierr eq 0) then begin &$
    print, '--- ', i, ful.z.itime, ful.z.time, format='(A,I4,I6,E15.8)' &$
    ;
    ; --- Now do the data handling (demo) ---
    print, 'Mean density: ', avg(ful.z.rho) &$
    ;
    i=i+1 &$
  endif &$
endwhile
```

All necessary counter information is stored in the structure `listdata`.

Note, that you can specify an entire group of files with e.g. `modelident='_*'`, `modelident='_??'`, `modelident='_3?'`, or `modelident='_{29,3[0-2]}'`.

5 Control and Data Files

Table 10 shows a list of all files necessary to run CO5BOLD. Figure 6 gives similar information but is not quite up to date. Executing the makefile produces an executable `rhd.exe`. Its name can of course be changed afterwards. The names of the control files `rhd.par`, `rhd.stop`, `rhd.cont`, and `rhd.dump` and of the status file `rhd.done` cannot be changed (without modification of the source code). The names of EOS, opacity, and CO5BOLD data files can be chosen freely in the parameter file `rhd.par`. Table 10 only contains dummy names.

File	Sect.	I/O	Type	Description
`rhd.exe`	3.2		executable	main program
`rhd.par`	5.3	I	control/data: UIO	central control file
`rhd.stop`	5.4	I	control	file to force controlled stop of simulation
`rhd.cont`	5.4	I	control	file to force continuation after stop
`rhd.dump`	5.4	I	control	file to request output of current model
`data.eos`		I	data: UIO	tabulated equation of state
`data.opta`		I	data	tabulated opacities
`rhd.sta`	5.1	I	data: UIO	start model (e.g. end file of last run)
`rhd.done`	5.4	O	status	exit status: written if run was successful
`rhd.end`	5.1	O	data: UIO	end model
`rhd.full`	5.1	O	data: UIO	sequence of (2D or 3D) snapshots, large
`rhd.mean`	5.2	O	data: UIO	derived data: mean flux, intensity
`rhd.snap`	5.4	O	data: UIO	file with model snapshot if requested
`rhd.out`	5.5	O	data: text	human readable text output
`data.dat`	5.6	I	data: text	chemical reaction data
`data.atom`	5.7	I	data: text	HION data file (model atom)
`edens.dat`	5.7	I	data: UIO	HION data file(electron density table)
`abundance.input`	5.7	I	data text	HION data file(abundances)
`pf_kurucz.dat`	5.7	I	data: UIO	HION data file(partition functions)
`HION.time.H.*.out`	5.8	O	data: UIO	HION: additional output
`HION.step.H.*.out`	5.8	O	data: UIO	HION: additional output

Table 10: List of all control and data files of CO5BOLD

5.1 Model Files: rhd.sta, rhd.end, rhd.full

If the UIO scripts (Sect. 4.6) are properly installed, you can view the contents (more precisely the headers of the data entries) of an UIO file with `uiolook filename`, e.g.

```
uiolook st35gm04n05_03.end
```

gives the output (slightly edited)

```
fileform uio form=unformatted convert=ieee_4 version=0.1.2000.11.26 &
  date='02.01.2002 16:17:26.036' system=craSHi machine=craSHi osrelease=10.0.0.6 &
  osversion=UoK.4 hardware='CRAY SV1' language=Fortran90 program=RHD

character file_id f=A8 b=8 n='File identification'
character description d=(1:1) f=A24 p=1 b=24 n='File description'
character history d=(1:20) f=A80 p=1 b=80 n='File history'
character version f=A80 b=80 n='Program version'

label dataset n='RHD model' date='02.01.2002 16:17:26.043'
  character dataset_id f=A10 b=10 n='Type of box hierarchy'
  real modeltime f=E13.6 b=4 n=time u=s
  real modeltime_db f=E23.15 b=8 n=time u=s
```

```
  integer modelitime f=I11 b=4 n='time step number' u=1
  real dtime f=E13.6 b=4 n='time step' u=s
  real time_out_full_last f=E13.6 b=4 n='Time of last output of full model' u=s
  real time_out_mean_last f=E13.6 b=4 n='Time of last output of averaged data' &
    u=s
  label box date='02.01.2002 16:17:26.049'
    character box_id f=A80 b=80 n='Block identification'
    integer dimension d=(1:2,1:3) f=I7 p=6 b=4
    real time f=E13.6 b=4 n=time u=s
    real time_db f=E23.15 b=8 n=time u=s
    integer itime f=I11 b=4 n='time step number' u=1
    real xc1 d=(-63:63,-63:-63,-63:-63) f=E13.6 p=4 b=4 &
    n='x1 coordinates of cell centers' u=cm ds=(0:0,0:1,0:1)
    real xc2 d=(-63:-63,-63:63,-63:-63) f=E13.6 p=4 b=4 &
      n='x2 coordinates of cell centers' u=cm ds=(0:1,0:0,0:1)
    real xc3 d=(-63:-63,-63:-63,-63:63) f=E13.6 p=4 b=4 &
      n='x3 coordinates of cell centers' u=cm ds=(0:1,0:1,0:0)
    real xb1 d=(-63:64,-63:-63,-63:-63) f=E13.6 p=4 b=4 &
      n='x1 coordinates of cell boundaries' u=cm ds=(0:1,0:1,0:1)
    real xb2 d=(-63:-63,-63:64,-63:-63) f=E13.6 p=4 b=4 &
      n='x2 coordinates of cell boundaries' u=cm ds=(0:1,0:1,0:1)
    real xb3 d=(-63:-63,-63:-63,-63:64) f=E13.6 p=4 b=4 &
      n='x3 coordinates of cell boundaries' u=cm ds=(0:1,0:1,0:1)
    real rho d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n=Density u=g/cm^3
    real ei d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Internal energy' u=erg/g
    real v1 d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Velocity 1' u=cm/s
    real v2 d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Velocity 2' u=cm/s
    real v3 d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Velocity 3' u=cm/s
  label endbox
label enddataset date='02.01.2002 16:17:43.322'
```

The UIO format is described in some detail in Sect 4. Each entry has a type (e.g. "`label`", "`real`", "`character`"), an identifier (e.g. "`box`", "`time`", "`description`"), and additional information about array size (e.g. "`d=(-63:63,-63:63,-63:63)`"), data format (e.g. "`f=E13.6 p=4 b=4`"), and properties of the quantity (e.g. "`n=Density u=g/cm^3`").

Each start ("`rhd.sta`") or final ("`rhd.end`") model file has a structure as shown above. The ("`rhd.full`") file usually contains a sequence of these data sets, which of course can also be used as start model of a simulation.

The axes `xc1`, `xc2`, and `xc3` describe the positions of the cell centers. The axes `xb1`, `xb2`, and `xb3` contain the positions of the cell boundaries: they have one element more than the corresponding cell centered quantity.

Cell boundaries should be centered in the middle between cell centers for the best representation of radiative fluxes with MSrad3D.

5.2 File with Additional Data: rhd.mean

A "`rhd.mean`" file contains derived data (averaged fluxes, other averaged quantities, surface intensities) in addition to the complete data sets in "`rhd.full`" files. It has more entries than a full model file. However, they are much smaller. Therefore, one can afford a higher output sampling rate.

Its format is usually Fortran "unformatted" (binary).

5.2.1 Organization of rhd.mean File

A mean file usually consists of several datasets. The overall structure is

```
fileform uio form=unformatted convert=ieee_4

character file_id f=A8 b=8 n='File identification'
```

```
character description d=(1:1) f=A14 p=2 b=14 n='File description'
character history d=(1:20) f=A80 p=1 b=80 n='File history'
character version f=A80 b=80 n='Program version'

label dataset n='RHD model'
...
label enddataset

label dataset n='RHD model'
...
label enddataset
.
.
.
```

Each dataset has the following structure (for a supergiant simulation):

```
label dataset n='RHD model' date='25.05.2001 09:41:29.405'
...

label box date='25.05.2001 09:41:29.408'
character box_id f=A80 b=80 n='Block identification'
rad
...
label endbox

label box date='25.05.2001 09:41:29.983'
character box_id f=A2 b=2 n='Block identification'
z1
...
label endbox

label box date='25.05.2001 09:41:30.078'
character box_id f=A2 b=2 n='Block identification'
z2
...
label endbox

label box date='25.05.2001 09:41:30.170'
character box_id f=A2 b=2 n='Block identification'
z3
...
label endbox

label box date='25.05.2001 09:41:30.260'
character box_id f=A1 b=1 n='Block identification'
r
...
label endbox

label box date='25.05.2001 09:41:30.359'
character box_id f=A80 b=80 n='Block identification'
z
...
label endbox
label enddataset date='25.05.2001 09:41:30.489'
```

There a six sub-blocks delimited with `box` and `endbox` labels. They contain surface intensity and flux arrays (`rad`), averages in the 23-plane (`z1`), the 13-plane (`z2`), the 12-plane (`z3`), and over spherical shells (`r`), and a 2D slice through the model (`z`).

5.2.2 Contents of Individual rhd.mean File Entry

An individual box inside a dataset entry in a mean file can have e.g. the following contents describing horizontal averages in a plane-parallel model. With

```
uiolook chro2D03co08_01.mean | less
```

you get this (and more):

```
label box date='06.11.2002 17:58:05.533'
  character box_id f=A2 b=2 n='Block identification'
integer dimension d=(1:2,1:3) f=I7 p=6 b=4
real time f=E13.6 b=4                              n=time &
                                                   u=s
real time_db f=E23.15 b=8                          n=time &
                                                   u=s
integer itime f=I10 b=4                            n='time step number' &
                                                   u=1
real xc1 d=(1:1,1:1,1:1) f=E13.6 p=4 b=4           n='x1 coordinates of cell centers' &
                                                   u=cm &
        ds=(0:0,0:1,0:1)
real xc2 d=(1:1,1:1,1:1) f=E13.6 p=4 b=4           n='x2 coordinates of cell centers' &
                                                   u=cm &
        ds=(0:1,0:0,0:1)
real xc3 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4         n='x3 coordinates of cell centers' &
                                                   u=cm &
        ds=(0:1,0:1,0:0)
real xb1 d=(1:2,1:1,1:1) f=E13.6 p=4 b=4           n='x1 coordinates of cell boundaries' &
                                                   u=cm &
        ds=(0:1,0:1,0:1)
real xb2 d=(1:1,1:2,1:1) f=E13.6 p=4 b=4           n='x2 coordinates of cell boundaries' &
                                                   u=cm &
        ds=(0:1,0:1,0:1)
real xb3 d=(1:1,1:1,1:121) f=E13.6 p=4 b=4         n='x3 coordinates of cell boundaries' &
                                                   u=cm &
        ds=(0:1,0:1,0:1)
real rho_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n=Density &
                                                   u=g/cm^3
real v1_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Velocity x1' &
                                                   u=cm/s
real v2_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Velocity x2' &
                                                   u=cm/s
real v3_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Velocity x3' &
                                                   u=cm/s
real v1_xmean2 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Velocity x1' &
                                                   u=cm/s
real v2_xmean2 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Velocity x2' &
                                                   u=cm/s
real v3_xmean2 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Velocity x3' &
                                                   u=cm/s
real rhov1_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Mass Flux x1' &
                                                   u=g/cm^2/s
real rhov2_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                   n='Mass Flux x2' &
```

```
                                                u=g/cm^2/s
real rhov3_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Mass Flux x3' &
                                                u=g/cm^2/s
real bc1_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Magnetic field 1' &
                                                u=G
real bc2_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Magnetic field 2' &
                                                u=G
real bc3_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Magnetic field 3' &
                                                u=G
real bc1_xmean2 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Magnetic field 1' &
                                                u=G
real bc2_xmean2 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Magnetic field 2' &
                                                u=G
real bc3_xmean2 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Magnetic field 3' &
                                                u=G
real ei_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n='Internal energy' &
                                                u=erg/g
real rhoei_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Internal energy' &
                                                u=erg/cm^3
real rhoek_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Kinetic energy' &
                                                u=erg/cm^3
real rhoeg_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Gravitational energy' &
                                                u=erg/cm^3
real t_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4  n=Temperature &
                                                u=K
real t_xmean4 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n=Temperature &
                                                u=K
real t_xmeankapparho d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n=Temperature &
                                                u=K
real p_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4  n=Pressure &
                                                u=dyn/cm^2
real s_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4  n=Entropy &
                                                u=erg/K/g
real rhos_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n=Entropy &
                                                u=erg/K/cm^3
real gamma1_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='1st Adiabatic Coefficient' &
                                                u=1
real gamma3_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='3rd Adiabatic Coefficient' &
                                                u=1
real delta_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Expansion coefficient' &
                                                u=1
real kapparho_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Absorption Coefficient' &
                                                u=1/cm
real quc001_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                                n='Number density of CO' &
```

```
                                                u=1/cm^3
rreal rhovb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Mass flux' &
                                                u=g/cm^ &
                ds=(0:0,0:0,0:1)
real frhov13b_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Momentum x1 flux x3 direction' &
                                                u=erg/cm^3 &
                   ds=(0:0,0:0,0:1)
real frhov23b_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Momentum x2 flux x3 direction' &
                                                u=erg/cm^3 &
                   ds=(0:0,0:0,0:1)
real frhov33b_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Momentum x3 flux x3 direction' &
                                                u=erg/cm^3 &
                   ds=(0:0,0:0,0:1)
real feipb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Enthalpy Flux' &
                                                u=erg/cm^2/s &
                ds=(0:0,0:0,0:1)
real fekb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Kinetic Energy Flux' &
                                                u=erg/cm^2/s &
              ds=(0:0,0:0,0:1)
real fegb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Gravitational Energy Flux' &
                                                u=erg/cm^2/s &
              ds=(0:0,0:0,0:1)
real fepb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Pressure Energy Flux' &
                                                u=erg/cm^2/s &
              ds=(0:0,0:0,0:1)
real fevb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Viscous Energy Flux' &
                                                u=erg/cm^2/s &
              ds=(0:0,0:0,0:1)
real ferb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                                n='Radiative Energy Flux' &
                                                u=erg/cm^2/s &
              ds=(0:0,0:0,0:1)
label endbox
```

The above list was slightly edited (by adding blanks) to improve readability.

The identifier of an entry together with the name (`n`='...') and the unit (`u`='...') should give a first hint about the meaning of the quantity. The suffix '`_xmean`' indicates a simple average. The suffix '`_xmean2`' indicates the root-mean-square average (note: the simple average is not subtracted).

Some entries (e.g. `ferb_xmean`) have a hidden `b` in their name, have one element more (e.g. 121 instead of 120) than most of the others, and are characterized by the `ds` keyword (see Table 6). These quantities are located at the cell boundaries in contrast to the usual cell-centered quantities. Clearly, there are also two sets of axes (e.g. `xc3` and `xb3`) corresponding to the cell- or boundary-centered quantities.

Note: The total energy flux can be written as sum

```
feb_total = feipkgvrb = feipb+fekb+fegb+fevb+ferb .
```

The flux `fepb` is already part of `feipb`.

5.3 Parameter File: rhd.par

The parameter file `rhd.par` also has the UIO format. But it will be usually Fortran "formatted" (ASCII).

It contains a list of parameter entries. which are collected in groups to make it easier to find an entry. Otherwise, the order is arbitrary (except for the very first `fileform uio` entry). If there are more than one entry with the same name, the first occurrence will be used by CO5BOLD. But the doubling of entries is strongly discouraged because it will almost certainly lead to confusion at some time. In addition, the IDL routine to read the parameter file will fail with an error message.

Additional entries can be added if the names differ from the standard ones described below. Theses entries will be ignored by CO5BOLD but read by the IDL input routine. They can be used to provide comments, additional information about the model, or control parameters for further processing.

5.3.1 Quickstart: How to Make a Proper Parameter File

You will never write a new parameter file from scratch. Typically, you take an old file (e.g. the one controlling the simulation which produced the model which is used to start the new run) and edit it:

1. Take the parameter file corresponding to the model you want the new simulation to start with.
2. Most of the parameters should be already OK. E.g. most of the parameters controlling the boundaries do not have to be changed.
3. Write a brief description of the purpose of the planned simulation into the `character description` array. You might but a remark about the parent file of the parameter file under construction and the current date into the `character history` array (see Sect. 5.3.2).
4. Check/modify the name of start model and output files: `infile_start`, `outfile_end`, `outfile_full`, `outfile_mean`. On a system with batch queue this has not to be done in the parameter file itself but in the external command file (see Sect. 5.3.16).
5. Check/modify the fundamental parameters including boundary condition specifiers (see Sections 5.3.3 and 5.3.4, respectively)
   - effective temperature control (`s_inflow`, `teff`, `luminositypervolume`, `C_radHtautop`)
   - gravity (`grav_mode`, `grav`, `mass_star`, ...)
   - abundances (`eosfile`, `opafile`, check the paths!)
6. If the gravity of the new model (and therefore the characteristic time scale) significantly deviates from the old one, the time specifications controlling the output frequency (`dtime_out_full`, `dtime_out_mean`), the total length of the simulation (if specified as stellar time: `endtime`, `plustime`), and absolute boundaries/specifications for the time step (`dtime_min`, `dtime_min_stop`, `dtime_max`, `dtime_start`) have to be scaled. Look for parameters with units `u=s` (see Sections 5.3.15 and 5.3.16).
7. The rest of the parameters controls additional details. Most of the constants are specified in dimensionless form and keep their value in a class of related simulations. The previously used values will probably be reasonable for the new simulation, too.

Of course, a complete control of CO5BOLD is only possible after studying of the meaning of the parameters in detail (e.g. by reading the following pages) AND – unfortunately – an accompanying look into the source code itself.

5.3.2 Header

The header of the parameter file contains information about the file format and contents. The `description` array can be used to specify the goal of the simulation, special model characteristics, or important parameter changes compared to a previous or standard model. The history array may contain the predecessor of the parameter file to simplify a tracing of parameter changes.

- `fileform uio`:
  The header of the parameter file, e.g.

  ```
  fileform uio form=formatted convert=ieee_4  date='01.01.2002' &
    program='by hand'
  ```

  can be abbreviated to

  ```
  fileform uio form=formatted convert=ieee_4
  ```

  which indicates that the file is in UIO form and Fortran "formatted" (ASCII). The specification of the conversion type ("`convert=ieee_4`") is more relevant for unformatted files. These terms should not be changed. But it can be of interest to append e.g. the date of the last modification (e.g. "`date='01.01.2002'`").

- `character file_id`:
  The file identification string

  ```
  character file_id  f=A80 b=80  n='File identification'
  rhd-parameter
  ```

  indicates the intended use of the file as parameter file for the RHD code CO5BOLD. Do not edit!

- `character description`:
  The header of the file can (should) contain a short description of the simulation, as in e.g.

  ```
  character description  d=(1:4) f=A80 p=1 b=80  n='File description'
  Parameter file for RHD code:
  Full size 3D Betelgeuse model: 5 M_Sun, 650 R_Sun
  Start with st35gm04n03_09.end (127^3 -> 171^3)
  Run with SHORTrad
  ```

  This entry is optional (it can be omitted completely) but it is recommended to put at least some relevant keywords into this array. If you change the number of lines (between 1 and 20) you have to adjust the size specification ("`d=(1:4)`" in the example above).

- `character history`:
  The file history has a similar purpose as the previous entry. It can be used to keep information about the "parent" parameter file, as in

  ```
  character history  d=(1:2) f=A80 p=1 b=80  n='File history'
  Taken from st35gm04n03_09.par
  Last Modification:           01.01.2002
  ```

  Its use is optional.

5.3.3 Fundamental Model Parameters

- `real teff`:
  The effective temperature is one of the basic model parameters and is specified e.g. with

```
real teff  f=F13.3 b=4  n='Effective Temperature' u=K
 3500.0
```

  (for a relatively cool star). Note that the actual effective temperature can only be determined a posteriori and that the entropy of the instreaming entropy (see below) is more important than `teff` itself. In fact, `teff` is only used to control material properties at the outer boundary. Its value should be close to the expected effective temperature of the model.

- `character grav_mode`:
  Gravity is another characteristic of a stellar atmosphere. The type (or geometry) of the external gravity field has to be specified e.g. with

```
character grav_mode  f=A80 b=80  n='Type of gravity field' &
  c0='constant/central'
central
```

  Three values are possible so far:

  - `constant`: In the standard "solar" case the constant gravity specified with `real grav` is directed downward in x3 direction.
  - `localboxtide`: This activates a simple model for the action of a tidal wave on convection in a local box model. It adds to the case of `constant` gravity a potential $\hat{\Phi}_{\rm ex}$ which is harmonic in space and time according to

$$\Phi_{\rm ex} = \hat{\Phi}_{\rm ex} \cos(k_{\rm h} x1 + \omega t). \tag{92}$$

    It is intended to mimic a travelling tidal wave. Since the setup is considered experimental the parameters are set by the `C_test` parameters according:
    $\hat{\Phi}_{\rm ex}$ = `C_test1` (amplitude of potential variations)
    $k_{\rm h}$ = `C_test2` (horizontal wavenumber)
    ω = `C_test3` (frequency)
    Boundary conditions: in order to be compatible with periodic lateral boundaries $k_{\rm h}$ should be an integer multiple of 2π times the inverse lateral box size.
  - `central`: For the "supergiant" case a central potential is assumed with an origin at x=0. The stellar mass as well as inner and outer smoothing radius have to be specified.

- `real grav`:
  In the case of a constant gravity the amount of the acceleration has to specified with

```
real grav  f=E15.8 b=4  n='Gravity' u=cm/s^2
27500.0
```

  Setting this value to zero switches off gravity (oh wonder).

- `real mass_star`:
  In the case of a central the mass (in cgs units) of the star has to be specified with

```
real mass_star f=E15.8 b=4 n='Stellar Mass'              u=g
 9.94500e+33
```

- `real r0_grav`:
  To avoid the central singularity in a 1/r potential it is smoothed in the center to give a central potential of 1/`r0_grav`, specified with

```
real r0_grav   f=E15.8 b=4 n='Inner Smoothing Radius'    u=cm
 9.45833e+12
```

This parameter should always be non-zero for a central potential.

- `real r1_grav`:
  The density in an atmosphere in hydrostatic equilibrium can decline to very low values. To artificial enlarge the pressure (and density) scale height in the outer layers of the star (the corners of the box) the gravity can be reduced by defining the potential at infinity to be 1/`r1_grav`, specified with

```
real r1_grav   f=E15.8 b=4 n='Outer Smoothing Radius'    u=cm &
  c0='0.0: Not used'
 11.35000e+13
```

  Setting this parameter to zero gives the usual 1/r behavior of the potential in the outer layers but also chooses another smoothing formula in the central part (where `real r0_grav` is relevant). But a value somewhat larger than the remotest corner of the box effectively cancels this artificial smoothing in the outer layers without changing the formula for the potential.

- `real r1_rad`:
  For a "Star-in-a-Box" and particularly when only "simple" ray directions are allowed in the radiation transport step the temperature in the outer corners of the box tends to become very small. To artificially increase the effect of radiative heating the parameter `real r1_rad` can specify a radius beyond which only positive contributions of the radiative energy transport to the energy budget are taken into account. This ruins the conservativity of the code in these layers and should be applied only in very remote corners which are then considered only as sort of extended boundary region but not as part of the "real" model. The parameter can be specified e.g. with

```
real r1_rad   f=E15.8 b=4 n='Outer radiation transport radius'    u=cm &
  c0='0.0: Not used'
  8.00000e+13
```

  A value of `0.0` (default) or below deactivates this feature.

- `real nu_rotation`:
  To transform onto a coordinate system rotation around the x3 axis, a rotation rate can be specified with e.g.

```
real nu_rotation   f=E15.8 b=4 n='Rotation frequency'    u=1/s
 0.0
```

  The potential is modified by adding terms due to a centrifugal force. In addition, a Coriolis force are applied during the hydrodynamics step.

5.3.4 Boundary Conditions

The boundary conditions at the six sides of the computational box cannot be specified independently. For the naming convention of the boundaries a gravitational acceleration in -x3 direction is assumed. Accordingly, there is a bottom and a top boundary, and four side boundaries.

All boundary conditions of the hydrodynamic case are available in the MHD module.

- `character side_bound`:
  The boundary condition at all four sides is given by e.g.

```
character side_bound   f=A80 b=80 n='side boundary conditions' &
  c0='closed, transmitting, periodic'
transmitting
```

Possible values are:

- `reflective`: closed wall, no gravity, no radiation. Like the velocity field, the magnetic field is mirrored at the boundary. This boundary condition is unphysical, because the magnetic field is an axial vector and it violates the divergence free property of the magnetic field. Therefore, this boundary condition should not be used in MHD simulations. Use `closed` boundary conditions instead.
- `constant`: open boundary with constant extrapolation of all values, no gravity, no radiation
- `closed`, `closedtop`: closed wall, can handle gravity, open for outward radiation Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
- `closedbottom`: closed wall, handles gravity, radiation in diffusion approximation. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
- `periodic`: periodic boundaries for hydrodynamics, radiation, and magnetic fields
- `transmitting`: transmitting boundary for hydro and outward radiation. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.

Any of these values can be specified. But in fact, not all of them are recognized by all modules. Therefore some parameters are for test purposes (e.g. shock calculations) only. In simulations of a solar-like star with the `MSrad` radiation transport module the side boundaries *have* to be `periodic`. In simulations of a red supergiant all boundaries (including the sides) will typically be `transmitting`. As an alternative, `closed` boundaries can be chosen in this case.

- `character top_bound`:
The boundary condition at the top of the model is given by for instance

```
character top_bound    f=A80 b=80 n='top boundary conditions'
transmitting
```

Possible values are:

- `reflective`: closed wall, no gravity, no radiation. Like the velocity field, the magnetic field is mirrored at the boundary. This boundary condition is unphysical, because the magnetic field is an axial vector and it violates the divergence free property of the magnetic field. Therefore, this boundary condition should not be used in MHD simulations. Use `closed` boundary conditions instead.
- `constant`: open boundary with constant extrapolation of all values, no gravity, no radiation
- `closed`, `closedtop`: closed wall, can handle gravity, open for outward radiation. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
- `periodic`: periodic boundaries for hydrodynamics, radiation, and magnetic fields
- `transmitting`: transmitting boundary for hydro and outward radiation. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.

In almost every simulation of stellar convection a `transmitting` top boundary will be selected, the `closed` one is an alternative. The `periodic` condition is only recognized by the hydrodynamics routines and not by any radiation transport routine.

- `character bottom_bound`:
  The boundary condition at the bottom of the model is given for instance by

```
character bottom_bound f=A80 b=80 n='bottom boundary conditions' &
  c0=closedbottom
transmitting
```

  Possible values are:

  - `reflective`: closed wall, no gravity, no radiation. Like the velocity field, the magnetic field is mirrored at the boundary. This boundary condition is unphysical, because the magnetic field is an axial vector and it violates the divergence free property of the magnetic field. Therefore, this boundary condition should not be used in MHD simulations. Use `closed` boundary conditions instead.
  - `constant`: open boundary with constant extrapolation of all values, no gravity, no radiation
  - `closed`, `closedtop`: closed wall, can handle gravity, open for outward radiation. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
  - `closedbottom`: closed wall, handles gravity, radiation in diffusion approximation. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
  - `periodic`: periodic boundaries for hydrodynamics, radiation, and magnetic fields
  - `transmitting`: transmitting boundary for hydro and outward radiation. The parameters `real c_tchange`, `real c_tsurf`, and `real c_hptopfactor` have to be specified. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
  - `inoutflow`: "classical" open lower boundary for deep convection, gravity and radiation possible. The parameters `real s_inflow`, `real c_schange`, and `real c_pchange` have to be specified. Magnetic field lines are orthogonal to the boundary, i.e. the tangential component of the magnetic field vanishes at the boundary.
  - `inoutflow2`: variant of the open lower boundary condition. The parameters `real s_inflow`, `real c_schange`, `real c_pchange`, and `real B1_inflow` have to be specified.

  In simulations of a solar-like star with the `MSrad` radiation transport module the bottom boundary is typically of type "`inoutflow`". A supergiant simulation will have a `transmitting` lower boundary.

- `character heat_mode`:
  The mode in which energy is supplied can be adjusted with this parameter. The classical choice is to leave it empty, in which case the mode is chosen from `s_inflow` (see Sect. 5.3.4) and `luminositypervolume` (see Sect. 5.3.4). Example:

```
character heat_mode  f=A80 b=80  n='Heating mode' &
  c0='-/bottom_entropy1/bottom_energy1'
bottom_entropy1
```

  Possible values, so far:

  - : (empty). The classical value. For local models the energy comes through the lower boundary, either by radiation (for a closed bottom boundary `closedbottom`) or by convection + radiation (for an open bottom boundary `inoutflow`).
  - `bottom_entropy1`: The entropy in the bottom layers (defined as being less than `r0_grav` above the bottom of the model) is adjusted towards `s_inflow` on a rate given by `c_schange`.

- `bottom_energy1`: Energy in the bottom layers is added according to `luminositypervolume`.

- `real luminositypervolume`:
The luminosity of a "Star-in-a-Box" or a local model with the appropriate `heat_mode` can be set with this parameter. To avoid numbers that do not fit into a 4 Byte real the luminosity per volume has to be specified as e.g. in

```
real luminositypervolume f=E15.8 b=4 n='Luminosity per core volume' &
  u='erg/cm^3/s'
4.5E-02
```

Reference volume is $4/3\,\pi\,r0_{\rm grav}^3$. If this parameter is set to a value of `0.0` or below the entropy of the material within the core (defined by as all cells within radius `r0_grav`) is adjusted instead.

- `real s_inflow`:
The entropy of the material streaming through an open boundary of type "`inoutflow`" into the model can be specified e.g. with

```
real s_inflow f=E15.8 b=4 n='Entropy of core material' &
  u=erg/K/g
3.25E+09
```

In the case of a `central` potential the entropy in a sphere with radius `r0_grav` is adjusted towards this entropy value. In both geometry (supergiant as well as solar) this value is very important as it finally (but indirectly) determines the luminosity and effective temperature of the star. A value of `0.0` (default) or below disables this energy input.

- `real c_schange`:
The entropy `s_inflow` of the material in the bottom layer (solar case, `inoutflow` boundary condition) or the central region of the model (supergiant case) is not just set to the specified but adjusted towards it. The adjustment rate can be controlled with e.g.

```
real c_schange f=E15.8 b=4 &
  n='Rate of entropy change for open lower boundary' u=1
 0.3
```

Guide values are

  - `1.0`: fast adjustment
  - `0.3`: typical value
  - `0.1`: slow adjustment
  - `<=0.0`: not allowed

- `real c_pchange`:
The `inoutflow` boundary condition not only controls entropy and velocity but also the pressure in the bottom layers: It is locally adjusted towards the global average to damp out possible instabilities. The adjustment rate can be specified e.g. with

```
real c_pchange f=E15.8 b=4 &
  n='Rate of pressure change for open lower boundary' u=1
 1.0
```

- `real c_tchange`:
In the case of a `transmitting` upper or outer boundary the temperature of the material streaming into the model is adjusted with a rate given e.g. by

```
real c_tchange f=E15.8 b=4 &
  n='Rate of temperature change for open upper boundary' u=1
 0.3
```

- `real c_tsurf`:
  In the case of a `transmitting` upper or outer boundary the temperature of the material streaming into the model is adjusted towards a temperature `teff`*`c_tsurf`. This temperature can be specified as fraction of the effective temperature e.g. with

  ```
  real c_tsurf f=E15.8 b=4 n='Temperature factor for open upper boundary' u=1
   0.62
  ```

  The value depends on where the outer boundary is located relative to the photosphere: If the boundary lies at a point where the solar photospheric minimum temperature is located, it can be fairly small. If the boundary is far away from the photosphere of a red supergiant, the value can be even smaller. On the other hand, if the boundary lies somewhere within the solar chromosphere even values above 1.0 might be reasonable.

- `real c_hptopfactor`:
  In the case of a `transmitting` upper or outer boundary the density stratification outside the model has to be extrapolated properly. Assumptions about this density affects the amount of mass flowing into the model. For the extrapolation it is assumed that the density scale H_ρ scales with the pressure scale height H_p as H_ρ=H_p/`c_hptopfactor`.

  ```
  real c_hptopfactor f=E15.8 b=4 &
    n='Correction factor for surface pressure scale height' u=1
  0.8
  ```

  Possible values are

  - C < `0.0`: No effect (actually, a value of `1.0` is chosen).
  - `0.0` ≤ C < `1.0`: The density scale height is enlarged to account for possible effects of turbulent pressure on the scale height: The density decays less rapidly with height than in an (isothermal) hydrostatic stratification.
  - C = `1.0`: Density scale height is pressure scale height.
  - C ≥ `1.0`: Density scale height is smaller than pressure scale height. Not really useful.

- `real c_radhtautop`:
  The `MSrad` radiation transport module needs the specification of the scale height of the optical depth at the upper boundary, e.g. with

  ```
  real c_radhtautop f=E15.8 b=4 n='Scale height of optical depth at top' u=cm
  60.0E+05
  ```

- `real rho_min`:
  During long periods of matter infall the density at an open outer boundary can become very low. To limit the decrease of the density a lower limit in the extrapolated ghost cells can be set e.g. with

  ```
  real rho_min f=E15.8 b=4 n='Minimum boundary density' u=g/cm^3
  1.0E-25
  ```

  The density within the model will typically not fall much below this value. A value of `0.0` (default) or below deactivates this feature.

- `real c_coredrag`:
  To damp the flow in the core of models with central potential a drag force restricted to the inner part of the model (r<`r0_grav`) can be applied. It is controlled e.g. with

  ```
  real c_coredrag f=E15.8 b=4 n='Core drag force parameter' u=1
  1.0
  ```

  A value of `0.0` (default) or below deactivates this feature.

5.3.5 Equation of State

- `character eosfile`:
  The equation of state file together with the opacity file implicitly determine the chemical composition. The EOS file can be specified for instance with

```
character eosfile f=A80 b=80 n='EOS file name' &
  c0=eos_gamma140.eos/eos_mm20_l.eos/eos_mm00_l3.eos
eos_mm00_l5.eos
```

  There exists an increasing number of files:

  - `eos_mm00_l3.eos`: Standard EOS file for solar composition with extra large density range (towards low densities). There exist two other files for the same composition but smaller density range (`eos_mm00.eos`, `eos_mm00_l.eos`)
  - `eos_XXXX_l4.eos`: Several EOS tables for various compositions.
  - `eos_mm00_l5.eos`: EOS file for solar composition, with temperature range extended to very low values by keeping μ fixed below 500 K. The number of points for the density sampling has been reduced. The number of points for the energy sampling has been increased.
  - `eos_mm20_l.eos`: Standard EOS file for metal-poor star ([M/H]=-2.0) with extended range in internal energy and density (towards lower values). The older file (`eos_mm20.eos`) did not reach far enough.
  - `eos_gamma140.eos`: EOS table for simple gas with constant Γ=1.4. In this case all quantities could be faster computed than by interpolation in a table. Nevertheless, for compatibility reasons (to be able to use the existing EOS Fortran routines), the table is provided.
  - `eos_gamma166.eos`: EOS table for simple gas with constant Γ=5/3.
  - `cpheos_mm00.eos`: Copenhagen EOS for (their) solar composition.

- `character eospath`:
  The equation of state file does not have to be in the working directory. Instead, its path can be specified e.g. with

```
character eospath f=A80 b=80 n='path of EOS file' &
  c0=/astro/b/bf/for/eos/dat
/home/a_bf/for/eos/dat
```

5.3.6 Opacities

- `character opafile`:
  The opacity file can be specified with e.g.

```
character opafile f=A80 b=80 n='opacity file name' &
  c0=g2va.opta/big_grey.opta &
  c1='empty -> no radiation transport'
phoenix_opal_grey.opta
```

  So far, there exist already a couple of files:

  - `davmf.opta`:
  - `f5v.opta`:
  - `g2va.opta`:
  - `g2v_lowhe.opta`:
  - `g2v_m20.opta`:

- g2v.opta:
- hmin_p00.opta:
- opal_lowhe.opta:
- opal_m05.opta:
- opal_m10.opta:
- opal_m20.opta:
- phoenix_dust_grey.opta:
- phoenix_dust_ob4.opta:
- phoenix_opal_grey.opta:
- ross_m05.opta:
- ross_m10.opta:
- ross_m20.opta:
- sunur1.opta:
- sunur2.opta:
- t5000g44mm20.opta:
- t5000g47mm20.opta:
- t6300g40mm20.opta:
- t6500g44mm20.opta:
- zzceti1g.opta:
- zzceti1.opta:

- `character opapath`:
  The opacity file does not have to be in the working directory. Instead, its path can be specified e.g. with

```
character opapath f=A80 b=80 n='path of opacity file' &
  c0=/astro/b/bf/for/opa/dat
/home/a_bf/for/opa/dat
```

5.3.7 Hydrodynamics Control (HD and MHD)

Allmost all parameters in the parameter file are valid for the HD and the MHD module. Only a few parameters for the hydrodynamics control (`character hdscheme`: Sect. 5.3.7, `character reconstruction`: Sect. 5.3.7, `real c_slopered`: Sect. 5.3.7) are slightly modified or extended for the MHD module.

- `character hdscheme`:
  With this parameter the type of the hydrodynamics scheme can be specified as in

```
character hdscheme f=A80 b=80 n='Hydrodynamics scheme' &
  c0='Roe (approximate Riemann solver of Roe type)' &
  c1='RoeMagKin (Roe solver + kinetic magnetic field transport)' &
  c2='None (skip hydrodynamics step entirely)'
Roe
```

  Possible values are

  - `None`: The hydrodynamics step is skipped entirely (for test purposes). Note that in this case some initializations necessary for the generation of the mean file are omitted, too.
  - `Roe`: (default) The standard Riemann solver of Roe type is activated. This value will in almost every case be chosen.

- `RoeMagKin`: The standard Roe solver is extended to transport passively a magnetic field. This is a test implementation to check if the general magnetic field handling works. For proper MHD simulations use `RoeMHD` instead.
- `RoeMHD`: Compile the MHD HLL solver.

- `character hdsplit`:
With this parameter the type of the hydrodynamics operator (directional) splitting scheme can be specified as in

```
character hdsplit f=A80 b=80 n='Hydrodynamics directional splitting scheme' &
  c0='123 (default): directional splitting' &
  c1='unsplit: new unsplit operator'
123
```

Possible values are

- `123`: (default) The standard directional splitting is activated, where the 1D operators for the individual directions are applied in the given order. So far, only the order `123` is possible.
- `unsplit`: The standard Roe solver is applied. However, the changes from the individual steps are computed from (and applied to) the same model configuration. The result is an unsplit scheme.

- `character reconstruction`:
This parameter determines the order and "aggressiveness" of the reconstruction scheme with e.g.

```
character reconstruction f=A80 b=80 n='Reconstruction method' &
  c0=Constant c1=Minmod/VanLeer/Superbee c2=PP
Minmod
```

Possible values are

- `Constant`: The run of the partial waves inside the cells is assumed to be constant. A highly dissipative first order scheme results. This values will usually only be used for test (or comparison) purposes.
- `Minmod`: Chooses the smallest slope which still results in a second order scheme. It is the most diffusive (and most stable) one in this class.
- `VanLeer`: (default) The recommended second order scheme.
- `Superbee`: The "most aggressive" stable 2nd order scheme. It results in the steepest shocks, which works well in some test cases but might be to difficult for the radiation transport module to handle.
- `PP`: Chooses the piecewise parabolic reconstruction of the PPM scheme ("Piecewise Parabolic Method", Colella & Woodward 1984). Results in 3rd order accuracy for the advection. This method can only be used with the standard `hdscheme Roe`, not with `hdscheme RoeMHD`.

Usually, the `VanLeer` reconstruction is a good choice. If a more stable (and diffusive) scheme is needed, take `Minmod`. The `PP` reconstruction gives the highest accuracy. However, it tends to produce somewhat "noisy" models with small wiggles e.g. in the velocity. The 2nd order piecewise parabolic reconstruction (PP) is not implemented in the MHD module. By specifying e.g. `VanLeer Superbee` it is possible to use the VanLeer scheme for the hydrodynamics scheme as such and Superbee only for the advection of additional `quc` quantities.

- `real c_slopered`:
  When `-Drhd_roe1d_slope_l01=2` is set (see Sect. 3.6), a new extra stabilization mechanism can be activated: If one of the reconstruction methods `VanLeer`, `Superbee`, or `PP` (see Sect. 5.3.7) is activated, the slope can be reduced (by averaging with the results from a `MinMod` reconstruction) by setting `c_slopered` to a positive non-zero value. This value can be set e.g. with

  ```
  real c_slopered f=E15.8 b=4 &
      n='Slope reduction parameter in case of strong density contrast' u=1 &
      c0='0.00: off (default), 0.02: reasonable value, 0.10: large value'
  0.02
  ```

  Typical choices are

  - `0.0`: Slope reduction switched off. Original reconstruction is used.
  - `0.02`: Moderate slope reduction in case of large density jumps.
  - `0.10`: More pronounced slope reduction in case of strong density contrast.

  This parameter is not recognized by the MHD module.

- `real c_hydpredfactor`:
  The "hydrostatic pressure correction" terms in the two acoustic waves are always present. However, for the entropy wave and the "ionization wave" it is not quite clear if the terms should be there (the classical default) or if they should be set to zero. The value of a factor in front of these terms can be set e.g. with

  ```
  real c_hydpredfactor f=E15.8 b=4 &
      n='hydrostatic pressure reduction in waves 3 and 6' u=1 &
      c0='0.0: Deactivation of pressure reduction terms' &
      c1='1.0: Activation of pressure reduction terms (default)'
  0.0
  ```

  Possible choices are

  - `0.0`: Deactivation of pressure reduction terms in waves 3 and "6" in Roe solver
  - `1.0`: Activation of pressure reduction terms in waves 3 and "6" in Roe solver (default)

  This parameter is not recognized by the MHD module.

- `integer n_hyditer`:
  After each complete hydiative time step the recommendation for the next time step will be chosen so that `n_hyditer` iterations will (probably) needed. The parameter can be set e.g. with

  ```
  integer n_hyditer f=I4 b=4 &
      n='Number of hydrodynamics iterations' c0=10
  8
  ```

  For a simulation of a solar-type star it will typically be set to `1`. E.g. for brown dwarfs with shorter hydrodynamical time scales values around `10` may be considered. Note, that the hydrodynamics iteration works somewhat differently than the radiation transport iteration: in the latter case the size of the actual time step can be determined after computing the fluxes, whereas the hydrodynamics step is (possibly) of at least second order in time and the time step has to be known in advance

- `integer n_hydmaxiter`:
  The absolute maximum number of hydro iterations can be specified e.g. with

  ```
  integer n_hydmaxiter f=I4 b=4 &
      n='Maximum number of hydro iterations' c0=14
  0
  ```

If more iterations are needed the computation for the current time step is stopped and resumed with a smaller one. Usually, `n_hydmaxiter` will either be set to a value somewhat larger than the recommended number of iterations (`n_hyditer`) or to `0` which disables the check for too many iterations completely. This can be safely allowed in many cases. To disable the iteration of the hydrodynamics sub-step set `n_hyditer=0`.

- `integer n_hydcellsperchunk`:
  In every directional sub-step neighboring 1D columns are independent from each other. They can be grouped and computed in chunks of arbitrary size. The approximate number of grid cells per chunk can be specified e.g. with

```
integer n_hydcellsperchunk f=I9 b=4 &
  n='Number of cells per hydro chunk' &
  c0='0 => one 2D slice at a time' &
  c0='1 => minimum chunk size (inefficient)' &
  c0='2500: reasonable value' &
  c0='1000000000: maximum chunk size (inefficient and memory intensive)'
20000
```

  The exact number is determined at run time to get (approximately) equal sizes of the individual chunks. The choice of this parameter does not affect the result of the computation but the memory usage and performance: Smaller (and more) chunks may result in an optimum cache usage and need the smallest amount of memory, but result in additional overhead due to frequent subroutine calls. Bigger (and less) chunks are to be preferred for vector machines and processors with large caches. Very rough guide values may be

  - `2500`: Pentium III, Core 2 Duo processor
  - `20000`: RISC processor
  - `100000`: Vector machine

  Note: For simulations with activated OpenMP on a parallel machine the chunk size has to be made small enough to allow at least as many chunks as processors available. This is particularly important for models with a small number of grid points (e.g. 2D models). An example is given for the Hitachi SR8000 in Sect. 3.7.8.

- `real c_visdrag`:
  This viscosity parameter controls the drag force which is (if requested) applied inside the hydrodynamics routines themselves. It does not act on velocity gradients as usual viscosity but applies a force proportional to the velocity itself (but with the opposite sign). The amount can be specified e.g. with

```
real c_visdrag f=E15.8 b=4 &
    n='Drag viscosity parameter' u=1
0.001
```

  The value gives the fraction the velocity is reduced per time step. Therefore, reasonable values lie between `0.0` and `1.0`. In almost every case the drag forces will be switched off (`c_visdrag=0.0`). If e.g. strong pulsation have to be damped in the initial phase of a simulation a value around `0.001-0.01` seems appropriate.

- `real c_visbound`:
  An additional drag force can be added locally in inflow cells in the outer layer when the `transmitting` boundary condition is chosen. The value can be set e.g. with

```
real c_visbound f=E15.8 b=4 &
    n='Boundary drag viscosity parameter' u=1
0.001
```

  This extra drag force is usually not necessary and should be switched off (with `c_visbound=0.0`).

- `real c_resb`:
  This parameter is only valid for the `hdscheme=RoeMHD` module. It specifies the electric conductivity. Values between 0.0 and 1.0 may be reasonable. Higher values are possible but reduce the time step. The default value is 0.0. Example:

```
real c_resb f=E15.8 b=4 &
    n='Parameter for numerical resistivity'                    u=1
0.1
```

  Note that this parameter has no effect in the current version of the MHD module because the explicit electric conductivity and the addidional energy diffusion have been removed. Therefore, you can set them to any value you want without consequences. However, these parameters may be used again in future versions of the module!

- `real c_resepsilon`:
  This parameter is only valid for the `hdscheme=RoeMHD` module. It controls the additional energy diffusion. Typical values are between 0.0 and 1.0. The default value is 0.0. Example:

```
real c_resepsilon f=E15.8 b=4 &
    n='Parameter for additional energy diffusion'              u=1
0.5
```

  Note that this parameter has no effect in the current version of the MHD module because the explicit electric conductivity and the addidional energy diffusion have been removed. Therefore, you can set them to any value you want without consequences. However, these parameters may be used again in future versions of the module!

- `real b1_inflow`:
  This parameter is only valid for the `hdscheme=RoeMHD` module. It controls the strength of the inflowing horizontal magnetic field ($B1$) at the lower boundary (`bottom_bound=inoutflow2`). The default value is 0.0. Example:

```
real b1_inflow f=E15.8 b=4 &
    n='Strength of inflowing horizontal magnetic field'        u=G
2.0
```

  The units are only certain up to a factor $\sqrt{4\pi}$ or so.

5.3.8 Tensor Viscosity Control

In many test problems it is not necessary to activate the 2D/3D tensor viscosity. But when strong slow shock fronts are aligned with the grid the Roe solver runs into problems and at least some additional 2D or 3D viscosity is necessary. And even if the Roe solver can handle sharp shocks by its own, the radiation transport algorithm might cause trouble because of the enormous opacity variations across a shock front. Here the tensor viscosity is useful, too.

- `real c_vissmagorinsky`:
  A turbulent viscosity of Smagorinsky type can be activated e.g. with

```
real c_vissmagorinsky f=E15.8 b=4 &
    n='Turbulent eddy viscosity parameter (Smagorinsky type)'  u=1
1.2
```

  In many cases values around `0.5` are sufficient to stabilize the code. Larger values (`1.2` in the example above) are only necessary for some nasty under-resolved supergiant models. Setting `c_vissmagorinsky` = `c_visartificial` = `c_visexpansion` = `c_vislinear` = `c_visp2pcoeff` = `0.0` skips the tensor viscosity step entirely.

- `real c_visartificial`:
  A standard artificial viscosity can be activated e.g. with

```
real c_visartificial f=E15.8 b=4 &
    n='Artificial viscosity tensor parameter'                    u=1
1.2
```

  In many cases values around `0.5` are sufficient to stabilize the code. Larger values (`1.2` in the example above) are only necessary for some nasty under-resolved supergiant models.

- `real c_visexpansion`:
  An additional viscosity can be activated e.g. with

```
real c_visexpansion f=E15.8 b=4 &
    n='Expansion viscosity tensor parameter'                     u=1
1.2
```

  While the standard artificial viscosity acts on compressed regions, this viscosity acts in expansion areas. Ususally, it is not activated (`c_visexpansion` = `0.0`). However, it might be useful in cases were strong localized expansions cause problems.

- `real c_vislinear`:
  Another viscosity can be activated e.g. with

```
real c_vislinear f=E15.8 b=4 &
    n='Linear viscosity tensor parameter'                    u=1
1.2
```

  In the formulae for the standard (artificial, compression, Smagorinsky) viscosity velocity gradients appear. That means that in regions with smooth small-amplitude flows these types of viscosity essentially vanish. Here, the linear viscosity comes in. It uses $\sqrt{R_{\rm gas}T}$ as approximation for the sound speed that is used in the formula for the kinematic viscosity. Ususally, it is not activated (`c_vislinear` = `0.0`). It might be useful to damp small-amplitude almost linear waves.

- `real c_visprturb`:
  The Prandtl number for turbulent mixing can be specified e.g. with

```
real c_visprturb f=E15.8 b=4 &
    n='Turbulent Prandtl number'                                 u=1
8.0
```

  Values between `1.0` and `10.0` appear reasonable. Note that larger values lead to smaller amounts of turbulent mixing! A value of `0.0` switches off the turbulent mixing terms (but not the entire tensor viscosity).

- `real c_vistensordiag`:
  The factor in the stress tensor in front of of the diagonal terms can be set with

```
real c_vistensordiag f=E15.8 b=4 &
    n='Diagonal factor for viscous stress tensor'                u=1 &
    c0='typically 1.0
1.0
```

  This is not really parameter one would try to adjust. The total amount of viscosity should be controlled with parameters like `real c_vissmagorinsky` and `real c_visartificial`. But the parameter can be used to tentatively switch off the diagonal terms completely or to change its importance compared to the other terms.

- `real c_vistensoroff`:
  The factor in the stress tensor in front of of the off-diagonal terms can be set with e.g.

```
real c_vistensoroff f=E15.8 b=4 &
    n='Off-diagonal factor for viscous stress tensor'            u=1 &
    c0='typically 0.5
0.5
```

  This is not really parameter one would try to adjust. The total amount of viscosity should be controlled with parameters like `real c_vissmagorinsky` and `real c_visartificial`. But the parameter can be used to tentatively switch off the off-diagonal terms completely or to change its importance compared to the other terms.

- `real c_vistensordiv`:
  The factor in the stress tensor in front of of the divergence terms (also on the diagonal) can be set with e.g.

```
real c_vistensordiv f=E15.8 b=4 &
    n='Divergence factor for viscous stress tensor'              u=1 &
    c0='typically -1./3.
0.0
```

  This is not really parameter one would try to adjust. The total amount of viscosity should be controlled with parameters like `real c_vissmagorinsky` and `real c_visartificial`. But the parameter can be used to switch off the divergence terms completely or to change its importance compared to the other terms. These divergence terms can be used to reduce the effect of the tensor viscosity in the case of isotropic compression. But this reduction (`c_vistensordiv` = `-0.333333` in 3D, `c_vistensordiv` = `-0.5` in 2D) is usually switched off.

- `integer n_viscellsperchunk`:
  The number of cells per box (or "chunk") treated by the tensor viscosity scheme at one call (and by one thread) can be set e.g. for an Intel Macintosh with

```
integer n_viscellsperchunk f=I9 b=4 &
  n='Number of cells per viscosity chunk' &
  c0='0 => old chopping' &
  c0='12000: reasonable value'
32000
```

  It can be adjusted to improve cache efficiency and to modify the work load distribution onto the threads (in case of parallel runs with OpenMP). Due to the special handling of boundary cells the overhead per call increases significantly for small chunks. Typically, larger chunk sizes (compared the the hydrodynamics chunk sizes set with `integer n_hydcellsperchunk`, see Sect. 5.3.7) are adequate. On the other hand they should not be too large to limit the usage of temporary memory and to allow parallelization (the distribution of chunks to threads): For simulations with activated OpenMP on a parallel machine the chunk size has to be made small enough to allow at least as many chunks as processors available. This is particularly important for models with a small number of grid points (e.g. 2D models). An example is given for the Hitachi SR8000 in Sect. 3.7.8.

In addition to the standard tensor viscosity described above, there is a more experimental "point-to-point" viscosity.
It relies on a completely different discretization. It should conserve angular momentum exactly and guarantee positivity of dissipated energy (for sufficiently small time steps). The current version should only be used for equidistant grids (same spacing in all directions, as for the supergiant models) by experienced users. If activated, the "point-to-point" viscosity is typically used in addition to the standard one.

- `real c_visp2pcoeff`:
  The strenght of the viscosity can be controlled with e.g.

```
real c_visp2pcoeff f=E15.8 b=4 &
    n='Point to point viscosity coefficient'                    u=1
0.20
```

  This parameter is somewhat analogous to `real c_visartificial`, see 5.3.8. A value of `0.0` switches it off.

- `real c_visp2pincl1`:
  The interaction with the edge neighbor cells with indices $(\pm 1 \pm 1 + 0)$ can be specified with e.g.

```
real c_visp2pincl1 f=E15.8 b=4 &
    n='Point to point viscosity inclined cell factor 1'         u=1
1.0
```

  Common values are `1.0` (interaction is considered) and `0.0` (no interaction with these cells). The usual value is `1.0`.

- `real c_visp2pincl2`:
  The interaction with the corner neighbor cells with indices $(\pm 1 \pm 1 \pm 1)$ can be specified with e.g.

```
real c_visp2pincl2 f=E15.8 b=4 &
    n='Point to point viscosity inclined cell factor 2'         u=1
0.0
```

  Common values are `1.0` (interaction is considered) and `0.0` (no interaction with these cells). The usual value is `0.0` to save some computation time.

5.3.9 Dust/Molecules/Hydrogen Ionization: General

CO5BOLD can now handle a number of additional density arrays. They can be used to describe e.g. the mass density of dust distribution moments or number densities of molecules. These species are properly advected with the gas density. There is also already a small number of dust/molecule formation models available. These models have to be improved in the future and the influence on the radiation field (opacities, radiation pressure on dust) has to be taken into account.

- `character dustscheme`:
  A scheme for dust or molecule formation and transport can be selected e.g. with

```
character dustscheme f=A80 b=80 n='Dust model' &
  c0='none (default), nosource, dust_simple_01, co_component01_01' &
  c1='dust_k3mon_01, dust_k3mon_02'
dust_k3mon_01
```

  The following values are currently possible:

  - `none`, `None`: No handling of any dust/molecule density at all.
  - `nosource`: Skip source term step for dust/molecules entirely, but do the transport.
  - `dust_simple_01`: Simple and unrealistic 'dust' formation model (only for testing of the numerics).
  - `co_component01_01`: Simple CO formation (from Matthias Steffen) with one component only but realistic time scales.

- `dust_k3mon_01`: Simple C-rich dust formation (routines from Susanne Höfner) with one component only but realistic time scales.
- `dust_k3mon_02`: Simple C-rich dust formation (routines from Susanne Höfner) with two components for dust density and free carbon density.
- `dust_k3mon_03`: Simple Forsterite dust formation (based on routines from Susanne Höfner) with two components for dust density and free "Forsterite monomer" density.
- `dust_bins_01`: Multi-size-bin Forsterite dust formation (based on Rossow's equations) with one bin for the monomers and several bins for the different grain sizes.
- `dust_moment04_c2`: C-rich dust chemistry, 4 moments (routines from Susanne Höfner).
- `chemreacnet`: chemical reaction networks (routines from Sven Wedemeyer-Böhm and Inga Kamp).
- `hiontd`: time-dependent hydrogen ionization (routines from Jorrit Leenaarts and Sven Wedemeyer-Böhm).

- `real c_dust0X`:
  There are ten parameters (`real c_dust01` to `real c_dust10`) to control each dust formation scheme in detail. A parameter can be given as in

  ```
  real c_dust01 f=E15.8 b=4 n='Dust parameter 1'
  0.0
  ```

  The meaning (and unit) can vary from scheme to scheme. The default value is `0.0` in each case.
  Important: The parameter `real c_dust01` must be set to `1.0` in order to activate advection of particle densities for the CHEM (`chemreacnet`) and the HION (`hiontd`) module. The default value is `0.0`, i.e. advection is switched off.

- `character chem_reacfile`:
  The name of the input file containing the chemical reaction network.

  ```
  character chem_reacfile f=A80 b=80 n='file name of reaction table'
  chem.dat
  ```

- `character chem_reacpath`:
  The path of the input file containing the chemical reaction network.

  ```
  character chem_reacpath f=A80 b=80 n='path of reaction table'
  /data/sven/cobold/dat/chem/
  ```

- `real chem_abumetal`:
  Abundance of the representative metal ('M', if present) relative to hydrogen ($\epsilon_{\mathrm{M}} = [M]/[H]$). A value of `1.0E-04` means there are 10^4 hydrogen atoms for every metal atom. The metal number density for each grid cell is then derived via $n_{\mathrm{H}} = \epsilon_{\mathrm{M}}\,\rho/m_{\mathrm{H}}$ (assuming a pure hydrogen gas). This parameter is ignored when a `quc` array for the metal is found in the input model.

  ```
  real chem_abumetal f=E15.8 b=4 n='Chemical abundance of repres. metal'
  1.0E-04
  ```

- `character hion_datapath`:
  The path of all input files for HION.

  ```
  character hion_datapath f=A80 b=80 n='HION data path'
  /data/sven/cobold/dat/hion/
  ```

- `character hion_atomfile`:
  The file name of the model atom for HION.

```
character hion_atomfile f=A80 b=80 n='HION atom file name'
H_6.atom
```

- `character hion_abufile`:
  The name of the HION input file containing the chemical abundances.

```
character hion_abufile f=A80 b=80 n='HION abundance file name'
abundance.input
```

- `character hion_edensfile`:
  The name of the HION input file containing the electron density table.

```
character hion_edensfile f=A80 b=80 n='HION electron density file name'
edens.dat
```

- `character hion_pffile`:
  The name of the HION input file containing the partition functions.

```
character hion_pffile f=A80 b=80 n='HION partition function file name'
pf_kurucz.dat
```

- `real dtime_out_hion`:
  Time increment for additional HION output. Positive values specify the time increment in seconds, negative values the increment in computational time steps. Setting the parameter to zero, suppresses the output.

```
real dtime_out_hion f=E15.8 b=4 n='Output file time step (HION)'
-10.0
```

- `integer hion_chunks`:
  Number of chunks to use for HION in order to limit the required memory. Do not make it bigger than the number of points in the x2 direction.

```
integer hion_chunks f=I9 b=4 n='Number of HION chunks'
1
```

5.3.10 Dust: dustscheme=dust_moment04_c2

In this section the parameters for `dustscheme=dust_moment04_c2` (4-bin (4 moments) dust scheme for carbon-rich dust) are described:

- `real c_dust01`:
  The carbon to oxygen ratio is specified with e.g.

```
real c_dust01 f=E15.8 b=4 n='C to O ratio'                    u=1
1.4
```

  Larger values mean more dust. Values below 1 make no sense for the current dust model.

- `real c_dust02`:
  The oxygen abundance is specified with e.g.

```
real c_dust02 f=E15.8 b=4 n='Oxygen abundance'                u=1
6.606934E-04
```

- `real c_dust03`:
  The cutoff for the integration of the degree of condensation is specified with e.g.

```
real c_dust03 f=E15.8 b=4 n='cutoff for integration of degree of condensation' &
                                                                          u=1
1.0E-05
```

- `real c_dust04`:
  The relative dust opacity factor is specified with e.g.

```
real c_dust04 f=E15.8 b=4 n='Relative dust opacity factor'              u=1
1.0
```

5.3.11 Dust: dustscheme=dust_k3mon_03

In this section the parameters for `dustscheme=dust_k3mon_03` (simple 2-bin dust scheme for Forsterite dust) are described:

- `integer n_dustgrainradius`:
  The number of dust grain radius bins (including one for the monomers) is specified with

```
integer n_dustgrainradius f=I8 b=4 n='Number of dust grain radius bins' &
  c1='Includes: bin for monomers'
2
```

  The default value is `1` (to avoid an empty array). The value should be the same as the upper dimension in `real ar_dustgrainradius`. For the current dust scheme, there should always be exactly two bins.

- `real ar_dustgrainradius`:
  The radii of the dust grains are specified with e.g.

```
real ar_dustgrainradius f=E10.4 b=4 p=1 d=(1:2) n='Dust grain radii' u=cm
0.0
1.0E-04
```

  The default value is `0.0`.

- `real c_dust01`:
  The density of the grain material is specified with e.g.

```
real c_dust01 f=E15.8 b=4 n='Density of grain material' u=g/cm^3
3.3E+00
```

- `real c_dust02`:
  The atomic weight of the "dust monomer" is specified with e.g.

```
real c_dust02 f=E15.8 b=4 n='Atomic weight of dust monomer' u=u
140.71
```

  The value `140.71` should be appropriate for Forsterite (Mg_2SiO_4). The unit is the atomic mass unit. The default value is `0.0`.

- `real c_dust03`:
  The number fraction of the rarest component is specified with e.g.

```
real c_dust03 f=E15.8 b=4 n='Number fraction of rarest component' u=1 &
  c0='For Mg2SiO4, Mg is the rarest, its fraction is 3.1187E-05' &
  c1='Mg2SiO4 contains 2 Mg -> * 1/2 -> 1.55935e-05'
1.55935e-05
```

For Mg_2SiO_4 the rarest component is (usually) Mg_2. So, half the magnesium abundance is required as value. The default value is `0.0`.

- `real c_dust04`:
  The lower dust limit fraction is specified with e.g.

```
real c_dust04 f=E15.8 b=4 n='Lower dust limit fraction' u=1
1.0E-10
```

  It is used in the calculation of the settling velocity where a division by the total density of monomers and dust is required. To prevent this denominator to become zero a term $c_{\rm dust04}\,\rho$ is added. The default value is `0.0`.

- `real c_dust05`:
  The minimum number of monomers during condensation is specified with e.g.

```
real c_dust05 f=E15.8 b=4 n='Minimum number of monomers during condensation' u=1
10.0
```

  For very small grains (just one or very few monomers) the condensation rates can be very small in this dust model: nucleation that would form already small clumps of monomers is not considered. Therefore, to speed things up a minimum number of monomers can be given that is considered for the condensation rate. With `1.0` or smaller values the enhancement is switched off. The default value is `0.0`.

- `real c_dust06`:
  The sticking coefficient for the condensation rate is specified with e.g.

```
real c_dust06 f=E15.8 b=4 n='Sticking coefficient' u=1 &
  c0='For C-rich dust: 0.37; can be between 0 and 1'
1.0
```

  The default value is `0.0`.

5.3.12 Dust: dustscheme=dust_bins_01

In this section the parameters for `dustscheme=dust_bins_01` (multi-size-bin dust scheme for Forsterite dust) are described:

- `integer n_dustgrainradius`:
  The number of dust grain radius bins (including one for the monomers) is specified with

```
integer n_dustgrainradius f=I8 b=4 n='Number of dust grain radius bins' &
  c1='Includes: bin for monomers'
8
```

  The default value is `1` (to avoid an empty array). The value should be the same as the upper dimension in `real ar_dustgrainradius`.

- `real ar_dustgrainradius`:
  The radii of the dust grains are specified with e.g.

```
real ar_dustgrainradius f=E15.8 b=4 p=1 d=(1:8) n='Dust grain radii' u='cm'
0.0
0.00390625E-04
0.0156250E-04
0.06250E-04
0.25000E-04
1.00000E-04
4.00000E-04
16.0000E-04
```

The default value is `0.0`.

- `real c_dust01`:
The density of the grain material is specified with e.g.

```
real c_dust01 f=E15.8 b=4 n='Density of grain material' u=g/cm^3
3.3E+00
```

- `real c_dust02`:
The atomic weight of the "dust monomer" is specified with e.g.

```
real c_dust02 f=E15.8 b=4 n='Atomic weight of dust monomer' u=u
140.71
```

The value `140.71` should be appropriate for Forsterite (Mg_2SiO_4). The unit is the atomic mass unit. The default value is `0.0`.

- `real c_dust03`:
The number fraction of the rarest component is specified with e.g.

```
real c_dust03 f=E15.8 b=4 n='Number fraction of rarest component' u=1 &
  c0='For Mg2SiO4, Mg is the rarest, its fraction is 3.1187E-05' &
  c1='Mg2SiO4 contains 2 Mg -> * 1/2 -> 1.55935e-05'
1.55935e-05
```

For Mg_2SiO_4 the rarest component is (usually) Mg_2. So, half the magnesium abundance is required as value. The default value is `0.0`.

- `real c_dust04`:
The lower dust limit fraction is specified with e.g.

```
real c_dust04 f=E15.8 b=4 n='Lower dust limit fraction' u=1
1.0E-10
```

If the density in a bin relative to the gas density falls below this value, the bin is completely emptied and the material is added to the bin with the largest dust or monomer density. Typical values are `1.0E-09` or so. The default value is `0.0`.

- `real c_dust06`:
The sticking coefficient for the condensation rate is specified with e.g.

```
real c_dust06 f=E15.8 b=4 n='Sticking coefficient' u=1 &
  c0='For C-rich dust: 0.37; can be between 0 and 1'
1.0
```

Typical values are between `0.0` (deactivating this process) and `1.0`. The default value is `0.0`. The standard choice is `1.0`.

- `real c_dust07`:
The sticking coefficient for the coagulation rate is specified with e.g.

```
real c_dust07 f=E15.8 b=4 n='Sticking coefficient for coagulation' u=1 &
  c0='Typically between 0 and 1'
1.0
```

Typical values are between `0.0` (deactivating this process) and `1.0`. The default value is `0.0`.

- `real c_dust08`:
The sticking coefficient for the coalescence rate is specified with e.g.

```
real c_dust08 f=E15.8 b=4 n='Sticking coefficient for coalescence' u=1 &
  c0='Typically between 0 and 1'
1.0
```

Typical values are between `0.0` (deactivating this process) and `1.0`. The default value is `0.0`.

- `real c_dust09`:
  The sticking coefficient for the nucleation rate is specified with e.g.

```
real c_dust09 f=E15.8 b=4 n='Sticking coefficient for nucleation' u=1 &
  c0='Typically between 0 and 1'
1.0
```

Typical values are between `0.0` (deactivating this process) and `1.0`. The default value is `0.0`. The standard choice is `1.0`.

5.3.13 Radiation Transport Control

In this part of the parameter file the radiation transport module has to be selected. Depending on this selection a couple of additional parameters have to be specified. Table 11 gives a list of the parameters and the modules they apply to. The standard routines are now in the MSrad module for local models and the SHORTrad module for global "Star-in-a-Box" models. The LHDrad module is not maintained very much anymore.

- `character radscheme`:
  So far, there exist three different radiation transport modules. The active on can be selected e.g. with

```
character radscheme f=A80 b=80 n='Radiation transport scheme' &
  c0='LHDrad/MSrad/SHORTrad' &
  c1='None (skip radiation transport step entirely)'
SHORTrad
```

  Possible values are

  - `None`: Skip radiation transport entirely.
  - `LHDrad`: (old "supergiant module") It uses long characteristics and is restricted to an equidistant grid and open boundaries at all surfaces. Note that the switch `-Drhd_r01=1` has to be set during compilation (see Sect. 3.6).
  - `MSrad`: ("solar module") It uses long characteristics. The lateral boundaries have to be periodic. Top and bottom can be closed or open. Note that the switch `-Drhd_r02=1` has to be set during compilation (see Sect. 3.6).
  - `SHORTrad`: (new "supergiant module") It uses short characteristics and is restricted to an equidistant grid and open boundaries at all surfaces. Note that the switch `-Drhd_r03=1` has to be set during compilation (see Sect. 3.6).

- `integer n_radminiter`:
  Usually the stability considerations dictate a radiative time step smaller than the hydrodynamics or tensor viscosity time step. To remedy this situation it is possible to allow several radiation transport steps per global time step. Hitherto, all three radiation transport modules support this iteration. The minimum number of iterations (radiative sub-steps) can be specified e.g. with

```
integer n_radminiter f=I4 b=4 &
  n='Minimum number of radiation transport iterations' c0=8
1
```

Parameter	Section	LHDrad	MSrad	SHORTrad
radscheme	5.3.13	*	*	*
n_radminiter	5.3.13	*	*	*
n_raditer	5.3.13	*	*	*
n_radmaxiter	5.3.13	*	*	*
radraybase	5.3.13	*	*	*
radraystar	5.3.13	*		*
n_radtheta	5.3.13		*	
n_radphi	5.3.13		*	
n_radsubray	5.3.13		*	
n_radthinpoint		*		
n_radthickpoint	5.3.13	*	*	
n_radtaurefine	5.3.13	*	*	
n_radband	5.3.13		*	
n_radrsyslevel	5.3.13		*	
n_radoutput	5.3.13		*	
c_radtcool	5.3.13		*	
c_raddcool	5.3.13		*	
c_radscool	5.3.13		*	
c_radtinci	5.3.13		*	
c_raddinci	5.3.13		*	
c_radimplicitmu	5.3.13	*		*
c_raditereps	5.3.13	*		*
c_raditerstep	5.3.13	*		*
c_radtvisdtau	5.3.13	*		
c_radtvis	5.3.13	*		
c_radhtautop	5.3.4		*	
c_radcourant	5.3.15	*	*	*
c_radcourantmax	5.3.15	*	*	*
c_radmaxeichange	5.3.15	*	*	*

Table 11: List of radiation transport control parameters and the modules they are relevant for.

If less iterations are needed the time step limit for the next step is increased. This value will in almost any case (for explicit radiation transport) be set to `1`. In the implicit case it is set to a higher value (typically `5`).

- `integer n_raditer`:
  After each complete radiative time step the recommendation for the next time step will be chosen so that `n_raditer` iterations will (probably) needed. The parameter can be set e.g. with

```
integer n_raditer f=I4 b=4 &
    n='Number of radiation transport iterations' c0=10
8
```

  For a simulation of a solar-type star (with comparatively long radiative time scales) it will typically be set to `1`. For stars with shorter radiative time scales values around `10` may be considered. All three radiation transport modules understand this parameter.

- `integer n_radmaxiter`:
  The absolute maximum number of iterations can be specified e.g. with

```
integer n_radmaxiter f=I4 b=4 &
    n='Maximum number of rad. transport iterations' c0=30
0
```

If more iterations are needed the computation for the current time step is stopped and resumed with a smaller one (which means that the hydrodynamics and the tensor viscosity step have to be done again). Usually, `n_radmaxiter` will either be set to a value somewhat larger than the recommended number of iterations (`n_raditer`) or to `0` which disables the check for too many iterations completely. This can be safely allowed in many cases and has the advantage that there is no need to save the initial model before calling the radiation transport module, which saves some memory. To disable the iteration of the radiation transport sub-step set `n_radminiter`=`n_raditer`=`n_radmaxiter`=`1`. All three radiation transport modules understand this parameter.

- `character radraybase`:
  Using the modules `LHDrad` or `SHORTrad` the orientation of the base axis system can be selected e.g. with

```
character radraybase f=A80 b=80 n='Base axis system' &
  c0='unity/random/randomgroup'
random
```

  Allowed values are

  - `unity`: (default) During all time steps and radiative sub-steps the direction of the rays stays the same.
  - `random`: At each time step (and radiative sub-step) a new base axis system is chosen at random
  - `randomgroup`: At each new time step a new base axis system is chosen at random. It is kept for all radiative sub-steps.

  Because typically only a relatively small number of rays is chosen per time step (with `radraystar`) it is advisable to vary the directions of the rays (by choosing `radraybase`=`random` or `randomgroup`) to cover the entire sphere at least over a longer time.

- `character radraystar`:
  Using the modules `LHDrad` or `SHORTrad` the list of ray directions (i.e. the number of rays and their coordinates) relative to the base axis system can be specified with e.g.

```
character radraystar f=A80 b=80 n='List of relative ray directions' &
  c0='x1(1)/x2(1)/x3(1)/oktaeder(3)/tetraeder(4)/cube(4)' &
  c1='ikosaeder(6)/dodekaeder(10)'
oktaeder
```

  Examples for allowed values are

  - `x1`: (N=1) one single ray along x1 axis (not enough to specify fluxes in all directions)
  - `x2`: (N=1) one single ray along x2 axis (not enough to specify fluxes in all directions)
  - `x3`: (N=1) one single ray along x3 axis (not enough to specify fluxes in all directions)
  - `oktaeder`: (N=3, default) octahedron
  - `tetraeder`: (N=4) tetrahedron
  - `cube`: (N=4)
  - `ikosaeder`: (N=6) icosahedron
  - `dodekaeder`: (N=10) dodecahedron
  - `list-01`, `list-01(3)`: Choose ray systems from a list (oktahedrons, tetrahedrons). If `character radraybase` is set to `unity` the rays will only be aligned to the axes or diagonals and thus avoid the time-consuming interpolation step of the short-characteristics method.

Several other choices are possible, which are meant for test purposes only. Choosing one of the five Platonic solids (Ops! "German-Greek" names only, so far) means that the 3 to 10 rays are equally distributed over the solid angle (from the center to each *corner* of the respective solid).

- `integer n_radtheta`:
  Using the `MSrad` module the ray directions have to specified in a different way: The number of ray sets in theta direction can be chosen with e.g.

```
integer n_radtheta f=I4 b=4 &
    n='NTHETA: Number of ray sets in theta direction' c0=2
2
```

- `integer n_radphi`:
  Using the `MSrad` module the number of ray sets in phi direction can be set e.g. with

```
integer n_radphi f=I4 b=4 &
    n='NPHI: Number of ray sets in phi direction' c0=2
2
```

- `integer n_radsubray`:
  Using the `MSrad` module the number of rays per cell (with the same direction) can be specified e.g. with

```
integer n_radsubray f=I4 b=4 n='KPHI: Number of rays per cell' c0=2
2
```

- `integer n_radthickpoint`:
  With the `MSrad` module the lower part of the model can be computed in diffusion approximation. The number of points in diffusion approximation can be set with e.g.

```
integer n_radthickpoint f=I4 b=4 &
  n='Number of grid points with optically thick (diff.) approximation' &
  c0='0: no diffusion approximation'
0
```

  The value should be choosen so that for all points in that region $\Delta\tau > 1$ is valid. Setting this value to `0` means that the diffusion approximation is not used in any part of the model.

- `integer n_radtaurefine`:
  With the `LHDrad` and the `MSrad` module the number of points on the rays can be finer than the number of points in the basic numerical grid. The refinement can be set e.g. with

```
integer n_radtaurefine f=I4 b=4 &
  n='Refinement factor'
0
```

- `integer n_radband`:
  It can be specified whether the grey opacity table or the binned frequency-dependent part of the opacity table is used during the computation. The grey part contains only one bin. The other (possibly non-grey) contains one or more bins depending on the table chosen. The parameter is specified with e.g.

```
integer n_radband f=I4 b=4 n='Number of frequency bins' &
  c0='1: grey opacities' &
  c1='2: non-grey opacities (if available from table)' &
  c2='3: two bands: 1.grey, 2.CO (density via XCO)' &
  c3='4: two bands: 1.grey, 2.CO (density from chemistry)'
1
```

Allowed values are

- 1: Use the grey part of the table
- 2: Use the other (possibly non-grey, frequency-dependent) part of the table
- 3: Use a continuum band plus an infrared band with CO opacity, calculated with CO equilibrium density
- 4: Use a continuum band plus an infrared band with CO opacity, calculated with CO density resulting from time-dependent chemistry

Only the MSrad module so far can handle non-grey tables.

- integer n_radrsyslevel:
This parameter specifies the "zero" point of the ray system, default: 0 (MSrad only). The parameter is specified with e.g.

```
integer n_radrsyslevel f=I4 b=4 n='Zero index of ray system' &
  c0='0: (default)' &
0
```

- integer n_radoutput:
This parameter controls additional output into the file 'rhd.qrad', default: 0 (MSrad only). The parameter is specified with e.g.

```
integer n_radoutput f=I4 b=4 n='Output level of MSrad' &
  c0='0: (default)' &
1
```

- real c_radtcool:
Parameter for surface cooling option (N_radband≤0) of MSrad. It can be activated with the parameter

```
real c_radtcool f=E15.8 b=4 &
  n='Surface cooling'            u=1 &
  c0='0.0: default'
0.0
```

- real c_raddcool:
Parameter for surface cooling option (N_radband≤0) of MSrad. It can be activated with the parameter

```
real c_raddcool f=E15.8 b=4 &
  n='Surface cooling'            u=1 &
  c0='0.0: default'
0.0
```

- real c_radscool:
Parameter for surface cooling option (N_radband≤0) of MSrad. It can be activated with the parameter

```
real c_radscool f=E15.8 b=4 &
  n='Surface cooling'            u=1 &
  c0='0.0: default'
0.0
```

- real c_radtinci:
Temperature of black body that emits incident radiation, default: 0.0, (MSrad only). It can be used e.g. with

```
real c_radtinci f=E15.8 b=4 &
  n='Temperature of black body that sends incident radiation' u=K &
  c0='0.0: default'
0.0
```

- `real c_raddinci`:
  Dilution factor $(R_*/d)^2$ of black body that emits incident radiation, default: 0.0, (MSrad only). It can be used e.g. with

```
real c_raddinci f=E15.8 b=4 &
  n='Dilution factor of black body that sends incident radiation' u=1 &
  c0='0.0: default'
0.0
```

- `real c_radimplicitmu`:
  So far, only the `LHDrad` and the `SHORTrad` module support implicit radiation transport. It can be activated with the parameter

```
real c_radimplicitmu f=E15.8 b=4 &
    n='Implicitness parameter for radiation transport'           u=1 &
    c0='0.0: explicit / 0.5: time centered / 1.0: fully implicit'
0.0
```

  Allowed values are

  - `0.0`: Fully explicit radiation transport (possible with all modules)
  - `0.0` < C < `1.0`: Partly implicit radiation transport
  - `0.5`: Radiation transport time-centered
  - `1.0`: Fully implicit radiation transport

  Values outside this range do not have much meaning. The implicit transport does not work efficiently yet: It does not yield significantly larger time steps than possible with a sequence of purely explicit sub time steps. Additionally, it turns out that the hydrodynamics runs into trouble if a too large time step (still well within the Courant condition) is requested.

- `real c_raditereps`:
  With activated implicit radiation transport (`LHDrad` module only) the requested convergence accuracy of the iteration can be set e.g. with

```
real c_raditereps f=E15.8 b=4 &
    n='Relative accuracy for radiation iteration'                u=1 &
    c0='Typical value: 1.0E-03'
2.0E-03
```

- `real c_raditerstep`:
  With activated implicit radiation transport (`LHDrad` module only) the step size of the iteration can be restricted with e.g.

```
real c_raditerstep f=E15.8 b=4 &
    n='Step size of radiation iteration'                         u=1 &
    c0='Typical values: 0.7,0.81'
1.0
```

  Allowed values are

  - `0.0` < `1.0`: Restricted step size
  - `1.0`: No restriction, standard step size
  - > `1.0`: Extra large steps

This value has to be chosen carefully to get optimal performance. Is the step size too small the convergence is safe but too slow. A too large step size inhibits convergence and leads to a decrease in the time step, which results in a bad performance, too.

- `real c_radtvisdtau`:
  Using the `LHDrad` module the limit in delta optical depth (rho*kappa*dx) below which the "radiative temperature viscosity" (=temperature smoothing) is to be applied can be set with e.g.

```
real c_radtvisdtau f=E15.8 b=4 &
  n='Optical depth limit for temperature viscosity' u=1
0.1
```

  The introduction of this "temperature diffusion" is a somewhat desperate and inelegant attempt to improve the behavior of the Greens function (hot cells should be cooled, cool cells should be heated). This diffusion is necessary for not well resolved models. It is switched off with `c_radtvisdtau` $\leq$ `0.0`.

- `real c_radtvis`:
  Using the `LHDrad` module the amount of the "radiative temperature viscosity" (=temperature smoothing) can be specified e.g. with

```
real c_radtvis f=E15.8 b=4 n='Temperature viscosity' u=1
1.6
```

  For well resolved models it should be switched off (with `c_radtvis` $\leq$ `0.0`). But often its use is necessary.

5.3.14 Process Time Management

In this group several parameters can be set which control the start of the time counting during a simulation and the total length of a job. If either one of the halt conditions below is met, CO5BOLD finishes the current step, writes a final model (plus some final information to other files), and stops execution.

For example on a CRAY one typically wants to use most of the CPU time given for an individual batch job. In this case one can set e.g. `real cputime_remainlimit=2000.0` and the values for the other halt conditions to `-1.0` or `-1`.

- `real starttime`:
  The start time of a simulation is usually taken from the start model file. But sometimes is simulation is to be started with the final model of a previous run but should start at time=0.0. This can be achieved by setting the start time with

```
real starttime f=E15.8 b=4 n='Start time'                    u=s
0.0
```

  Allowed values are

  - $\geq$ `0.0`: Set the initial time of the simulation to this value and override value from start model.
  - $<$ `0.0`: (default) Take the initial time from start model.

- `integer starttimestep`:
  The start time step count of a simulation is usually taken from the start model file. But sometimes is simulation is to be started with the final model of a previous run but should start at time step=0. This can be achieved by setting the start time step count with

```
integer starttimestep f=I11 b=4 n='Start time step number'   u=1
0
```

Allowed values are

- $\geq$ 0: Set the initial time step of the simulation to this value and override value from start model.
- $<$ 0: (default) Take the initial time step count from start model.

- `real cputime`:
  Because of the long simulation time usually CO5BOLD will run in some sort of batch mode which might impose limits on the execution time per run. On a CRAY the CPU time that is left can be accessed with a special subroutine (in `call tremain` in `rhd_mac_cray_module.f90`). On other machines it is possible to specify the allowed total time for the job e.g. with

  ```
  real cputime f=E15.8 b=4 n='CPU time'                                    u=s
  1000000.0
  ```

  During the run of CO5BOLD the leftover CPU time is computed by subtracting the used CPU time (which is given by `e_time=etime(tarray)` in `rhd_mac_sun_module.f90`) from the specified total CPU time for the job.

- `real cputime_remainlimit`:
  Because CO5BOLD needs some time to finish the last time step it should start exiting well before all CPU time is used up. This amount of buffer CPU time can be specified e.g. with

  ```
  real cputime_remainlimit f=E15.8 b=4 n='maximum remaining CPU time'    u=s
  2000.0
  ```

  Its value depends on the size of the model and the speed of the machine (more precisely the maximum CPU time per time step).

- `real endtime`:
  If the simulation should run up to a certain (stellar) time, its values can be specified e.g. with

  ```
  real endtime f=E15.8 b=4 n='total simulation time limit'                 u=s
  10000.0
  ```

  A value $<$ `0.0` deactivates this halt condition: it is not checked at all. If this parameter is set to a non-negative value a follow-up simulation should not use the same parameter file: it would stop immediately.

- `real plustime`:
  If the initial model should be advanced by a certain (stellar) time span, this value can be set e.g. with

  ```
  real plustime f=E15.8 b=4 n='simulation advance time'                    u=s
  5.0E+07
  ```

  A value $<$ `0.0` cancels this halt condition: it is not checked at all. This condition assures (if it is the only one) that all individual simulation runs cover (approximately) the same stellar time.

- `integer endtimestep`:
  If the simulation should run up to a certain time step, its values can be specified e.g. with

  ```
  integer endtimestep f=I11 b=4 n='total simulation time step number'    u=1
  1234
  ```

  This might be useful to advance the simulation up to a point shortly before a previous simulation crashed. A value $<$ `0` cancels this halt condition: it is not checked at all.

- `integer plustimestep`:
  If the initial model should be advanced by a certain number of time steps their number can be set e.g. with

```
integer plustimestep f=I11 b=4 n='simulation advance time step number' u=1
2000
```

  A value $<$ `0` deactivates this halt condition: it is not checked at all.

5.3.15 Time Step Control

In this group parameters to control the time step restrictions can be set.

They are important because decide about performance and stability of CO5BOLD. They should be tested and adjusted for a simulation of a new type of object. But all the dimensionless parameters can stay unchanged for a group of similar simulations. Only the parameters with an explicit time dimension should be checked in all cases (they scale with characteristic timescales and depend particularly on gravity).

- `real dtime_start`:
  The initial time step recommendation of a simulation is usually taken from the start model file. It can be overwritten e.g. with

```
real dtime_start f=E15.8 b=4 n='Start time step'                    u=s
1.0E+03
```

  A value $<$ `0.0` means that the original value from the start model is used.

- `real dtime_min`:
  In some rare cases it might be useful to specify explicitly the minimum time step with e.g.

```
real dtime_min f=E15.8 b=4 n='Minimum time step'                    u=s &
  c0='dtime_min=0.0 => no restriction'
1.0
```

  This value is used even if restrictions from the Courant condition try to enforce a smaller value. A fixed time step can be prescribed by setting `dtime_min` = `dtime_max` to some positive value. A value `dtime_min` ≤ 0.0 means that this time step restriction is completely ignored, which is the case that should usually be chosen.

- `real dtime_max`:
  It is possible to explicitly specify the maximum time step too, e.g. with

```
real dtime_max f=E15.8 b=4 n='Maximum time step'                    u=s &
  c0='dtime_max=0.0 => no restriction'
1.0E+05
```

  A fixed time step can be prescribed by setting `dtime_min` = `dtime_max` to some positive value. A value `dtime_max` ≤ 0.0 means that this time step restriction is completely ignored, which is the case that should usually be chosen.

- `real dtime_min_stop`:
  Sometimes a simulation can run into a pathological state where the time step decreases rapidly without recovering. To prevent a simulation in such a case from running forever (or until some other process time restriction applies) without actually advancing significantly in time, it is possible to specify an absolute minimum time step, e.g. with

```
real dtime_min_stop f=E15.8 b=4 n='Minimum time step'               u=s &
  c0='dtime_min_stop=0.0 => no restriction' &
  c1='dtime < dtime_min_stop => program stop'
1.0
```

If the actual time step falls below this value, the simulation finishes gracefully. This values has to specified as absolute time and has to be chosen carefully for each individual model (or each group of models). This time step restriction can be switched off by setting `real dtime_min_stop=0.0`. But in general, one should keep it activated and try to find a proper positive value.

- `real dtime_incmax`:
  Sometimes a time step restriction can lead to a sudden drastic drop in the time step. To prevent unwanted oscillations in the size of the time step its increase can be restricted e.g. with

```
real dtime_incmax f=E15.8 b=4 n='Maximum time step increment factor' u=1 &
  c0='dtime_max<1.0 => no restriction' c1='typically 1.1'
1.2
```

  This value specifies the maximum factor by which the time step can be increased from step to step (even if the new Courant condition etc. would allow more). A value value < 0.0 deactivates this restriction.

- `real c_courant`:
  A typical Courant factor for each 1D hydrodynamics step can be specified with e.g.

```
real c_courant f=E15.8 b=4 n='HD Courant factor'                    u=1 &
  c0='range: 0.0 < C_Courant <= 1.0, typically: 0.5'
 0.5
```

  From the minimum cell crossing time of a partial wave and this factor a recommendation for the *next* time step is computed. A value of `1.0` is the upper limit which guarantees stability for some simple linear test problems. Values around `0.5` are recommended for fully non-linear simulations.

- `real c_courantmax`:
  A typical Courant factor for each 1D hydrodynamics step can be specified with e.g.

```
real c_courantmax f=E15.8 b=4 n='maximum HD Courant factor'          u=1 &
  c0='range: C_Courant < C_Courantmax <= 1.0, typically: 0.9'
 0.8
```

  From the minimum cell crossing time of a partial wave and this factor an upper limit for the *current* time step is computed. If this limit is exceeded the computation is interrupted and resumed with a smaller time step (based on `c_courant`). Usually this parameter should be restricted by `c_courant` $<$ `c_courantmax` $\leq$ `1.0`. A value around `0.8` appears to be a good choice.

- `real c_hydexpcourant`:
  In addition to the usual Courant condition one could restrict the maximum expansion between two adjacent grid cells with e.g.

```
real c_hydexpcourant f=E15.8 b=4 n='HD expansion Courant factor'     u=1 &
  c0='range: 0.0 < C_hydExpCourant < C_hydExpCourantmax, typically: 0.3'
 0.2
```

- `real c_hydexpcourantmax`:
  This parameter can be set e.g. with

```
real c_hydexpcourantmax f=E15.8 b=4 n='HD max. expansion Courant factor' u=1 &
  c0='range: 0.0 < C_hydExpCourant < C_hydExpCourantmax, typically: 0.5'
 0.3
```

The pair `c_hydexpcourant`/`c_hydexpcourantmax` works analogously to the pair `c_courant`/`c_courantmax`.

- `real c_maxeichange`:
The relative change in internal during a single 1D hydrodynamics step can be used to restrict the time step by specifying

```
real c_maxeichange f=E15.8 b=4 n='maximum hydro energy change'       u=1 &
  c0='range: 0.1 - 1.0, typically 0.5, off:0.0'
 0.5
```

The default is `0.9`. Nevertheless, since the Roe solver is constructed to handle shocks and rapid changes in density and energy, this check is usually not needed. It can be switched off by setting `c_maxeichange`=`0.0`.

- `real c_radcourant`:
The radiation transport routines are subject so time step restrictions, too. And in typical scenarios, its the radiative timescale are the shortest one and poses the tightest restriction. Contrary to the hydrodynamics routines the timescale relevant for the stability of the radiation transport scheme can only be estimated using the characteristic timescale of a small sinusoidal temperature disturbance with a wavelength of the grid size in a homogeneous background and grey radiative energy exchange. The "radiative Courant" factor can be set e.g. with

```
real c_radcourant f=E15.8 b=4 n='RAD Courant factor'                u=1 &
  c0='range: 0.0 < C_radCourant, typically: 1.0'
 2.5
```

If the estimate of the timescale would be correct a value of `2.0` would cause the temperature fluctuation on the shortest scale to flip its sign, setting the absolute stability limit. A value of `1.0` would lead to a damping of theses fluctuations within one time step. But in practice, even higher values (for example `2.5`) show a reasonable behavior. This might be due to the effect that the shortest radiative timescale only occurs at single points (or in 2D layers) but that already the immediate neighbors have longer timescales and can damp the "most sensitive points". Based on `real c_radcourant` the recommended typical radiative time step is computed.

- `real c_radcourantmax`:
With this parameter the maximum allowed radiative time step is prescribed as e.g. in

```
real c_radcourantmax f=E15.8 b=4 n='maximum RAD Courant factor'     u=1 &
  c0='range: C_radCourant <= C_radCourantmax, typically: 2.0'
 3.0
```

This value will typically be somewhat larger than `real c_radcourant`.

- `real c_radmaxeichange`:
The relative energy change per radiative sub step can be restricted e.g. with

```
real c_radmaxeichange f=E15.8 b=4 n='maximum radiative energy change' &
  u=1 c0='range: 0.01 - 1.0'
 0.25
```

The default is `0.5`. Values between `0.1` and `0.5` seem reasonable. A value $\leq$ `0.0` deactivates this time step check. However, the check of the radiative energy change should usually be performed. A way to maximize the radiative time step (and therefore the performance of the entire code) can be to first set `real c_radmaxeichange` to a proper value (say `0.25`). Then, `real c_radcourant` (and `real c_radcourantmax`) are adjusted (by trial and error) in a way that the radiative time step is almost always restricted by the "Courant" condition and only sometimes in extreme cases by the maximum energy change restriction. The computed output intensity should be checked for the size of its fluctuations due to a possibly too large value of `c_radmaxeichange`.

- `real c_radthintimefac`:
  In the `LHDrad` module only the radiative time step restriction due to energy changes can be relaxed further in the optically thin by specifying e.g.

```
real c_radthintimefac f=E15.8 b=4 &
  n='time scale reduction in optically thin'                    u=1 &
  c0='range: 0.1 - 1.0, typically: 0.5'
 0.60
```

  A value $\leq$ `0.0` or `real c_radtvisdtau` $\leq$ `0.0` switches off this relaxation.

- `real c_viscourant`:
  The tensor viscosity routines have their own time step restriction. The recommended typical viscous time step can be set e.g. with

```
real c_viscourant f=E15.8 b=4 n='viscous Courant factor'        u=1 &
  c0='range: 0.0 < C_visCourant, typically: 0.5-1.0, better 0.25'
 0.5
```

  As the corresponding viscous timescale is typically longer than the radiative one (and even the Courant timescale from the Roe hydrodynamics routines) this factor is often irrelevant. The absolute upper stability limit is located at `c_viscourant`=`2.0`. Values around `0.5` to `1.0` are more typical. In some extreme cases in simulations of the solar chromosphere it has turned out that an even lower value (`0.2`) is necessary to prevent some spikes in the neighborhood of strong colliding shocks.

- `real c_viscourantmax`:
  The absolute upper limit for the viscous time scale can be set with

```
real c_viscourantmax f=E15.8 b=4 n='maximum viscous Courant factor'  u=1 &
  c0='range: C_visCourant <= C_visCourantmax, typically smaller than 2.0'
 1.0
```

  Its value should be slightly above `c_viscourant` and below `2.0`.

5.3.16 Input/Output Control

With this group of parameters the start model and the type and amount of output can be specified. Parameters with the suffix "`_start`" describe the initial model, these with suffix "`_end`" the corresponding final model. Additional data can be written into the file described by the parameters with suffix "`_full`" (full 2D/3D model dumps, huge, see Sect. 5.1) or into the file described by the parameters with suffix "`_mean`" (additional information, see Sect. 5.2).

- `real dtime_out_full`:
  The interval between datasets in the `full` file can be set e.g. with

```
real dtime_out_full f=E15.8 b=4 n='Output time step'            u=s &
  c0='dtime_out_full < 0.0 => no output' &
  c1='dtime_out_full = 0.0 => output every time step'
 2.0E+06
```

  Allowed values are

  - $<$ `0.0`: No output to this file
  - $=$ `0.0`: Output at every time step. Attention: This can produce HUGE files in no time.
  - $>$ `0.0`: Output to `full` file approximately every `dtime_out_full` seconds.

Some examples: The "classical" value for this output for simulations of solar granulation is 20 sec. To save memory this can be increased to 30 sec. But in this case chromospheric shocks are very badly resolved. To cover them properly, a sampling rate of 10 sec or below is needed.

- `real dtime_out_end`:
  The interval between outputs into the `end` file can be set e.g. with

```
real dtime_out_end f=E15.8 b=4 n='Output time step'                    u=s &
  c0='dtime_out_end < 0.0 => output only at very end' &
  c1='dtime_out_end = 0.0 => output every time step' &
  c1='dtime_out_end > 0.0 => output every dtime_out_end seconds (and at end)'
 1.0E+04
```

  Allowed values are

  - $<$ `0.0`: Output only at very end of run (classical behavior).
  - $=$ `0.0`: Output at every time step. Attention: This can produce lots of I/O operations and can take a long time. However, it will not produce a large file. Instead, the `end` file is written over and over again.
  - $>$ `0.0`: Output to `end` file approximately every `dtime_out_end` seconds (and at the very end of the simulation).

  The standard value is `-1.0`, not enabling any additional output into this file. A value a reasonable factor smaller than `real dtime_out_full` seems appropriate.

- `real dtime_out_mean`:
  The interval between datasets in the `mean` file can be set e.g. with

```
real dtime_out_mean f=E15.8 b=4 n='Output time step'                  u=s &
  c0='dtime_out_mean<0.0 => no output'
 0.5E+06
```

  Allowed values are

  - $<$ `0.0`: No output to this file
  - $=$ `0.0`: Output at every time step.
  - $>$ `0.0`: Output to `mean` file approximately every `dtime_out_mean` seconds.

  Because the size of one `mean` dataset is much smaller than one `full` dataset, it is possible to request a higher sampling rate without using too much disk space.

- `integer n_outslicedim_mean`:
  The index of the optional slice in the mean output file can be specified with e.g.

```
integer n_outslicedim_mean f=I4 b=4 n='index of slice in mean output file' u=1 &
  c0='0: no output of slice' &
  c1='1, 2, 3: output of slice with plane perpendicular to this direction'
2
```

  With a value of `0` the output is suppressed. A value of `1, 2, 3` indiciates the direction of the normal to the output plane: for instance, in a local 3D "box-in-a-star" model with gravity along direction 3 a value of `3` gives a horizontal plane in the middel of the model (useful only in special cases) whereas a value of `2` (or `1`) gives a vertical slice with a horizontal and the vertical axis – useful for movies of 2D slices. The grid index of the slice cannot be specified.

- `character infile_start`:
  The filename of the initial model is specified e.g. with

```
character infile_start f=A80 b=80 n='File name of start model'
rhd.sta
```

Default is `rhd.sta` (for a parameter file used within a batch system). Typical filenames are `st35gm04n01_01.sta` or `gt57g44n20dz.end`.

- `integer istep_in_start`:
  The index number of the dataset in the start model file to be used can be specified, e.g. with

```
integer istep_in_start f=I4 b=4 n='Number of dataset to read as start model' &
  u=1 c0='1: first dataset (default), 2: second dataset, ...'
1
```

- `character outfile_end`:
  The file name for the final model can be specified with e.g.

```
character outfile_end f=A80 b=80 n='Output file name'
rhd.end
```

  The default is `rhd.end`. Leaving it empty means that no final model is written. This of course inhibits follow-up simulations but can be useful to save time and disk space for some tests.

- `character outfile_full`:
  The name of the file for the output of additional full models at regular intervals (see Sect. 5.1) can be given with e.g.

```
character outfile_full f=A80 b=80 n='Output file name'
rhd.full
```

  Leaving it empty means that no file of this type is written.

- `character outfile_mean`:
  The name of the file for the output of additional information (average stratification, mean fluxes, surface intensities) at regular intervals (see Sect. 5.2) can be specified with e.g.

```
character outfile_mean f=A80 b=80 n='Output file name'
rhd.mean
```

  Leaving it empty means that no file of this type is written.

- `character outform_end`:
  The format (see Sect. 4.3.1) of the final model files can be chosen e.g. with

```
character outform_end f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

  Allowed values are

  - `unformatted`: (default) fast compact (possibly machine-dependent) output: strongly recommended
  - `formatted`: slow (machine-independent) output, big files

- `character outconv_end`:
  The conversion type (see Sect. 4.3.1) of the final model files can be specified e.g. with

```
character outconv_end f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen.

- `character outform_full`:
  The format (see Sect. 4.3.1) of the `full` model files can be chosen e.g. with

```
character outform_full f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

  Allowed values are

  - `unformatted`: (default) fast compact (possibly machine-dependent) output: strongly recommended
  - `formatted`: slow (machine-independent) output, big files

- `character outconv_full`:
  The conversion type (see Sect. 4.3.1) of the `full` model files can be specified e.g. with

```
character outconv_full f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

  The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen.

- `character outform_mean`:
  The format (see Sect. 4.3.1) of the additional data files can be chosen e.g. with

```
character outform_mean f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

  Allowed values are

  - `unformatted`: (default) fast compact (possibly machine-dependent) output: strongly recommended
  - `formatted`: slow (machine-independent) output, big files

- `character outconv_mean`:
  The conversion type (see Sect. 4.3.1) of the additional data files can be specified e.g. with

```
character outconv_mean f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

  The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen.

5.3.17 Additional Information, Obsolete and Test Parameters

- `real abux`:
  This optional information parameter can be specified with

```
real abux f=E15.8 b=4 n='hydrogen abundance (number fraction)' u=1 &
              c0='standard solar mixture'
 0.90851003E+00
```

It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

- `real abuy`:
  This optional information parameter can be specified with

```
real abuy f=E15.8 b=4 n='helium abundance (number fraction)'   u=1 &
          c0='standard solar mixture'
 0.90850003E-01
```

  It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

- `real qmol`:
  This optional information parameter can be specified with

```
real qmol f=E15.8 b=4 n='mean molecular weight'                u=u &
          c0='standard solar mixture'
 0.13018000E+01
```

  It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

- `real gamma`:
  This optional information parameter can be specified with

```
real gamma f=E15.8 b=4 n='Adiabatic coefficient'               u=1 &
          c0='0.0/1.6666666666666/1.4'
 0.0
```

  It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

- `real c_visneu1`:

```
real c_visneu1 f=E15.8 b=4 &
    n='Linear viscosity parameter (von Neumann-Richtmyer type)'   u=1
0.0
```

- `real c_visneu2`:

```
real c_visneu2 f=E15.8 b=4 &
    n='Quadratic viscosity parameter (von Neumann-Richtmyer type)' u=1
0.0
```

- `real c_radkappasmooth`:
  In the `LHDrad` module the opacity along each ray can be smoothed. The amount of smoothing can be set e.g. with

```
real c_radkappasmooth f=E15.8 b=4 n='Opacity smoothing parameter' u=1 &
    c0='0.0: no smoothing, 0.25: light smoothing, 0.666: strong smoothing'
0.0
```

  The smoothing can perhaps reduce the noise in the intensity images somewhat but has no general beneficial effect and should usually not be used.

- `real c_radtsmooth`:
  In the `LHDrad` module the 3D temperature array can be smoothed. The amount of smoothing can be set e.g. with

```
real c_radtsmooth f=E15.8 b=4 n='Temperature smoothing parameter' u=1 &
    c0='0.0: no smoothing, 0.5: reasonable smoothing, 1.0: max. smoothing'
0.0
```

The smoothing can sometimes reduce the noise in the intensity images but causes/amplifies some anomalies of the radiative Greens function: Some cool cell just above the sharp subphotospheric temperature drop are not heated but cool further down. Negative temperature spikes may result. This smoothing should not be used anymore.

- `character radpressure`:
  In the `LHDrad` module there exists a simple prescription for the radiative pressure (reasonable in the optically thin) which can be activated with

  ```
  character radpressure f=A80 b=80 n='Radiation pressure mode' &
    c0='on/off'
  on
  ```

  Allowed values are

  - `on`: Radiation pressure on.
  - `off`: Radiation pressure off.

  The scheme is pretty slow and wrong in the optically thick. Do not use!

- `real c_radtintminfac`:
  In the `LHDrad` module: The fraction the interpolated temperature (at a point on the ray) may exceed the minimum temperature at its four neighbors on the HD grid can be set e.g. with

  ```
  real c_radtintminfac f=E15.8 b=4 &
    n='Temperature interpolation parameter' u=1 &
    c0='<1.0: only bilinear, 1.1: reasonable weighting between min. und bil.'
  0.0
  ```

  The introduction of this parameter was an attempt to reduce the negative (cooling) effect of a single hot cell on its cool neighbors. It should be switched off e.g. by setting it to `0.0`.

- `integer dtimestep_out_fine`:
  This parameter can be specified but there is no corresponding output file in CO5BOLD yet.

  ```
  integer dtimestep_out_fine f=I4 b=4 n='Output time step number'       u=1 &
    c0='dtimestep_out_fine<0 => no output'
  -1
  ```

- `character outfile_fine`:
  The name of the file for the output of additional information at regular (small) intervals can be specified with e.g.

  ```
  character outfile_fine f=A80 b=80 n='Output file name'
  rhd.fine
  ```

  Leaving it empty means that no file of this type is written. Specifying it means the same (yet).

- `character outform_fine`:
  The format (see Sect. 4.3.1) of the files with frequent output can be chosen e.g. with

  ```
  character outform_fine f=A80 b=80 n='Output file format' &
    c0='formatted/unformatted'
  unformatted
  ```

Allowed values are

- `unformatted`: (default) fast compact (possibly machine-dependent) output: strongly recommended
- `formatted`: slow (machine-independent) output, big files

This parameter can be specified but there is no corresponding output file in CO5BOLD yet.

- `character outconv_fine`:
  The conversion type (see Sect. 4.3.1) of the files with frequent output can be specified e.g. with

```
character outconv_fine f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

  The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen. This parameter can be specified but there is no corresponding output file in CO5BOLD yet.

5.4 Additional Control and Status Files: rhd.stop, rhd.cont, rhd.done, and rhd.dump

Before each time step CO5BOLD checks in the working directory whether the file `rhd.stop` exists. If it has been generated (e.g. with `touch rhd.stop`), the code exits gracefully, i.e. it produces a proper final model, which can be used to restart the code. This method of stopping a simulation is to be preferred over a simple `kill` or `qdel` command because it allows to analyze the state of the model just at the end of the simulation and a smooth restart.

Before the restart the `rhd.stop` file has to be deleted! The simulation can be continued by just initiating a new run. If the file `rhd.cont` exists at the beginning of a simulation, the code tries to resume an interrupted computation: The initial model will not be taken from the start model file (`infile_start`) but from the final model (`outfile_end`). The data for the full and the mean file is not written into new files but will be appended to the existing ones.

In this way a simulation can be interrupted and continued in a fairly safe way. It is possible to analyze the final model and to changes values in the parameter file. Keep in mind that after a restart with `rhd.cont` the specifications about the length of the job (e.g. the number of time steps) will be counted from the restart point and not from the beginning of the original simulation.

To interrupt a job with `rhd.stop` can be very handy. The continuation with `rhd.cont` and the old parameter file is not to be preferred over an ordinary restart with a new parameter file.

At the beginning of every time step CO5BOLD checks in the working directory whether the file `rhd.dump` exists. If it has been generated (e.g. with `touch rhd.dump`) and the file `rhd.snap` does *not* exist, the current model is written into `rhd.snap`. It has the same file properties (format and conversion) as the regular `rhd.end` file. The run of the simulation itself is not modified. This feature might be useful for debugging purposes.

If a run was successful i.e. it was completed because one of the regular termination conditions was fulfilled (e.g. the requested number of time steps was performed) the exit status file `rhd.done` is produced. Currently, it contains the date and time of its generation. The existence of this file can be checked within a script to determine if the simulation was successful (and should be continued). Note: the existence of an `rhd.end` file only indicates that CO5BOLD managed to exit gracefully – due to an error or in a regular way.

5.5 Text Output: rhd.out

During execution – expecially during the initialization phase – CO5BOLD writes lots of information to standard output:

After the header its with a block “Compiler call”, e.g.

```
pgf90 -byteswapio -fast -Mvect=sse -Mcache_align -Minfo=inline -Minline=rhd_hyd_a
  vg,rhd_hyd_upwind,rhd_hyd_pred0,rhd_hyd_predm,rhd_hyd_predp,rhd_hyd_alpha,rhd_h
  yd_constanteq,rhd_hyd_minmodeq,rhd_hyd_minmod,rhd_hyd_vanleereq,rhd_hyd_vanleer
  ,rhd_hyd_superbeeeq,rhd_hyd_superbee,rhd_hyd_ppeq,rhd_hyd_pp,rhd_hyd_hdflux,rhd
  _hyd_entropyfix -Minline=rhd_rad3d_raylhd,rhd_rad3d_solve,rhd_rad3d_solveeq,rhd
  _shortrad_operator,rhd_shortrad_dtauop -Drhd_hyd_roe1d_l01=0 -Drhd_r02 -Drhd_r0
  3 -DMSrad_raytas1 -Drhd_hyd_entropyfix_p01=1 -Drhd_roe1d_step_t01 -Drhd_roe1d_f
  lux_t01 -Drhd_vis_t01 -Drhd_bound_t01 -Drhd_shortrad_step_t01 -Drhd_shortrad_fo
  rmal_t01 -Drhd_shortrad_lambda_t01
```

These lines were produced by the configure script (see Sect. 3.5) and written into the file

```
  compiler_flags.info
```

which is accessed from `rhd.F90` via `include` during compilation.

Various modules now have a routine "`XXX_switchinfo`" that prints the values of the compiler switches used during the compilation of that particular module. The output can look e.g. like

```
Compiler switches: rhd_hyd_module .......................
  IDF:                              0
  rhd_hyd_gravcorr_p01:             5
  rhd_hyd_entropyfix_p01:           1
  rhd_hyd_upwind_p01:               0
  rhd_hyd_roe1d_l01:                0
  rhd_roe1d_step_l01:               0
  rhd_roe1d_slope_l01:              0
  rhd_roe1d_flux_l01:       undefined
  rhd_bound_t01:              defined
  rhd_roe1d_flux_t01:         defined
  rhd_roe1d_step_t01:         defined
```

See Sect. 3.6 for more information about the meaning of the values.

The reading of the parameter file starts with

```
ACTION: Read parameter file <<<<<<<<
```

After a parameter is read, its value is printed (see Sect. 5.3)

The line

```
ACTION: Load EOS data <<<<<<<<
```

indicates the start of the reading of the equation of state data. It is followed by some information about the EOS table in use.

Similarly, the line

```
ACTION: Load opacity tables <<<<<<<<
```

indicates the start of the reading of the opacity data. The information that follows is taken directly from the header of the opacity table.

Currently, the last file to be read is the start model, which is announced by

```
ACTION: Read start model <<<<<<<<
```

and followed by some information about the start model, e.g. the number of grid points and a new section showing the quantities actually read, e.g.

```
Properties of start model:
  time       "time"                                    [s]
  xc1        "x1 coordinates of cell centers"          [cm]
  xc2        "x2 coordinates of cell centers"          [cm]
  xc3        "x3 coordinates of cell centers"          [cm]
  xb1        "x1 coordinates of cell boundaries"       [cm]
  xb2        "x2 coordinates of cell boundaries"       [cm]
  xb3        "x3 coordinates of cell boundaries"       [cm]
  rho        "Density"                                 [g/cm^3]
  ei         "Internal energy"                         [erg/g]
  v1         "Velocity 1"                              [cm/s]
  v2         "Velocity 2"                              [cm/s]
  v3         "Velocity 3"                              [cm/s]
  quc001     "Number density of CO"                    [1/cm^3]     advect(1)
  bb1        "Magnetic field 1"                        [G]
  bb2        "Magnetic field 2"                        [G]
  bb3        "Magnetic field 3"                        [G]
```

It might follow

```
ACTION: Initialize MS radiation transport routines <<<<<<<<
```

And finally

```
ACTION: Open output files <<<<<<<<
```

which indicates that the `rhd.full` file (see Sect 5.1)) and the `rhd.mean` file (see Sect 5.2)) have been opened and now contain a header.

The end of the initialization phase and the beginning of the proper simulation is marked by e.g.

```
================================ Start Computation ================================
=== Time step number: itime=    47050  time=  2.5821813E+08  t_job= 8.510000E+00 ===
```

The output for a typical simulation time step can look like (for a supergiant model with SHORTrad radiation transport)

```
--- Time step number: itime=    49048  time=  2.6822680E+08  t_job= 1.272180E+06 ---
dtime= 5.3047E+03 HD= 1.4838E+04 RAD= 5.3047E+03 VIS= 1.0723E+05
Luminosity per core volume:  4.49999049E-02
HYD 1: N_cellsperchunk, n_chunks:      10000  1410
HYD 2: N_cellsperchunk, n_chunks:      10000  1410
HYD 3: N_cellsperchunk, n_chunks:      10000  1410
VIS3D: N_cellsperchunk, n_chunks:      10000  1360

=== Start of rhd_shortrad_step ===
n_subdtime:    1
minmax(T)        1.111651E+03 1.630733E+05
Main ( 1/ 3) ray direction 2:   0.000000  1.000000  0.000000 ------------------------
Main ( 2/ 3) ray direction 3:   0.707105  0.000000  0.707109 ------------------------
Main ( 3/ 3) ray direction 3:  -0.707105  0.000000  0.707109 ------------------------
Time step ratio: dtime/dtime_rad:   1.750409E+01
dtime_:rad,drhoei,limit_this,all:  6.667E+02 2.510E+03 6.276E+02 0.000E+00
n_subdtime:    2
minmax(T)        1.116348E+03 1.630658E+05
Main ( 1/ 3) ray direction 1:   1.000000  0.000000  0.000000 ------------------------
Main ( 2/ 3) ray direction 3:   0.000000  0.707105  0.707109 ------------------------
Main ( 3/ 3) ray direction 3:   0.000000 -0.707105  0.707109 ------------------------
Time step ratio: dtime/dtime_rad:   1.836970E+01
dtime_:rad,drhoei,limit_this,all:  6.353E+02 3.188E+03 7.971E+02 6.276E+02
...
```

```
n_subdtime:    8
minmax(T)        1.118540E+03 1.630164E+05
Main ( 1/ 3) ray direction 2:  -0.707105  0.707109  0.000000 ----------------------
Main ( 2/ 3) ray direction 2:   0.707105  0.707109  0.000000 ----------------------
Main ( 3/ 3) ray direction 3:   0.000000  0.000000  1.000000 ----------------------
Time step ratio: dtime/dtime_rad:   1.791384E+01
dtime_:rad,drhoei,limit_this,all:  6.515E+02 3.894E+03 8.884E+02 4.814E+03
=== End of rhd_shortrad_step =====
```

A simulation ends with e.g.

```
=== Time step number: itime=    49050  time=  2.6823742E+08  t_job= 1.273407E+06 ===
================================= End Computation ===================================
```

A proper exit is indicated by

```
-------------------------------------------------------------------------------
Exit information: Requested number of time steps done
Exit status:        0
-------------------------------------------------------------------------------
```

In this case a file `rhd.done` (see Sect. 5.4) is produced. A messages like

```
*******************************************************************************
Severe error: SHORTRAD: Time step below absolute limit
Error index:      100
Interrupt computation
*******************************************************************************
```

marks an exit with an error and without `rhd.done` file. A message about the final model like

```
ACTION: Write final model <<<<<<<<
Model file 'rhd.end' opened on channel  12
===============================================================================
```

is followed by some timing information like e.g.

```
Timing statistics (rate x factor=   1000000 x     10000)
=======================================================

Process                            Samples     Total time      Mean time
                                                    [sec]          [sec]
-------------------------------------------------------------------------
RHD code                                 1     410.830017     410.830017
uio output routines                     27      37.469997       1.387778
HYD: bound_3Dcenter                   2000       3.540000       0.001770
Hydrodynamics routines                2000   48944.660156      24.472330
HYD: 1                                2000   16350.610352       8.175305
HYD: 2                                2000   16052.459961       8.026230
HYD: 3                                2000   16520.798828       8.260400
Viscosity routines 3D                 2000   25446.400391      12.723200
VIS: make_box(modelvis)               2000       0.010000       0.000005
VIS: copy_box(modelvis)               2000    1750.960083       0.875480
VIS: delete_box(modelvis)             2000       0.000000       0.000000
Radiation transport routines          2000  243729.000000     121.864502
SHC: step                             2020  244064.515625     120.824020
SHC: step: dtime: init: EOS          16024   49312.738281       3.077430
SHC: step: dtime: explicit           16024  174542.343750      10.892558
SHC: formal                          16024  170085.437500      10.614418
SHC: formal: init                    16024   35591.378906       2.221129
SHC: formal: dirloop                 16024  133010.687500       8.300717
SHC: formal: exp                     28014    9014.280273       0.321778
```

```
SHC: formal: exp: expl2t            28014    3950.409912       0.141016
SHC: formal: dir3                   36083   63222.242188       1.752134
SHC: time: dir3                     36083   19676.009766       0.545299
SHC: formal: limitei                16024    1306.419922       0.081529
SHC: step: dtime: final             16024   12730.129883       0.794441
SHC: formal: dir2                   11959   22205.000000       1.856761
SHC: time: dir2                     11959    5731.149902       0.479233
SHC: formal: dir1                    4044   10674.429688       2.639572
SHC: time: dir1                      4044    1893.760010       0.468289
SHC: step: dtime: final(output)       181    8620.870117      47.629116
Radiation trans.: output only          20     335.929993      16.796499
```

In this example the value for the overall time ("rhd code 410.830017 sec") is not useful because of an overflow in the counter. However, it is evident that the radiation transport consumes most of the time (243729.000000 sec), followd by the hydrodynamics routines (48944.660156 sec) and the tensor viscosity routines (25446.400391 sec). Some of these values are split further.

5.6 Chemistry Input

The number densities of the chemical species must be provided as cell-centred quantities `quc` in cm^{-3} (see Sect. 3.6). The array (UIO) headers must be named following this example: "Number density of H2".

The chemistry input file contains all data for the reaction network. It is a text file with a strict format following the *UMIST 99 ratefile* standard:

```
FORMAT(I4,5(A8,1X),2(1X,A4),1X,1PE8.2,3X,0PF5.2,2X,0PF8.1,A16)
```

It consists of 12 columns with the following meaning:

col.	meaning	format
1	reaction ID	I4
2-4	reactants (max. 3 symbols with 8 characters)	3(A8,1X)
5-8	products (max. 4 symbols, first two with	2(A8,1X),2(1X,A4)
	8 characters, last 2 with 4 characters	2(A8,1X),2(1X,A4)
9	reaction coefficient α	1PE8.2
10	reaction coefficient β	0PF5.2
11	reaction coefficient γ	0PF8.1
12	reference	A16

The symbols are usually the chemical symbols of the involved species, e.g. C for carbon. The present species are recognised automatically. Molecules consisting of more than one atom of the same chemical element, e.g. H_2, are also possible (`H2`). A special case is the representative metal `M` which is a catalytic element only, i.e. it must appear as reactant *and* product. The special symbol `PHOTON` represents a photon as reaction product. Currently no photon can be used as reactant ionising or exciting another species.

The reaction coefficients are needed to calculate the chemical rates at runtime. The basic rate is then given by

$$k \;=\; \alpha \; {T_{300}}^{\beta} \; e^{-\gamma/T} \quad , \tag{93}$$

where $T_{300} = T/300$ K with T the gas temperature. For catalytic reactions which involve a representative metal also the number density n_{M} of the metal enters:

$$k \;= n_{\mathrm{M}} \; \alpha \; {T_{300}}^{\beta} \; e^{-\gamma/T} \quad . \tag{94}$$

An input file could look like this:

```
5001 H       H       H2      H2      H2              9.00E-33   -0.6       0.0  -  AK
5002 H       H       H       H2      H               4.43e-28   -4.0       0.0  DBDDG72
4069 H2      H2              H2      H       H       1.00e-08    0.00   84100.0L 28034
4071 H2      OH              O       H2      H       6.00e-09    0.00   50900.0L 16964
```

```
  66 C       OH              O       CH              2.25e-11   0.50   14800.0L  4934
  67 C       OH              CO      H               1.81e-11   0.50       0.0  -  W80
3707 C       O               CO      PHOTON          1.58e-17   0.34    1297.4C BDD90
7001 C       O       H       CO      H               2.14e-29  -3.08   -2114.0D DBDDG76
4076 CO      M               O       C       M       2.79e-03  -3.52  128700.0D CBDDG76
```

Refer to [Wedemeyer-Böhm et al. (2005)] for more details.

5.7 HION Input

Several input files are required for the time-dependent treatment of hydrogen ionization. Currently, they need to be stored in the same input directory as specified with the parameter `hion_datapath`. There are four input files:

- model atom: The following formatting rules apply. Currently we only provide a hydrogen atom file `H_6-2.atom`. The module might be extended for other species in a future version.
- electron density look-up table (`edens.dat`) as function of total number density of hydrogen in cm^{-3} or m^{-3}, gas temperature in K, and ionization degree of hydrogen.
- chemical abundances (`abundance.input`)
- partition functions (`pf_kurucz.dat`)

The first two files are always needed, whereas the files containing chemical abundances and partition functions are required the initial LTE electron densities for very first time step of a model sequence (and for creating electron density tables). Once the first time step has been calculated the last two input files are obsolete. We plan to implement another initial guess for the LTE densities so that only the model atom and the electron density look-up table are necessary.

Refer to [Leenaarts & Wedemeyer-Böhm (2005)] for more details.

5.8 HION Output

The HION module can produce two types of output. The first is the standard output of the `quc` arrays in the `.full` and `.end` files, holding the level populations. This is all that is needed to restart a computation. The second (optional) output is a HION specific output system that generates files in UIO format after a prescribed number of simulation timesteps or alternatively after a prescribed time interval (see parameter `dtime_out_hion`). Output after a fixed number of timesteps is mainly useful for debugging. The files are named `HION.aaaa.bb.cccc.out` with `aaaa` either '`step`' or '`time`', indicating output after a fixed number of timesteps or a fixed amount of solar time, `bb` the atom identifier and `cccc` the number of the output file, e.g. `HION.step.H.0001.out`. The HION files can be read with the IDL `uio_dataset_rd ('filename')` function. The resulting data structure contains mass density, gas temperature, electron density of the atmosphere, as well as the axes in the `atmos` substructure. The `atom` substructure contains the time-dependent populations `ntd`, the LTE populations `nstar`, the total population `ntot`, a number of atomic parameters and `l_ntr` and `c_ntr`, arrays of the z-index per column where the radiation temperature in a transition starts to deviate from the gas temperature.

Refer to [Leenaarts & Wedemeyer-Böhm (2005)] for more details.

6 Running a Simulation

6.1 Quickstart: How to Run CO5BOLD

The generation of a start file and the modification of the parameter file is a somewhat complex process. In short, the following steps have to be performed.

1. Produce an executable `rhd.exe` (see Sect. 3.1) and put it into your working directory.
2. Choose a start model (e.g. the final model of an earlier simulation or a model produced with an IDL routine).
3. Edit the parameter file `rhd.par`: typically, you will start with an existing file and edit it. You should check that the paths and names of EOS, opacity, and start file are set correctly (Watch the username!). For details about the parameter file see Sect. 5.3.1.
4. Start the simulation with
   `nice nohup rhd.exe > rhd.out &`
5. You can see how the simulation proceeds with
   `tail -f rhd.out`
6. The other data files usually are in a binary format (this can be changed to ASCII "formatted" in `rhd.par`). Their contents can be read and analyzed with IDL routines (see Sect. 4.7.3).

For machines with batch queue there is a script, which can handle an entire sequence of simulations (see Sect. 6.2).

6.2 Running CO5BOLD on a Machine with Batch System

For longer simulations it is inconvenient to restart the individual jobs by hand. This task is done by a script originally from Hans-Günter Ludwig. Its basic function is sketched in Fig. 6.

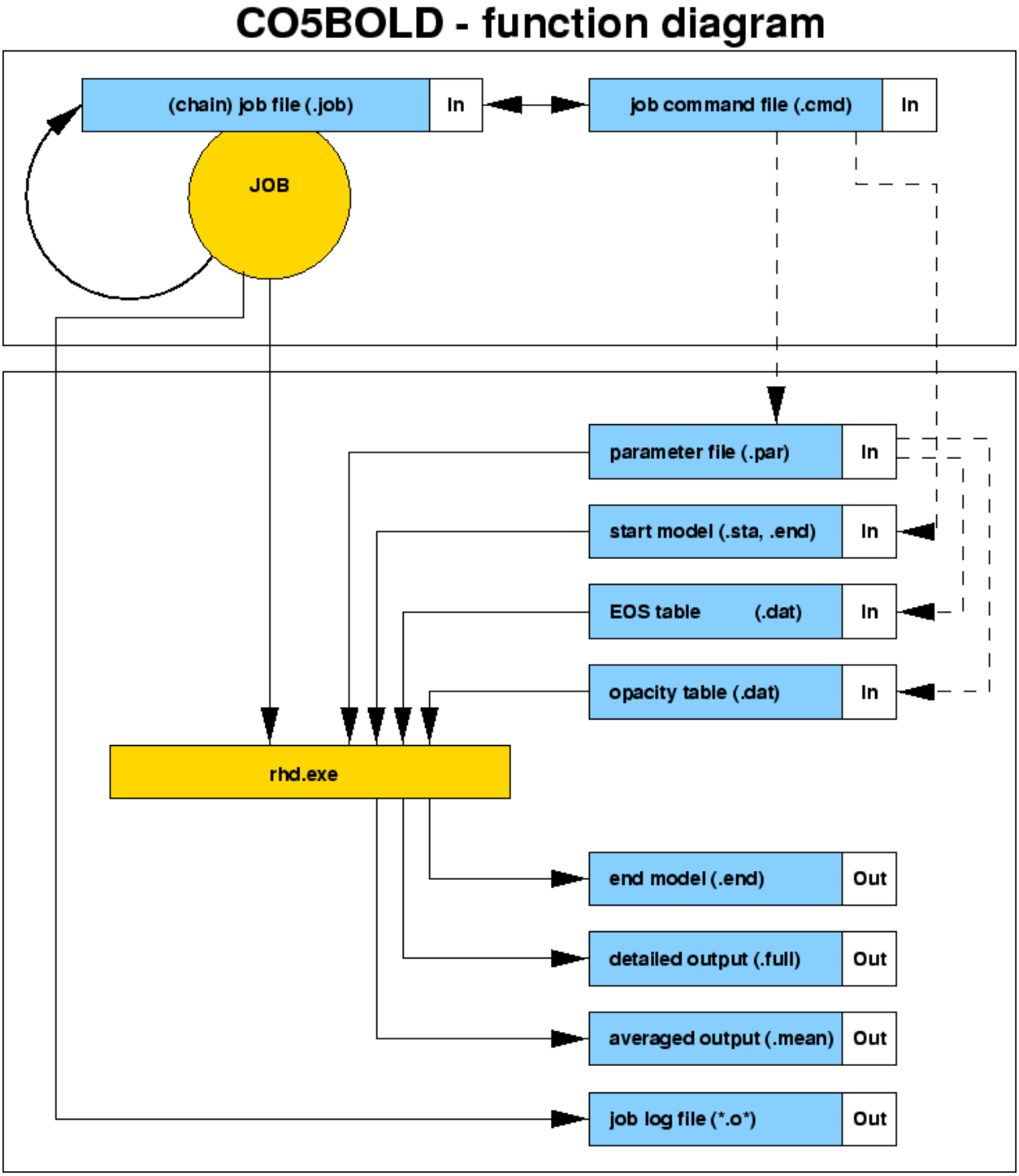


Figure 6: Program scheme

Here comes an example of the script (`rhd1.job`) for a system without dedicated batch system. The submission of a job is done via `nohup rhd1.job &`:

```
#!/bin/sh
#--- PBS -N rhd1
#--- PBS -l walltime=72:00:00
#--- PBS -l nodes=1:ppn=4
#
# --- Job file for the execution of RHD on gunnar (Itanium 2, Uppsala) ---
# --- Source: rhd1.job, original from HGL                              ---
# --- Last modification: 2002-12-13                                    ---
```

```
#
#set -xv
#
BASEDIR=/users/bf/dat/job/j1
STADIR=${BASEDIR}/sta      # Start directory: contains *.par, rhd1.cmd, rhd1.job
WRKDIR=${BASEDIR}/wrk      # Work directory
BAKDIR=${BASEDIR}/bak      # Backup and output directory
RHDEXE=$STADIR/rhd.exe     # RHD program to be executed
#
#export NCPUS=4
#echo $NCPUS
export OMP_NUM_THREADS=1
#
# --- Jump into work directory ---
cd $WRKDIR
#
# --- Loop: execute RHD code (possibly) several times in one job --------------
for IRUN in 1
do
  echo
  echo 'CO5BOLD Run #' $IRUN
  date
  #
  # --- Clear up work directory ---
  #set +e
  rm *
  #set -e
  #
  ###############################################################################
  #
  #   --- Get old command file, select actual command line ---
  #   --- and read variables from command line             ---
  #
  cp -p $STADIR/rhd1.cmd rhd1.cmd
  #
  awk \
  '      /#/   { print; next}
        /\*/   { print; next}
        /\+/   { print; next}
   DONE!="T"   { print >"cmdline"; printf "%-77s*\n", $0; DONE="T"; next}
               { print} ' rhd1.cmd | cat > dummy_nrhd.cmd
  #
  read INFILE OUTFILE PARFILE ACT < cmdline
  mv dummy_nrhd.cmd ${OUTFILE}_nrhd.cmd
  echo ${INFILE}
  echo ${OUTFILE}
  echo ${PARFILE}
  echo ${ACT}
  #
  ###############################################################################
  #
  if [ "${ACT}" != dum ]
  then
    ###############################################################################
    #
    #   --- RHD execution ---
    #
    # --- Copy parameter file ---
    cp -p ${STADIR}/${PARFILE} rhd.par
    #
    # --- Copy start file ---
    if test -s ${BAKDIR}/${INFILE}
    then
      cp -p ${BAKDIR}/${INFILE} rhd.sta
    else
      cp -p ${STADIR}/${INFILE} rhd.sta
      cp -p rhd.sta ${BAKDIR}/${INFILE}
```

```
  fi
  # --- Copy executable ---
  cp -p ${RHDEXE} rhd.exe
  #
  # --- Execute RHD ---
  ./rhd.exe > rhd.out
  RHD_EXIT=$?
  #
  if [ "$RHD_EXIT" != 0 ] || [ ! -s rhd.done ]
  then
    # --- Exit status not zero, ---
    # --- error may have occurred during execution of rhd.exe ---
    if [ "$RHD_EXIT" != 0 ]
    then
      echo 'Non-zero exit status ' $RHD_EXIT ' occurred during execution of RHD!'
    else
      echo 'No rhd.done file found: assume error during execution of RHD!'
    fi
    echo 'Execution of job chain terminated!'
    # --- Modify nrhd.cmd, set termination character "+" ---
    awk \
    '      /#/   { print; next}
          /\*/   { print; next}
          /\+/   { print; next}
     DONE!="T"   { printf "%-77s+\n", $0; DONE="T"; next}
                 { print} ' rhd1.cmd | cat > nrhd.cmd
    # --- Terminate chain by simulating ${ACT} = eoc ... ---
    ACT=eoc
  else
    # --- Modify command file: add '*' in appropriate column to indicate ---
    # --- proper execution                                               ---
    awk \
    '      /#/   { print; next}
          /\*/   { print; next}
          /\+/   { print; next}
     DONE!="T"   { print >"cmdline"; printf "%-77s*\n", $0; DONE="T"; next}
                 { print} ' rhd1.cmd | cat > nrhd.cmd
  fi
  #
  ls -l
  #
  # --- Move data into backup directory ---
  cp -p rhd.par  ${BAKDIR}/${PARFILE}
  mv rhd.out  ${BAKDIR}/${OUTFILE}.out
  mv rhd.par  ${BAKDIR}/${OUTFILE}.par
  #mv rhd.sta  ${BAKDIR}/${OUTFILE}.sta
  mv rhd.end  ${BAKDIR}/${OUTFILE}.end
  mv rhd.full ${BAKDIR}/${OUTFILE}.full
  mv rhd.mean ${BAKDIR}/${OUTFILE}.mean
  chmod go+r ${BAKDIR}/${PARFILE} ${BAKDIR}/${OUTFILE}.*
  chmod go-w ${BAKDIR}/${PARFILE} ${BAKDIR}/${OUTFILE}.*
  #
  ##############################################################################
fi
#
#
##############################################################################
#
# --- Dispose modified command file for next job ---
cp -p nrhd.cmd $STADIR/rhd1.cmd
#
# --- Exit loop if end of chain reached ---
if test ${ACT} = eoc
then
  break
fi
#
```

```
  # --- End of loop ------------------------------------------------------
done
#
# --- Submit next job if not end of chain reached---
if test ${ACT} != eoc
then
  cd $STADIR
  echo "Resubmit job"
#  /usr/local/bin/qsub rhd1.job
#  qsub rhd1.job
#  nice nohup rhd1.job &
  nohup rhd1.job &
else
  echo "End of job chain"
fi
#
###############################################################################
```

A more detailed description of the script will come sometime in the future (e.g. from Sven's manual...).

7 Data Analysis with IDL

In this section some basic commands for handling CO5BOLD data in IDL are described. See also Sect. 4.7

7.1 Preparations

Make the UIO IDL routines visible to IDL – somehow. There are several ways to do that. Three are described below:

We recommend to create an initialization file (e.g. named `start.pro`) which should be called after starting IDL (e.g. `@start`). This is necessary to define relevant paths of IDL subroutines and to provide the UIO package. Thus, the file should contain the following:

```
; --- Add user IDL directory to search path ---
addpath=expand_path('+$UIOPATH/idl')
addpath=addpath + ':' + expand_path('+$HOME/HYDRO/IDL/rhdpro')
if strtrim(addpath,2) ne '' then !path=addpath+':'+!path
delvar, addpath
; --- Initialize uio-routines ---
uio_init, progrm='by hand'
```

Note: Before using IDL the environment variables for the CO5BOLD paths should have been set. Use setarcdeppaths.sh (or .ksh, .csh) for this purpose. Important is `${UIOPATH}` which specifies where to find the IDL routines for the UIO handling in the script above.

Alternatively, one might set the IDL path variable accordingly like

```
export IDL_PATH="+$UIOPATH/idl"
```

for example in the `.bashrc` file before starting IDL.

Or, you just make a symbolic link from the UIO IDL routines at their original location to a sub-directory of the main IDL directory, which should be in the IDL path anyway.

The initial (single) call of `uio_init` is necessary in any case.

7.2 CO5BOLD Data in IDL

Important to know is that all operations can be performed in the command line of IDL. This allows an interactive processing of CO5BOLD data. Moreover, there are already prepared IDL scripts for this purpose but most of them are rather complex and still have to be edited (e.g. changing file names – Huuhh!). For the beginning it is more clear to use single commands. We give a short overview of some essential commands.

7.2.1 Loading the Parameter File

```
IDL> parfile='mymodel.par'
IDL> par=uio_struct_rd(parfile)
```

All control parameters are provided in the structure `PAR`.

7.2.2 Loading CO5BOLD Data (.full, .sta, .end)

```
IDL> modelfile='/home/user/mymodel.full' & n=0
IDL> ful=uio_dataset_rd(modelfile,n=n)
```

First the name and full path (if not in the actual directory) of the model file and the wanted time step should be defined. Here, time step means the consecutive number of the model snapshot in the file. Declaring a time step number greater than the number of snapshots contained in the file will cause an error.
Otherwise all data of the particular time step `n` will be provided in the structure `FUL`.
Loading more than one timestep from the same file could be achieved as follows:

```
IDL> uio_openrd, nc, modelfile, outstr, ierr
IDL> for i=0,ntime-1 do begin &$
IDL>   ful=uio_dataset_rd(modelfile, channel=nc,ierr=ierr, outstr=err_msg) &$
IDL> endfor &$
IDL> uio_closrd, nc
```

Again, this operation would cause an error if the wanted time step is not contained in the file. Via checking the error flag `ierr` of the routine `uio_dataset_rd` such errors can be avoided. This way it is unnecessary to know exactly of how many time steps the model file consists.

```
IDL> uio_openrd, nc, modelfile, outstr, ierr
IDL> i=0
IDL> repeat begin &$
IDL>   ful=uio_dataset_rd(modelfile, channel=nc, ierr=ierr) &$
IDL>   if (ierr eq 0) then begin &$
IDL>     ;--- Do the data processing here ---
IDL>     i=i+1 &$
IDL>   endif else begin &$
IDL>     print,'IDL> Reached EOF.' &$
IDL>   endelse &$
IDL> endrep until (ierr ne 0) or (EOF(nc))
IDL> uio_closrd, nc
```

To read a number of entries from a list of files in sequence the routine `uio_datasetlist_rd.pro` (see Sect. 4.7.3) is appropriate.

7.2.3 Loading the Equation of State

```
IDL> eosfile='../eos/dat/'+par.eosfile
IDL> tabinter_rdcoeff,eosfile, eos
```

The table for the equation of state is provided in the structure `EOS`.
NOTE: Always check file name and path!

7.2.4 Loading the Opacity Table

```
IDL> opafile='../opa/dat/' + par.opafile
IDL> dfopta, opafile
```

The opacity table will be stored as common block `OPTA_COMMON`. **NOTE: Always check file name and path!**

7.2.5 Computation of Deduced Quantities

After having read the model data `FUL` and the tables for the equation of state (`EOS`) and opacity (`OPTA_COMMON`) (see Sects. 7.2.3, 7.2.4), more quantities can be calculated:

```
IDL> eosbox, ful, eos=eos , /opa ,ierror=ierror
```

This operation adds the tags `EOS` and `OPA` to the data structure `FUL`, which contain more quantities like e.g. the temperature (see Sect. 7.3).

Based on the thermodynamic quantities now present in the `FUL` structure, further quantities can be computed with `combox.pro`, as for instance in

```
IDL> cs=combox('cs',ful)
```

7.3 IDL Data Structure

The data structure `FUL` contains the following variables and substructures. Use `help,/str,ful`, to get this information. See also the short description of the contents of a model file in Sect. 5.1 and particularly the man-page of the script `uiolook` in Sect. 4.6.2 which gives you even more detailed information directly from the file:

```
** Structure <8287a0c>, 9 tags, length=78404128, refs=1:
   TYPE               STRING    'uio'
   HEAD               STRUCT    -> <Anonymous> Array[1]
   DATASET_ID         STRING    'single_box'
   MODELTIME          FLOAT           10050.1
   MODELITIME         LONG            64088
   DTIME              FLOAT             0.176381
   TIME_OUT_FULL_LAST FLOAT           10050.1
   TIME_OUT_MEAN_LAST FLOAT           10040.0
   Z                  STRUCT    -> <Anonymous> Array[1]
```

If the command in Sect.7.2.5 has been performed, the following substructures are present:

```
   EOS                STRUCT    -> <Anonymous> Array[1]
   OPA                STRUCT    -> <Anonymous> Array[1]
```

The substructure `FUL.Z` contains the original data arrays from the model file like the spatial axes, density `rho`, internal energy `ei`, and the three spatial components of the velocity (`v1`, `v2`, `v3`):

```
** Structure <8274184>, 16 tags, length=78403900, refs=2:
   TYPE               STRING    'uio'
   BOX_ID             STRING    'z'
   DIMENSION          LONG      Array[2, 3]
   TIME               FLOAT           10050.1
   ITIME              LONG            64088
   XC1                FLOAT     Array[140, 1  , 1  ]
   XC2                FLOAT     Array[1  , 140, 1  ]
   XC3                FLOAT     Array[1  , 1  , 200]
   XB1                FLOAT     Array[141, 1  , 1  ]
   XB2                FLOAT     Array[1  , 141, 1  ]
   XB3                FLOAT     Array[1  , 1  , 201]
   RHO                FLOAT     Array[140, 140, 200]
   EI                 FLOAT     Array[140, 140, 200]
   V1                 FLOAT     Array[140, 140, 200]
   V2                 FLOAT     Array[140, 140, 200]
   V3                 FLOAT     Array[140, 140, 200]
```

Spatial axes: `XC1`, `XC2`, `XC3`, `XB1`, `XB2`, `XB3`:

The indices stand for `1`:x, `2`:y, `3`:z (or h) `C` for the grid cell centre, `B` for the boundaries. Most of the quantities are defined for the cell centres. In case of doubt, this can be found out by checking the array dimensions.

The substructure `FUL.Z` can contain additional arrays in case of dust formation, chemical reaction networks or time-dependent hydrogen ionization:

```
   QUC001          FLOAT     Array[140, 140, 200]
   QUC002          FLOAT     Array[140, 140, 200]
   QUC003          FLOAT     Array[140, 140, 200]
   QUC004          FLOAT     Array[140, 140, 200]
```

The magnetic field components are also stored in this substructure:

```
   BB1             FLOAT     Array[141, 140, 200]
   BB2             FLOAT     Array[140, 141, 200]
   BB3             FLOAT     Array[140, 140, 201]
```

The magnetic field is defined on the cell boundaries in the direction of the spatial components, e.g. `BB1` in direction 1, and in the cell-centres for the other directions. The resulting array dimensions differ from the cell-centred quanties like, e.g., `rho`. The array values must be multiplied with a factor $\sqrt{4\pi}$ in order to obtain the field strength in Gauss.

The substructure `FUL.EOS` (which is present only after a call of, e.g., `eosbox.pro`) contains important quantities like the temperature `T`, gas pressure `P`, entropy `S`:

```
** Structure <826a03c>, 6 tags, length=109760000, refs=2:
   P               FLOAT     Array[140, 140, 200]
   DPDRHO          FLOAT     Array[140, 140, 200]
   DPDEI           FLOAT     Array[140, 140, 200]
   T               FLOAT     Array[140, 140, 200]
   DTDEI           FLOAT     Array[140, 140, 200]
   S               FLOAT     Array[140, 140, 200]
```

The substructure `FUL.OPA` only contains the opacity `KAPPA`:

```
** Structure <826a5b4>, 1 tags, length=15680000, refs=2:
   KAPPA           FLOAT     Array[140, 140, 200]
```

7.4 More IDL routines

In the directory `IDL/bflib/` a lot of useful routines can be found which can be used for further processing and visualisation of CO5BOLD data. For the visualisation of 2-D models or 2-D data slices in general we recommend `plotfield.pro`. With `combox.pro` further quantities can be calculated.

Furthermore, we currently develop a widget-based analysis tool called **CO5BOLD AT** (abbrev.: CAT) which will help to work with CO5BOLD data without having to write and edit own IDL code. The routines are stored (if available) in the directory `IDL/COBOLDAT` and have to be started with `@cat`. A more detailed documentation is planned.

8 Document history

- 2002-02-16: First version on the web
- ... lots of extensions and changes in between...
- 2004-02-23: SGI Origin compiler settings section modified (for CINES machines) 3.7.16, 3.7.17
- 2004-02-23: short example for `uio_datasetlist_rd.pro` usage: 4.7.3
- 2004-03-02: Intel compiler settings section modified (`LD_ASSUME_KERNEL=2.4.19`): 3.7.11
- 2004-03-02: SGI Origin compiler settings section modified: 3.7.16
- 2004-03-03: IBM compiler settings section added: 3.7.9
- 2004-03-04: Document history started (pretty late...)
- 2004-03-04: Dedicated OpenMP section: 3.7.1
- 2004-03-04: Dedicated inlining section: 3.7.2
- 2004-03-04: Parameter for core drag force: 5.3.4
- 2004-03-04: New EOS table for solar composition: 5.3.5
- 2004-03-04: Trademarks: 10
- 2004-03-04: List of new dust files (the table was split into two): 3.4
- 2004-03-04: Installation of UIO UNIX scripts with configure: 4.6.1
- 2004-05-03: Thermodynamic relations: 2.3
- 2004-05-14: Point-to-point "tensor" viscosity: 5.3.8
- 2004-07-26: New gravitational potential mimicking a travelling tidal wave: 5.3.3
- 2004-08-18: New control files `rhd.dump` and `rhd.snap` to request a snapshot of current model: 5.4
- 2005-03-08: New control parameter `dtime_out_end`: 5.3.16
- 2006-07-28: Preparation for major code release (beta version) with the new modules CHEM (5.6), and HION(5.7), including new parameters (5.3.9) and switches for the configure script (3.5)
- 2006-08-14: MHD section: 2.2, MHD parameters: 5.3.7, 5.3.4
- 2007-02-12: Hydro section with new modii and parameters: heat mode: 5.3.4, rotating coordinate system: 5.3.3, possible hydrodynamics iteration: 5.3.7, new pressure correction scheme: 3.6 unsplit hydrodynamics operator possible: 5.3.7.
- 2007-10-22: Double precision time as additional scalar in model file: 5.1
- 2007-12-18: Rather stable version and parameter-rearrangements for dust model `dustscheme=dust_k3mon_03` (5.3.11) and `dustscheme=dust_bins_01` (5.3.12).
- 2008-03-13: Expansion Courant number `C_hydExpCourant`, `C_hydExpCourantmax`: 5.3.15
- 2008-03-17: "Hydrostatic pressure correction" in waves 3 and "6" switch-on-and-offable with `C_hydPredfactor`: 5.3.7

- 2008-04-27: Expansion viscosity `C_visExpansion`: 5.3.8
- 2008-07-03: Linear viscosity `C_visLinear`: 5.3.8
- 2008-08-13: Parameters `N_radrsyslevel`, `N_radoutput`, `C_radTcool`, `C_radDcool`, `C_radscool` in MSrad: 5.3.13, parameters `C_radTinci` and `C_radDinci` to control incident radiation in MSrad: 5.3.13
- 2008-08-14: Compiling double precision code: 3.7.3
- 2008-08-19: Some parameters (possibly) valid for MHD module: 5.3.7
- 2008-08-28: Rather old parameters for additional I/O control: `integer n_outslicedim_mean`: 5.3.16, `integer istep_in_start`: 5.3.16

9 Glossary

- **CO5BOLD** or **COBOLD** is the short form of "COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with l=2,3".
- **EOS**: "Equation Of State"
- **HION**: "Hydrogen IONization"
- **MHD**: "Magneto-HydroDynamics"
- **RHD**: "Radiation HydroDynamics"
- **UIO**: the "Universal Input Output" format. It is used in CO5BOLD for parameter, model, mean, and EOS files.

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