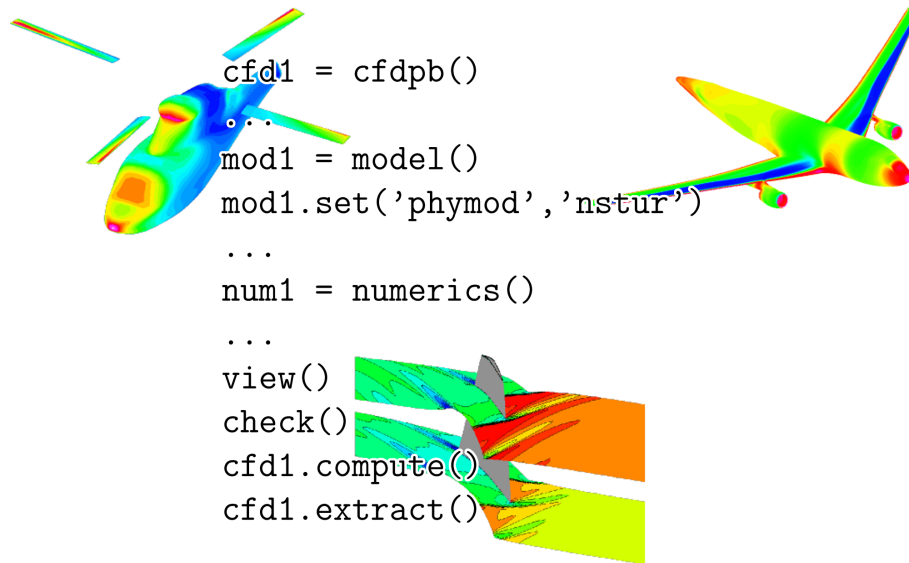


Design and Implementation Tutorial



Quality	For the authors	For the reviewers	Approver
Function	Integration manager, Head of design method	Quality manager	Project head
Name	M. Gazaix, A. Gazaix-Jollès	A.M. Vuillot	L. Cambier

Visa

Software management : ELSA SCM
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1. INTRODUCTION

1.0.1 Document's purpose

The intent of this document is to provide developers with design information necessary to contribute to *e/sA* software development. A companion document, "Development Process Tutorial" (/ELSA/MDEV-03036), provides additional information.

1.0.2 Content

The document starts with a brief summary of CFD basic concepts (chapter 2), and of Object-Oriented design (chapter 3).

An overview of *e/sA* general architecture is given in chapter 4; then the *e/sA* kernel design is presented in chapter 5.

Individual modules are described in chapter 6 to 13, with an emphasis over design and implementation technical choices.

2. THEORETICAL BACKGROUND

elsA is dedicated to numerical simulation of **single-species laminar** or **turbulent** (including transition) **compressible** flows, on **3D** (or 2D, or axisymmetric) **block-structured** grids.

The equations to be solved are the **Navier-Stokes** (NS) equations, in which turbulence is modelled via a statistical approach (turbulent fields are decomposed into a sum of mean and fluctuating fields). By carrying out the averaging operation upon the NS equations, one obtains the **Reynolds Average Navier-Stokes** (RANS) equations. Finally, these equations are expressed in the general **Arbitrary Lagrangian-Eulerian** (ALE) formulation, so that arbitrary grid motions (rigid system of body, deformation) can be taken into account.

A thorough description of the modeling and numerical methods implemented in *elsA* can be found in the Theoretical Manual [/ELSA/STB-97020].

The next section presents briefly the key concepts involved when performing CFD computations with *elsA*.

2.1 Overview

2.1.1 Numerical formulation

elsA solves the compressible **Navier-Stokes** (viscous) and **Euler** (viscous effects neglected) equations in a **cell-centered finite-volume formulation**, using space and time discretization. In the cell-centered approach, unknowns are interpreted as mean cell values. The central assumption in the numerical formulation used in *elsA* is the so-called "*Principle of Conservation*". This principle requires that the equations must be written in **conservative form**.

2.1.2 Discretization

The spatial discretization algorithm governs the computation of flux and source terms:

- **Fluxes** must be computed on each cell interface;
- **Source terms**, if any, are computed inside each computational cell.

After space discretization, these equations are translated in simple local **balances**. One can argue that the accurate and efficient computation of fluxes and source terms is the most important part of the *elsA* kernel. In *elsA*, the basic unit where these balances are done is the cell which must be hexaedric (in 3D).

The spatial discretization leads to an Ordinary Differential Equation (ODE) system which is solved using a (pseudo)-unsteady time integration solver. This translates into a **(pseudo)-time loop**. Inside this loop:

- fluxes and source terms are computed;
- boundary conditions are taken into account;
- auxiliary quantities (such as pressure, viscosity, ...) are computed if required;
- timestep can be computed and convergence acceleration techniques may be applied.

In **steady** simulations, the loop is iterated until convergence (or maximum number of iterations) is reached. In **unsteady** simulations, the computation stops when the specified final time is reached.

2.1.3 *Mesh and Grids*

Mesh generation is essentially outside the area of *elsA*: meshes, created by an external mesh generator, are given as input. *elsA* uses direct oriented structured meshes. Meshes must be 3D, structured, hexaedric; they can be multi-zone. In that case, communication between them is done through "join" boundaries.

Mesh objects are not essential inside *elsA*; instead, from the mesh point coordinates, *elsA* is able to build **grid** objects.

The conservative relationships are applied to grid cells. Grid objects are very important, and must be fully mastered by every application developer. Grids have two essential roles:

1. a grid object provides with the connectivity information (**topological relations** between geometrical entities: cells, interfaces, nodes and edges);
2. a grid object can provide the **metrics**: volume of the cells, surface of the cell interfaces.

2.2 **Description of the main features available**

2.2.1 *Space discretization schemes*

2.2.1.1 *Convective fluxes*

The **convective fluxes** can be discretized either by a **centered scheme** with **artificial viscosity**, or by an **upwind scheme**:

- **Jameson's** centered scheme with a choice of several artificial dissipation formulations;
- upwind schemes: **van Leer**, **Roe**, **Coquel-Liou** fluxes are available. First order and second order are available when combined with **MUSCL extrapolation**.

The additional equations arising from turbulence transport equations are, most of the time, solved in a **decoupled** way: the convective fluxes of the turbulent system are then discretized with the **Roe scheme** in association with the **Harten entropic correction**.

2.2.1.2 Diffusive fluxes

The discretization of the **diffusive fluxes** requires the evaluation of the flux densities, whose expression uses the **gradients** of **velocity**, **temperature** and possibly **turbulent quantities**.

Gradients can be evaluated either in cell centers, or in interface centers.

2.2.2 Time integration

2.2.2.1 Explicit stage

In the **explicit stage**, the time integration is based either on a **4-step Runge-Kutta** algorithm, or on a **backward-Euler** algorithm.

In the case of **steady flows**, time can be considered as an iterative parameter allowing to converge towards steady solution. If the Runge-Kutta time integration scheme is used, the convective flux is recomputed for each Runge-Kutta step, whereas the diffusive fluxes, numerical dissipation (if any) and source terms, are computed only at the first step, in order to save computation time. To accelerate convergence, the timestep can be a local timestep (different from one cell to another). The CFL number, introduced to ensure the stability of the numerical scheme, has to be defined by the user.

For **unsteady applications**, time accuracy must be preserved: a global timestep has to be chosen. If the Runge-Kutta time integration scheme is used, the calculation of the diffusive fluxes, numerical dissipation and source terms are done at the first and fourth Runge-Kutta steps.

2.2.2.2 Implicit stage

Implicit time integration methods can strongly reduce the total computational time, increasing the numerical stability of the schemes and thus allowing the use of larger timesteps.

The available implicit methods are:

- **Implicit Residual Smoothing (IRS)** is used in association with centered Jameson's scheme, with Runge-Kutta 4-step algorithm;
- **LU** or **LUSSOR** are used with both centered and upwind schemes, with backward-Euler time integration.

2.2.3 Calculation strategy

The system of mean NS equations (**mean flow**) and the system of transport equations (**turbulent quantities**) are solved using a **decoupled** algorithm. One carries out the following stages:

Before entering time loop:

1. **initialize** the **turbulent eddy viscosity**;

then at each iteration:

1. **integrate** (with **turbulent eddy viscosity frozen**) the **mean field** system using either Jameson's centered scheme with artificial viscosity or an upwind scheme, associated with a Runge-Kutta algorithm (or backward-Euler);
2. **integrate** (with **mean field frozen**) the **turbulent system** using the upstream space approximation according to Roe with Harten entropic correction, associated with Runge-Kutta (or backward-Euler) algorithm;
3. **update** the **turbulent eddy viscosity**.

2.2.4 Turbulence modeling

2.2.4.1 Modeling assumptions

In *elsA*, most turbulent models rely on the **Boussinesq hypothesis**; their common feature is the use of the eddy viscosity, which can be calculated either by **algebraic turbulence models**, or using **transport equations**.

EARSM models are also available; this class of transport equation models assumes a non-linear relation between the Reynolds stress tensor and the velocity gradients, in order to provide a better description of the turbulence anisotropy. They are characterized by an ASM closure instead of the Boussinesq closure. This closure relation is used to express the Reynolds stress tensor.

Large-eddy simulation (LES), with **Smagorinski model**, has also been introduced in *elsA*. LES allows the use of coarser meshes, by resolving directly only the largest scales of the flow, while small scales, referred to as subgrid scales, are represented through a statistical model.

2.2.4.2 Algebraic models

Among the turbulent models based on the Boussinesq hypothesis, the algebraic models are based on an algebraically defined turbulent viscosity according to a mixing length hypothesis. Their predictive value is limited, but their advantage is robustness and economy. **Michel-Quemard-Durant** and **Baldwin-Lomax** models are available.

2.2.4.3 Transport equation models

Many turbulence models with transport equations are available in *elsA*. Among them:

- one transport equation : **Spalart-Allmaras** model, with DES correction option;
- two transport equations:
 - **k-l Smith** model;
 - **k-omega** model with different options:

- * Zheng limiter;
- * cross diffusion term in the omega equation;
- * SST correction;
- * different treatments of the wall boundary condition: wall roughness or $1/y^{**2}$ extrapolation.
- **BSL k-omega Menter** model with SST correction option;
- **low Reynolds k-epsilon** Jones and Launder model, **high Reynolds k-epsilon** model with SST correction option;
- four transport equations: **multi scale** energy / spectral flux model.

2.2.5 Transition

For all the available turbulence models, transition effects can be included. Transition can be imposed or calculated; in the latter case, the transition **criterion** which can be **local** or **non local**.

2.2.6 Techniques of convergence acceleration

- Multigrid technique (V-cycle or W-cycle, cell to cell and node to cell prolongation); presently, multigrid technique can only be used for the resolution of the mean flow;
- Dual Time Stepping (DTS);
- Low speed preconditioning.

2.2.7 Rotation frame and ALE technique

In some problems, a formulation of the conservative laws in the entrained reference frame can be judicious (existence of a permanent flow in this reference frame). In *elsA*, helicopter and turbomachinery applications are treated in the relative entrained frame:

- in an absolute velocity formulation for the helicopter applications;
- in a relative velocity formulation for the turbomachinery applications.

2.2.8 Types of join boundary

In *elsA*, the available types of "join" boundaries are:

- coincident adjacent and partially coincident adjacent boundaries;
- adjacent boundary non coincident line;
- no match boundary;
- multistage boundary.

2.3 Not discussed in this document

2.3.1 *Chimera technique*

2.3.2 *Hierarchical Mesh Refinement (HMR)*

3. WHAT IS OBJECT-ORIENTED SOFTWARE?

3.1 Object-Oriented Programming Concepts

If you've never used an object-oriented language before, you need to understand the underlying concepts before you begin writing code. You need to understand what an object is, what a class is, how objects and classes are related, and how objects communicate by using messages. The next sections sum up the concepts behind object-oriented programming.

3.2 Object, interface, encapsulation

An **object** is a software "bundle" of **methods (behaviour)** and **attributes (data)**. At a given time, the set of all the attribute values is called the object **state**.

Everything an object can do is expressed through its **interface**. The interface can be seen as a **protocol**.

Providing access to an object only through its interface, while keeping the implementation details **private** (implementation masked), is called **information hiding**, or **encapsulation**. The benefit is that the private part of an object (both private data and private methods) can be changed at any time without affecting the other objects that depend on it.

Encapsulation means any kind of hiding:

1. Data hiding: data members (attributes) are kept private.
2. Class hiding: the actual class is hidden behind an abstract class or interface. In fact, polymorphism, which allows clients to ignore the true object type, can be viewed as an encapsulation mechanism.
3. Implementation hiding: clients are only aware of an opaque pointer, or *handle* (see **Do not systematically provide accessor methods**).

Encapsulation improves **maintenance**, facilitates **extensibility**. Obviously, many examples of encapsulation can be found in *elsA*; see for example section 6.2, *p. 26*.

3.3 Collaboration between objects

A single object, working isolated from any other objects, is usually not very useful. Instead, an object usually appears as a component of a larger program that contains many other objects. Through the **collaboration** of a large number of (relatively) simple objects, complex behaviour can be achieved. This collaborative technique greatly facilitate **flexibility** and **interoperability**.

3.3.1 Messages and methods

It is sometimes said in the OO community that objects interact and communicate by sending/receiving messages. In C++, messages correspond closely to (public) methods:

- as seen from the client side, the client sends a message: this means asking to another object to execute one of its methods;
- as seen from the receiver side, the receiver object executes the corresponding (public) method.

3.3.1.1 Example of collaborative work

A diffusive flux object (the sender) asks a k-l turbulent model object (the receiver) to perform its method `TurKL::compMut()`. Here, the *message* corresponds to the method:

```
FxdFlux::message()  
{  
    turObject -> compMut();  
}
```

3.4 Class

A **class** is a **prototype** that defines the attributes and the methods common to all the instances of the class. The individual instances are called objects. In practice, in C++, a new class is equivalent to a new **type**. A **factory** is used to manufacture object instances from the class definition.

Note:

The factory itself may be an instance, (usually a unique one: a *singleton*) of a specialized class.

3.5 Inheritance

Object-Oriented programming allows classes to be defined in terms of other classes. For instance, class `TurKL` **inherits** from class `TurBase`. `TurKL` is a **subclass** of the base class `TurBase`. Similarly, `TurBase` is the **superclass** (base class) of all the classes in charge of turbulence modeling.

Inside inheritance tree, methods and data are inherited down through the levels:

- In **abstract** classes, methods are **declared**, but partially (or not) implemented. Abstract classes define the **polymorphic** behaviour: all the derived classes will provide this behaviour.
- Each subclass inherits attributes (state) and methods (behaviour) from the superclass.
 - Subclasses can add their own data and methods to data and methods inherited from the superclass.
 - Subclasses can override (that is, specialize) virtual inherited methods by providing specialized implementations for those methods.

- When implementing a new specialized subclass, developers can **reuse** the code (the implementation) defined in superclasses. However, inheritance is really much more powerful than code factoring, which is of course available in any decent language (C and Fortran, for exemple). With the help of inheritance, developers can reuse the **interface**.

Inheritance greatly simplifies the software extensibility and maintenance tasks. The most important polymorphic hierarchies in *elsA* are:

- Implicit algorithms (`LhsBase` and derived classes).
- Boundary conditions (`BndBase` and derived classes; see **Bnd component**).
- Turbulence models (`TurBase` and derived classes; see **Tur component**).
- "Operators" (fluxes and source terms) (`OperBase` and derived classes; see **Oper component**).

Basically, developing a new implicit algorithm, a new boundary condition, or a new turbulence model, amounts to very similar tasks:

- Starting from the base class interface (`public` and `protected`), the developer must adapt it to his wishes; most of the time, the interface changes are very limited (usually some additional private attributes and a few private implementation methods).
- The developer must implement the abstract method(s) specific to the hierarchy:
 - `compLhs()` for the `Lhs` hierarchy;
 - `compBoundaryValue(...)` for the `Bnd` hierarchy (see **How to introduce a new boundary condition?**);
 - `compMutInModel()` for the `Tur` hierarchy (see **How to introduce a new turbulent model?**).
 - `compInterior()` for the `OperFlux` hierarchy.

3.6 And see other examples:

<http://www.softwaredesign.com/objects.html>

4. GENERAL ARCHITECTURE

4.1 *elsA* library and applications

elsA provides an **Object-Oriented (OO) CFD library**, together with a **stand-alone application** *elsA.X*, using Python as scripting language.

4.1.1 *Object-Oriented architecture*

elsA design and implementation are based both on Object-Oriented technology:

- *elsA* design uses the UML (Unified Modeling Language) modeling approach to obtain an accurate decomposition of the complex CFD problem into *static* classes, and to model the *dynamic* interacting objects (instances of classes).
- *elsA* kernel is implemented in the Object-Oriented language C++. Only the most CPU time-consuming computing loops are coded in Fortran, without impairing in any way the OO design.

4.1.1.1 *elsA* extensibility

elsA Object-Oriented architecture improves software extensibility through two basic mechanisms:

- **polymorphism**: developers can design and implement new features, such as a new turbulence model, a new boundary condition, a new implicit time integration algorithm,... in an *independent* way. By this we mean that code is *extended* through addition of new files, not *modified*, thus greatly decreasing integration time, by removing any conflicts.
- **encapsulation**: Object-Oriented technology encourages a clear distinction between private and public part of a component. Clients of the component only use the public interface, so they will not be affected by any changes in the private (implementation) part of the component. This greatly reduce maintenance costs.

4.1.2 *elsA* input data

To run a computation, *elsA* users must provide:

- geometric data, basically mesh coordinates (and possibly geometric coefficients in chimera);
- topological data: connectivity between blocks;
- physical data, to initialize the time-iterative loop; this physical data may be a constant thermodynamic state, or, more generally, come from data file (restart file).
- definition of boundary conditions; this may be only a boundary type identifier, or additional data may be needed (for example transition data can be prescribed in a fully general way with additional files).

4.1.2.1 *Definition of mesh points*

Mesh generation is not addressed by *elsA*: users must provide mesh point coordinates, as computed from external tools such as ICEM-CFD or NUMECA IGG¹.

¹Note however that mesh deformation algorithms are available (ALE, fluid-structure coupling).

A mesh file (binary, or ASCII Tecplot format) must be associated with each block. This greatly simplifies the parallel treatment, and is inherently scalable to massively parallel computations. To improve ergonomics, it is advised to put all mesh files in a single directory, and to use a consistent file naming. In that case, users do not have to care about the potentially large number of files, they are only aware of the directory name, which is just a "super-file".

4.1.2.2 *Restart files*

We use exactly the same mechanism as for mesh files. Again, the individual files associated with each block can be grouped into a single directory.

4.1.2.3 *Boundary information*

The generation of the complete boundary definition information can be time consuming and error prone. An automatic script generator is available to generate this information from ICEM-CFD input. It is often convenient to put boundary definition in a separate Python script file (module), which is imported by the main (driver) script:

- boundary definition are nearly always kept unchanged;
- several computations (with different numerical parameters, or Mach number,...) can *share* boundary definition, thus avoiding potential errors when duplicating boundary data.

4.1.2.4 *DAMAS database*

A tool using as input a DAMAS database is also available.

Note:

In future releases, it will be optionnaly possible to read mesh coordinates, as well as restart data and boundary definition data (at least for the "usual" boundary types) directly from a CGNS database.

4.1.3 *Simulation control*

elsA users control their CFD simulations through the Python scripting interface. This can be done in three ways:

- interactive text mode; this is limited to very basic test cases.
- through a Graphical User Interface (GUI), called **PyGelsA**, documented in the **PyGelsA** Graphical User interface User's Manual (<http://elsa.onera.fr/ExternDocs/user/MU-02044.pdf>).;
- through a Python script file; this is the preferred way for complex simulations. It is fully described in the *elsA* User Reference Manual (<http://elsa.onera.fr/elsA/doc/refdoc.html>).;

Using Python as the scripting interface greatly reduces the time required to develop and maintain the user interface. Moreover, Python provides with a high level versatile programming interface, allowing novice as well as expert users to interact with *elsA* in an optimized way. Let us give a small (non exhaustive!) list of useful Python features in the context of CFD simulation:

- Script files can be splitted in several modules, allowing *reuse* of well-tested blocks of settings, thus avoiding many potential errors.
- Simple Python programming enables basic numerical treatment in pre- or post-processing phase, such as normalization, directly in the script file, thus again avoiding inconsistent data arising from incompatible data coming from different independent tools.

- Users can write specific functions, or even Python classes, to automate specific tasks.
- Users can benefit from the large number of additional scientific Python modules available.

4.1.3.1 *Default value mechanism*

Users are not required to set explicitly all the control data necessary to define completely a simulation. Default parameters are provided through Python dictionary. The complete set of default parameters can be customized to suit the requirements specific to a specific user community. Python dictionaries can be modified at any time, thus allowing dynamic site customization without code recompilation.

4.1.3.2 *Connecting Python and C++: Use of SWIG*

elsA can be viewed as a standard Python module, `elsA.py`: it can be *imported*, as any other Python module. The task of generating the "glue" code necessary to access C++ code from the Python interpreter is done automatically by *swig*, a public domain tool (*cf.* 13, p. 68).

4.1.4 *Parallel mode*

elsA can run in parallel, using MPI communication library. *elsA* uses a coarse-grained parallelization strategy: taking advantage of *elsA* multiblock capability, each processor is responsible for the computation of a *subset* of the blocks belonging to the configuration. *elsA* uses the SPMD (Single Program Multiple Data) paradigm:

- each executable runs exactly the same program, reading the same Python scripting file (Python interpreter is embedded inside each parallel executable);
- each executable is responsible for local file pre- and post-processing: for example, if block 3 and 5 are allocated to processor 2, processor 2 is responsible for reading mesh data files corresponding to blocks 3 and 5. This should avoid bottleneck problems arising from centralized I/O treatment (for example through rank 0 processor) in massively parallel computations.

The mapping between blocks and processors can be done either "manually, or with the `Split` module. To achieve acceptable load balancing, splitting the initial configuration in a larger number of blocks may be necessary. This optional splitting stage can also be done through the `Split` module.

4.1.5 *Multidisciplinary Coupling*

Several coupling strategies can be used to couple *elsA* with other computational software. Let us give several examples:

- External coupling, basically through file exchange, with *elsA* used in black box:
 - in an optimization chain;
 - weak coupling with the boundary layer code COULEUR;
 - weak coupling with NASTRAN (static aeroelastic wing deformation computation).
- Use of a dedicated *coupler*, such as CALCIUM or PALM. A small number of "plugging" points have been identified and implemented inside *elsA* and tested.
- Modification of the internal algorithmic structure, to obtain full control and efficiency. This has been realized for complex fully coupled aeroelastic simulations.
- *elsA* has been coupled with the structural mechanics code HOST, using a proprietary protocol based on CGNS semantics.

4.1.6 Optimization module *Opt*

The *Opt* module implements the discrete Adjoint approach. It has been used inside automatic aerodynamic shape optimization process.

4.1.7 Access to CFD databases (CGNS, DAMAS)

indexdatabase (CFD)@database (CFD) To be written

4.1.8 Log file

For each run, *elsA* generates a log file (standard output), with some basic information:

- *elsA* version.
- precision (single or double precision)
- compiler options (DEBUG or optimized version)
- warning, or errors, if any.

Additionally, users can augment the log file by a large number of additional output: in fact, most post-processing available in *elsA* can be output either to a specific file, or to the log file.

Note:

In parallel mode, to avoid a "scrambled" log file (on some platforms, all the computing processors write in an essentially random order), there is one log file associated with each processor, with some information given only by the root (rank 0) processor.

4.1.9 Post-processing

4.1.9.1 Restart files can be generated by specifying a directory name.

This directory can then be used as input for a subsequent computation.

4.1.9.2 Global residuals

With default parameter GLOBAL_RESIDUAL set to YES, residuals for the complete configuration are automatically extracted.

4.1.9.3 General post-processing

A very fine control of post-processing is available.

- *Local* quantities: a wide range of local quantities (Mach, pressure,...) can be extracted.
- *Global* quantities: global quantities (lift, drag, mass flow, residuals,...) are available, with a simplified syntax when defined on predefined window families (for example, one family may correspond to the wing, another one to the fuselage).

5. KERNEL DESIGN

5.1 Classification and Design organization

CFD concepts can be classified as: geometrical, topological, numerical and physical concepts. In order to solve a CFD problem, we have defined a limited number of basic classes responsible of the following actions:

1. to take into account the fluid physical properties in the flow;
2. to build and control the numerical space region where the system of equations is solved;
3. to build the system of equations: compute the terms arising from the spatial discretization (flux, source terms); controls the application of the boundary conditions;
4. to control the time evolution of the solution.

So, the kernel has been designed as a set of consistent **modules** (or components). A module is **responsible** for a set of well-defined functionalities. Ideally, developers should be able to work inside a module, without having to know the implementation details of any other modules. Achieving a good decomposition is very important to improve ease of development and maintenance.

Moreover, this OO model has been split into sub-models with the aim to keep dependencies as local as possible. These modules are organized into **layers** in such a way that each layer should only affect the layers above. The goal of this organization is to achieve **mono-directional relationships**. The advantage is then that the maintenance becomes much easier, since one layer's interface affects only the upper layers. Avoiding cyclic dependency greatly simplifies test policy.

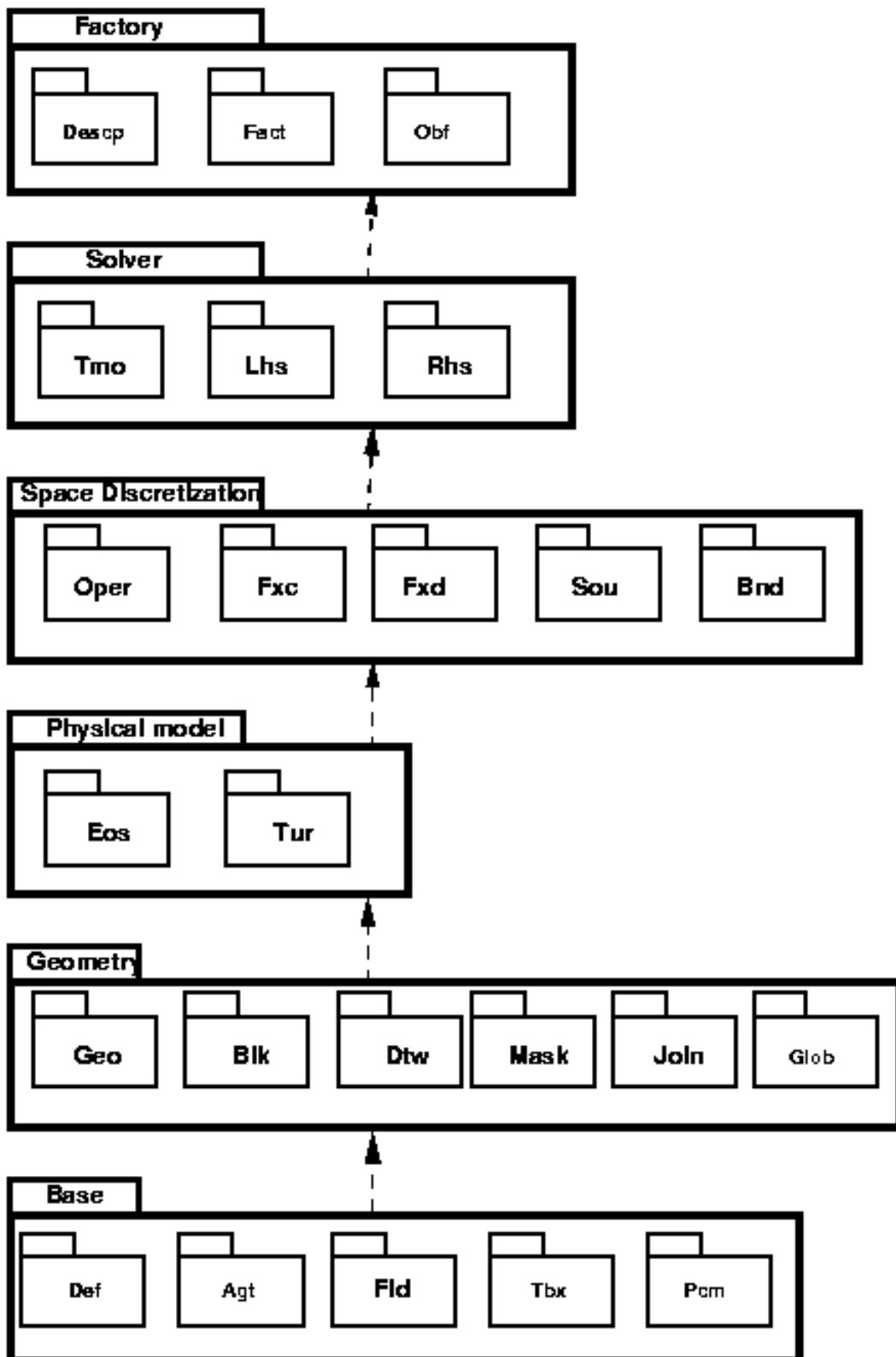
5.1.1 Naming convention

Each module is identified by a key of 3 to 5 letters, the first one being capitalized. Inside each module, each class name is then prefixed by the key of the module it belongs to. Example: TurKL belongs to the Tur module.

5.2 Overview of the layers

elsA kernel includes about 400 classes grouped in 26 modules specialized for a given CFD task. These modules are further organized in 6 layers:

- **Base;**
- **Geometry;**
- **Physical model;**
- **Space Discretization;**
- **Solver;**
- **Factory** (top level).



5.2.1 Base layer

Base layer gathers all **low-level** modules, among which the `Fld` and `Pcm` modules.

- `Fld`: **data storage** classes; these classes encapsulate dynamic memory needed to store any computational data. Their interface provide with monitoring methods, optimized array-like syntax (much like FORTRAN 90) and methods to communicate with FORTRAN routines. `Fld` classes are built in order to provide the highest efficiency (both in CPU and memory); a comparable efficiency could not be achieved through STL containers.
- `Pcm`: deals with **parallel** implementation; it "encapsulates" message passing interface (presently, MPI).

5.2.2 Geometry layer

Geometry layer gathers all **geometrical** and **topological** modules:

- `Blk`: defines the **block** notion. A `block` corresponds to a region of the discretized physical space defined by a mesh, to which are associated boundary and initial conditions. Blocks are specialized to take into account grid motion, ALE, chimera and HMR (Hierarchical Mesh Refinement) features. In most simulations, several blocks are needed.
- `Geo`: defines the abstraction of the **computational grid**; provides all geometrical ingredients used by a finite volume formulation:
 - **Metrics**: volume of cells, surface of cell interfaces.
 - **Topological relations** between geometrical entities: cells, interfaces, nodes. Recently, ghost cells have been introduced in `elsA`. Thanks to these ghost cells, most indirections have been suppressed in computational loops, and important improvement in CPU efficiency has been obtained.
- `Dtw`: gathers all **distance** and **boundary-layer integral thickness** computations.
- `Mask`: defines concepts used in the **Chimera technique**.
- `Join`: deals with **multi-block** computations. Multi-zone interface connectivity can be 1-to-1 abutting, 1-to-n abutting, or mismatched abutting.

5.2.3 Physical model layer

It includes two modules:

- `Eos`: computes quantities such as **pressure, temperature, laminar viscosity**;
- `Tur`: deals with **turbulence modeling** and **transition prediction**.

5.2.4 Space Discretization layer

This layer is responsible for the computation of the equation **terms** and of the **boundary conditions**:

- `Oper`: each operator class is responsible for the computation of a single term in the CFD equations:
 - `Fxc`: convective fluxes;
 - `Fxd`: diffusive fluxes;
 - `Sou`: source terms.
- `Bnd`: deals with boundary conditions.

5.2.5 *Solver layer*

This layer is responsible for:

- `Rhs`: builds the right hand side of the equation system;
- `Lhs`: gathers implicit methods; each implicit class has to build and invert the matrix resulting from a specific linearization of the system of equations;
- `Tmo`: time integration module; manages the main iterative (pseudo-)time loop.

It is probably the most complex part of the kernel, since many algorithms have to be taken into account: multi-block, multigrid, HMR, mesh motion, deformation, ...

5.2.6 *Factory layer (elsA top layer)*

This layer is responsible of the dynamic creation of all kernel objects: the `Fact` module implements several object "factories" to **build** object instances from user input data coming from the Python interface.

6. FLD COMPONENT

6.1 Basic numerical containers

Fields are the most basic objects manipulated by *elsA*. They are used as containers for the numerical values (real, integer, boolean) arising in CFD simulations.

It is useful to distinguish two general types:

- `FldArray` : stores numeric values, without any location information;
- `FldField` : stores numeric values defined on a grid. In that case, it can be also very useful to distinguish between:
 - values defined at grid nodes: `FldNode`;
 - values defined at centers of grid cells: `FldCell`;
 - values defined at centers of grid interfaces: `FldInt`.

So, we use `typedef` to express the specificity of each entity; for example:

```
typedef FldFieldF FldCellF;
```

This automatically gives important information upon the programmer's intent, and so facilitates code understanding and maintenance.

These containers must contain homogeneous collection of floats, integers, or booleans. To fulfill this requirement, *elsA* provides different versions of `FldArray` and `FldField`; the last letter of the class name identifies the contained element type:

- **F** stands for Float,
- **I** stands for Integer,
- **B** stands for Boolean.

Note:

`FldFieldB` is not implemented.

6.2 Public interface

Externally, for application programmers, fields are viewed as two-dimensional structures:

- the first dimension index goes from 0 to `_size-1`;
- the second dimension index goes from 1 to `_nfld`; if the second dimension is 1, it can be omitted.

Note:

The conventions used for first and second dimensions are inconsistent (0 instead of 1 for first index). This comes from historical reasons, and may be changed in future releases (just modify the constant `NUMFIELD0`, defined in `FldArray.h`, and recompile).

The field interface provides all the methods required to do numerical computations:

- construction;
- initialization;
- copy of an existing field into a new one;
- addition, subtraction, multiplication.

(See `FldFieldF` doxygen documentation for additional details).

6.2.1 Examples of `Fld` client code

1. Construction of a field which stores the unknowns of the CFD problem (`ro`, `rou`, `rov`, `row`, `roE`):

```
E_Int nfld = 5;
FldCellF wCons(ncell, nfld);
```

Construction of a field which stores fluxes:

```
FldIntF flux(3*ncell, nfld);
```

2. Construction of a field which stores mesh coordinates:

```
FldNodeF x(ncell, 3);
FldNodeF y(ncell, 3);
FldNodeF z(ncell, 3);
```

3. `FldArray` or `FldField` can be used to store values without geometric links, such as:

```
FldArrayF TurKO::getModConst() const
{
    FldArrayF modConst (7);
    modConst[0] = _kappa;
    modConst[1] = _sigma1;
    modConst[2] = _sigmae1;
    modConst[3] = _beta1;
    modConst[4] = _wsig1;
    modConst[5] = _betae;
    modConst[6] = _Sr;
}
```

4. To access individual elements, a syntax similar to Fortran is used:

```
FldArrayF f(100,2);
f(3,2)=3.14159; // assigns pi to the fourth element of component 2

FldArrayF g(100);
g[0] = 2.22;
```

Note:

`FldArray` is really an implementation class; it would be probably better to avoid using it directly, using `FldField` instead (additional memory associated with `FldField` own attributes is negligible).

6.2.2 Check of memory access, control of memory initialization

Fld classes should almost always be preferred to C/C++ arrays (see also **Prefer Fld objects (FldArray, FldField) to C arrays**), because they provide:

- memory usage check control; in DEBUG mode, we can check that access to container elements is valid:
- full control over data initialization; programmers can choose to initialize newly allocated memory with some "bad value" or, better, with Nan ("Not a number"); this will insure that access to non-initialized memory value can be trapped.

Subscript index checking and memory initialization control are very helpful to debug newly written code.

6.3 Passing field data to Fortran

In *elsA*, it is frequently necessary to communicate with Fortran 77 subroutine. Fortran 77 only knows scalars and arrays, and subroutine arguments are always passed by address. This means that we must, in some way, give the address of the piece of memory which is dynamically allocated by a FldField field to this subroutine (to know more about that, just look at the next section **FldArray internal structure**).

6.3.1 FldArray internal structure

Internally, a FldArray object stores its elements in a contiguous piece of memory. This memory is dynamically allocated. One can see FldArray as a convenient "wrapper" encapsulating raw C pointer-managed memory. Attribute `_data` in class FldArray points to this memory. This one-dimensional arrangement exactly matches the traditional Fortran or C arrangement.

However, it remains to choose a specific ordering between the two directions. Presently in *elsA*, the first index increases first; this choice corresponds to the Fortran way. Note that, in C++, we can turn to the other ("transpose") way quite easily: we would have to modify the implementation of exactly **one** method, leaving the class interface strictly unchanged. Instead of:

```
inline E_Float  
FldArrayF::operator()(E_Int l, E_Int fld) const  
{  
    return (_data[l + (fld-1)*_size]);  
}
```

We would have the *transpose* (or *swapped*) implementation:

```
inline E_Float  
FldArrayF::operator()(E_Int l, E_Int fld) const  
{  
    return (_data[fld-1 + l*_nfld]);  
}
```

When the *elsA* programmer uses a Fld object, he uses the public class interface, so he doesn't know how the data are actually stored and he should not be "disturbed" by any modification of the internal structure of the Fld classes. In Fortran obviously, it is another matter...

6.3.2 Examples

If called from inside a C++ method, a Fortran subroutine has first to be declared in a prototype, such as ¹:

```
extern "C"
{
void
denconvec_(const E_Int& ncell, const E_Int& neqtot, const E_Int& neq,
           const E_Int& ro, const E_Int& rou, const E_Int& roe,
           const E_Int& rog, const E_Int& roug, const E_Int& roeg,
           const E_Float* consvar, const E_Float* press,
           E_Float* fdx, E_Float* fdy, E_Float* fdz);
}
```

It is important to note that each argument is passed by address (reference for scalar, pointer for array), not by value (see **Calling Fortran subroutine**).

Then, in the C++ method, the Fortran subroutine is called by:

```
denconvec_(ncell, neqTot, nbEqMoyComp,
           rho, mom, ene, rhoG, momG, eneG,
           wCons.begin(), press.begin(),
           fdx.begin(), fdy.begin(), fdz.begin() );
```

The use of `fdX.begin()` allows to point on the beginning of the piece of memory where the values of the field `fdX` are stored. To get this address, it is convenient to use the iterator mechanism whose member functions are `begin()`, `end()`.

Notation: `fdX.begin()` stands for `fdX.begin(1)` (1 is the default value). If it is needed to manipulate the second field (corresponding to `rou`) the method `begin` has to be used with the argument 2: `fdX.begin(2)`.

It is obvious to see that if we change the two-dimensional structure choice (first index increases first), the method `begin()` will not provide the same collection of entities. In this case, and if dimensions of `fdX` are: `ncell x neq`, values of `fdX` will be stored in the following order:

```
fdX(      0,1), fdX(0,2), fdX(0,3), ..., fdX(      0,neq),
...,
fdX(ncell-1,1), ..., fdX(ncell-1,neq)
```

instead of:

```
fdX(0,  1), fdX(1,1),fdX(2,1), ..., fdX(ncell-1,  1),
...,
fdX(0,neq), ..., fdX(ncell-1,neq)
```

Finally, in the Fortran subroutine, we find the following implementation:

```
      SUBROUTINE denconvec(ncell, neqtot, neq,
&                          ro, rou, roe,
&                          rog, roug, roeg,
```

¹See also "*elsA* Coding Rules"

```
&          w, p,  
&          fdx, fdy, fdz)  
  IMPLICIT NONE  
  
C_IN  
  INTEGER_E ncell, neqtot, neq  
  REAL_E    w(0:ncell-1,neqtot) ! Conservative Variables  
  REAL_E    p(0:ncell-1)       ! Pressure  
  
C_OUT  
  REAL_E    fdx(0:ncell-1,neq) ! Convective Flux X-Component  
  REAL_E    fdy(0:ncell-1,neq) ! Convective Flux Y-Component  
  REAL_E    fdz(0:ncell-1,neq) ! Convective Flux Z-Component  
  
  [.....]  
  DO icell = 0, ncell-1  
    roi = ONE / w(icell,rog)  
  
    fdx(icell,ro) = w(icell,roug)  
    fdy(icell,ro) = w(icell,rovg)  
    fdz(icell,ro) = w(icell,rowg)  
  [.....]
```

6.3.3 Remark on Fortran convention

In the example above, the following convention has been followed in the two-dimensional array addressing:

- the first dimension index varies from 0 to ncell-1;
- the second dimension index varies from 1 to neq.

This choice has been made here in order to be the same as the C++ choice, but it is not mandatory. We could of course also write:

```
...  
  REAL_E    w(ncell,neqtot)  
  
C_OUT  
  REAL_E    fdx(ncell,neq)  
  REAL_E    fdy(ncell,neq)  
  REAL_E    fdz(ncell,neq)  
  
  [.....]  
  DO icell = 1, ncell  
    roi = ONE / w(icell,rog)  
  
    fdx(icell,ro) = w(icell,roug)  
    fdy(icell,ro) = w(icell,rovg)  
    fdz(icell,ro) = w(icell,rowg)  
  [.....]
```

7. GEO COMPONENT

GeoGrid objects are widely used in the CFD kernel, because many CFD classes need a pointer on GeoGrid objects. GeoGrid is a composition of two classes: GeoGridMetrics and GeoConnect. It is responsible for:

- **metrics**, issued from methods of GeoGridMetrics class;
- **index counting** and **position** (connectivity), issued from methods of GeoConnect class.

7.1 Ghost geometric entities

The number of ghost entities is controlled through 6 global variables:

GHOST_I1 and GHOST_I2 in the "I" direction,
GHOST_J1 and GHOST_J2 in the "J" direction,
GHOST_K1 and GHOST_K2 in the "K" direction.

elsA uses the following convention:

7.1.1 Ghost cell numbering

- GHOST_I1 ghost cells in IMIN, GHOST_I2 ghost cells in IMAX,
- GHOST_J1 ghost cells in JMIN, GHOST_J2 ghost cells in JMAX,
- GHOST_K1 ghost cells in KMIN, GHOST_K2 ghost cells in KMAX.

7.1.2 Ghost interface numbering

- GHOST_I1 ghost interfaces in IMIN, GHOST_I2-1 ghost interface in IMAX,
- GHOST_J1 ghost interfaces in JMIN, GHOST_J2-1 ghost interface in JMAX,
- GHOST_K1 ghost interfaces in KMIN, GHOST_K2-1 ghost interface in KMAX.

7.1.3 Ghost node (mesh points) numbering

- GHOST_I1 ghost nodes in IMIN, GHOST_I2-1 ghost node in IMAX,
- GHOST_J1 ghost nodes in JMIN, GHOST_J2-1 ghost node in JMAX,
- GHOST_K1 ghost nodes in KMIN, GHOST_K2-1 ghost node in KMAX.

7.1.3.1 Ghost defaultvalues

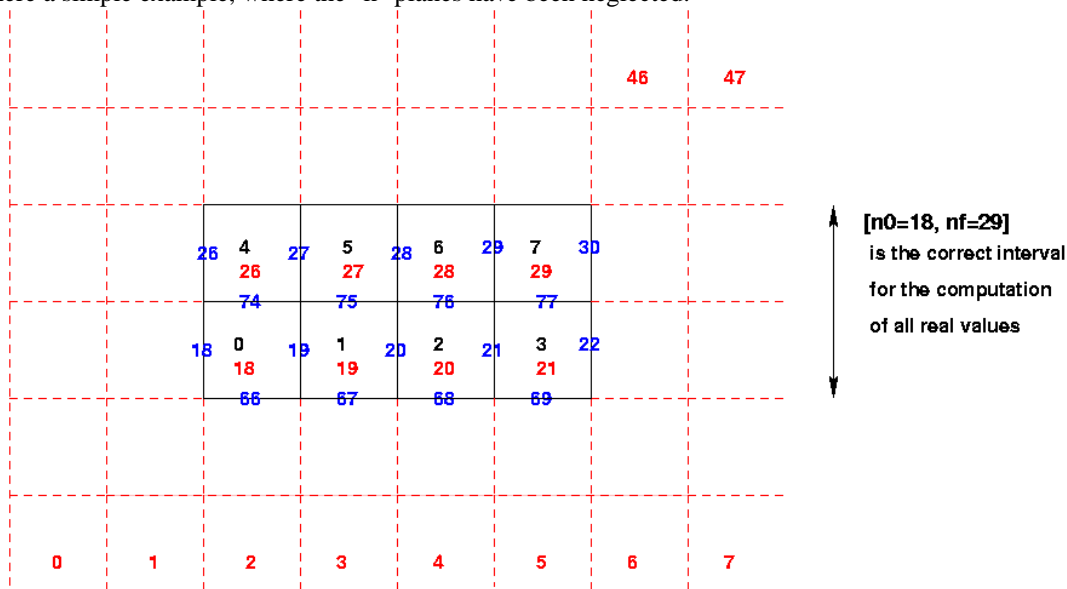
The default values are:

```
GHOST_I1 = 2; GHOST_I2 = 2;  
GHOST_J1 = 2; GHOST_J2 = 2;  
GHOST_K1 = 2; GHOST_K2 = 2;
```

Users can change these default values at the beginning of each run by calling `DesCfdPb::set_ghostcell()` (usually to reduce CPU time on some platforms).

7.1.4 Simplified example

We give here a simple example, where the "k" planes have been neglected:



- real cells numbering
- real and ghost cells numbering
- real and ghost interfaces numbering

7.1.5 Identical numbering of cell / interface / node

The benefit of this choice is that we have a simple relation between cell, interface and node indexes, which enables easy looping over cells, interfaces or nodes.

```

DO n=n0cell, nfcell           ! loop on cells
  ni1 = n                     ! "i" interface (left)
  nj1 = n + ncell            ! "j" interface (down)
  nk1 = n + 2*ncell          ! "k" interface (back)
  ....
  ni2 = n + inccell(1,0,0)    ! "i" interface (right)
  nj2 = n + ncell + inccell(0,1,0) ! "j" interface (up)
  nk2 = n + 2*ncell + inccell(0,0,1) ! "k" interface (front)

```

As a consequence of this choice, we have exactly the same number of cells, nodes, and interface in direction I, J or K (so, the total number of interfaces is three time the number of cells).

```

inline E_Int

```



```
GeoConnect::getNbCell() const
{
    return ((_im - 1 + GHOST_I1 + GHOST_I2)*
            (_jm - 1 + GHOST_J1 + GHOST_J2)*
            (_km - 1 + GHOST_K1 + GHOST_K2));
}

inline E_Int
GeoConnect::getNbInti() const
{
    return getNbCell();
}
```

7.2 Address and increment methods

The expression of the address methods is directly issued from the following points:

- by convention:
 - the first "real" (non ghost) cell corresponds to (1, 1, 1);
 - the IMIN (left) I interface of cell (1, 1, 1) corresponds also to (1, 1, 1);
 - the JMIN (lower) J interface of cell (1, 1, 1) corresponds also to (1, 1, 1);
 - the KMIN (back) K interface of cell (1, 1, 1) corresponds also to (1, 1, 1);
- ghost geometric entities have to be taken into account; for example, the indices of the two "extreme" cells are:


```
imin = - GHOST_I1 + 1; imax = im -1 + GHOST_I2;
jmin = - GHOST_J1 + 1; jmax = jm -1 + GHOST_J2;
kmin = - GHOST_K1 + 1; kmax = km -1 + GHOST_K2;
```
- data are always stored first considering the "i"-direction, then the "j"-direction, and lastly the "k"-direction;
- in the case of interfaces, we first consider the "i"-interfaces (for "i", then for "j", then for "k"), then the "j"-interfaces (for "i", "j", "k"), and finally the "k"-interfaces (for "i", "j", "k");

Address methods dealing with index counting and position, which are available in class `GeoConnect`, must be used in all the C++ kernel classes. If `im`, `jm`, `km` are the number of mesh points in the directions "i", "j", "k", then the numbering of cells, nodes, interfaces in the total grid (real + ghost entities) are:

Address methods:

```
-----
adrCell(i, j, k) = i - 1 + GHOST_I1
                  +(j - 1 + GHOST_J1)*(im -1 + GHOST_I1 + GHOST_I2)
                  +(k - 1 + GHOST_K1)*(im -1 + GHOST_I1 + GHOST_I2)
                  *(jm -1 + GHOST_J1 + GHOST_J2)

adrInti(i, j, k) = adrCell(i, j, k)
adrIntj(i, j, k) = adrCell(i, j, k) + nCell
adrIntk(i, j, k) = adrCell(i, j, k) + 2*nCell

adrNode(i, j, k) = adrCell(i, j, k)
```

Increment methods:

```
-----  
incrementCell (i,j,k) = i + j*( im-1+GHOST_I1+GHOST_I2)  
                        + k*((im-1+GHOST_I1+GHOST_I2)*(jm-  
1+GHOST_J1+GHOST_J2))  
  
increment[IJK](i,j,k) = incrementCell(i,j,k)  
                        = incrementNode(i,j,k)
```

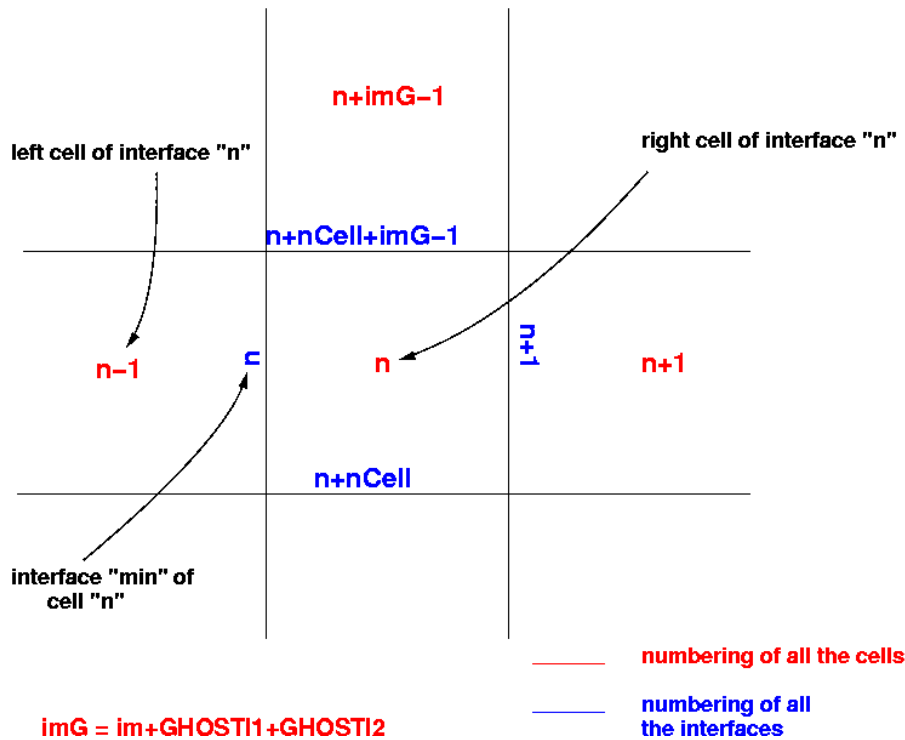
If needed inside Fortran subroutines, the following statement functions have to be used, by including the file `Geo/Grid/GeoAdrF.h`

```
INTEGER_E idummy, jdummy, kdummy  
INTEGER_E im_dummy, jm_dummy, km_dummy  
INTEGER_E adrcell, adrcellg, inccellg  
INTEGER_E adrnodeg, incnodeg  
  
adrcellg(idummy,jdummy,kdummy, im_dummy, jm_dummy, km_dummy) =  
&      (idummy-1+IFIC1)  
&      + (jdummy-1+JFIC1)*(im_dummy-1+IFIC1+IFIC2)  
&      + (kdummy-1+KFIC1)*(im_dummy-1+IFIC1+IFIC2)*  
&      (jm_dummy-1+JFIC1+JFIC2)  
  
adrnodeg(idummy,jdummy,kdummy, im_dummy, jm_dummy, km_dummy) =  
&      (idummy-1+IFIC1)  
&      + (jdummy-1+JFIC1)*(im_dummy-1+IFIC1+IFIC2)  
&      + (kdummy-1+KFIC1)*(im_dummy-1+IFIC1+IFIC2)*  
&      (jm_dummy-1+JFIC1+JFIC2)  
  
incnodeg(idummy,jdummy,kdummy, im_dummy, jm_dummy, km_dummy) =  
&      idummy  
&      + jdummy*(im_dummy-1+IFIC1+IFIC2)  
&      + kdummy*(im_dummy-1+IFIC1+IFIC2)*(jm_dummy-1+JFIC1+JFIC2)  
  
inccellg(idummy,jdummy,kdummy, im_dummy, jm_dummy, km_dummy) =  
&      idummy  
&      + jdummy*(im_dummy-1+IFIC1+IFIC2)  
&      + kdummy*(im_dummy-1+IFIC1+IFIC2)*(jm_dummy-1+JFIC1+JFIC2)
```

These methods (address and increment) allow to deal with connectivity between cells and interfaces as it is usual in finite volume formulation.

Note:

`adrcellg` (`adrnodeg`, `adrintg`) will be renamed as `adrcell` (respectively `adrnode`, `adrint`) in future releases.



7.2.1 Example: Centered convective fluxes

In this example, the loop index is an interface index. Cell flux density values are used to compute the flux interface values.

```

DO n = n0Int, nfInt
  int = n + incI
  flux(int, fld) = 1/2 * [Qx(n,fld)+Qx(n-inc,fld)]*surfx(int,1)
                    + [Qy(n,fld)+Qy(n-inc,fld)]*surfy(int,1)
                    + [Qz(n,fld)+Qz(n-inc,fld)]*surfz(int,1)
END DO

with:
interfaces "I"
-----
inc = 1 = incCell(1,0,0, im,jm,km)
incI = 0

interfaces "J"
-----
inc = im-1+GHOST_I1+GHOST_I2 = incCell(0,1,0, im,jm,km)
incI = nCell

interfaces "K"
-----
inc = (im-1+GHOST_I1+GHOST_I2)*(jm-1+GHOST_J1+GHOST_J2)
    = incCell(0,0,1, im,jm,km)
incI = 2*nCell

```

7.2.2 Example: Flux balance

In this example, the loop index is a cell index. Interface flux values are used to compute the cell flux balance values.

```
l1 = 1                      = incell(1,0,0, im,jm,km)
l2 = im-1+GHOST_I1+GHOST_I2 = incell(0,1,0, im,jm,km)
l3 = l2*(jm-1+GHOST_J1+GHOST_J2) = incell(0,0,1, im,jm,km)
```

```
DO n      = n0Cell, nfCell
  intI = n
  intJ = n +   nCell
  intK = n + 2*nCell
  fluxBal(n,nfld) = + flux(intI + l1, fld)
                   - flux(intI   , fld)
                   + flux(intJ + l2, fld)
                   - flux(intJ   , fld)
                   + flux(intK + l3, fld)
                   - flux(intK   , fld)
END DO
```

8. TUR COMPONENT

8.1 Definition of the public interface

This section details the design of the turbulence models based on the **Boussinesq hypothesis**.

The most important design activity is to identify the classes, together with their **public interface**. The UML class diagram is a very useful tool to present:

- classes;
- relations between classes;
- interfaces.

The first **analysis** stage is to identify what actions turbulence models are responsible for. The aim of turbulence models is to compute:

- **turbulent eddy viscosity**;
- **total stress tensor** (viscosity tensor + Reynolds tensor) used in momentum and energy equations;
- possibly other **quantities** needed **for the integration of transport equations** (source terms, coefficients for the computation of the density of the diffusive turbulent fluxes).

Moreover, the design solution must allow association of **transition** with any turbulence model.

More precisely, depending on algebraic model or transport equation model, we have to distinguish which computations have to be made and how they can be made :

- for algebraic models, the computation of the eddy viscosity only requires the knowledge of the conservative variables and the distance to wall;
- for turbulence models using transport equations, a system of equations must be integrated. Source terms, additional coefficients needed to compute the diffusive fluxes, and also eddy viscosity have to be computed.

This analysis shows that the **public methods** of the turbulence component **interface (Object-Oriented Programming Concepts)** are:

1. compute the eddy viscosity;
2. compute the total stress tensor;
3. apply transition.

Methods 2 and 3 can be defined in the same way whatever turbulence model; conversely, it is clear that the eddy viscosity implementation depends on the model.

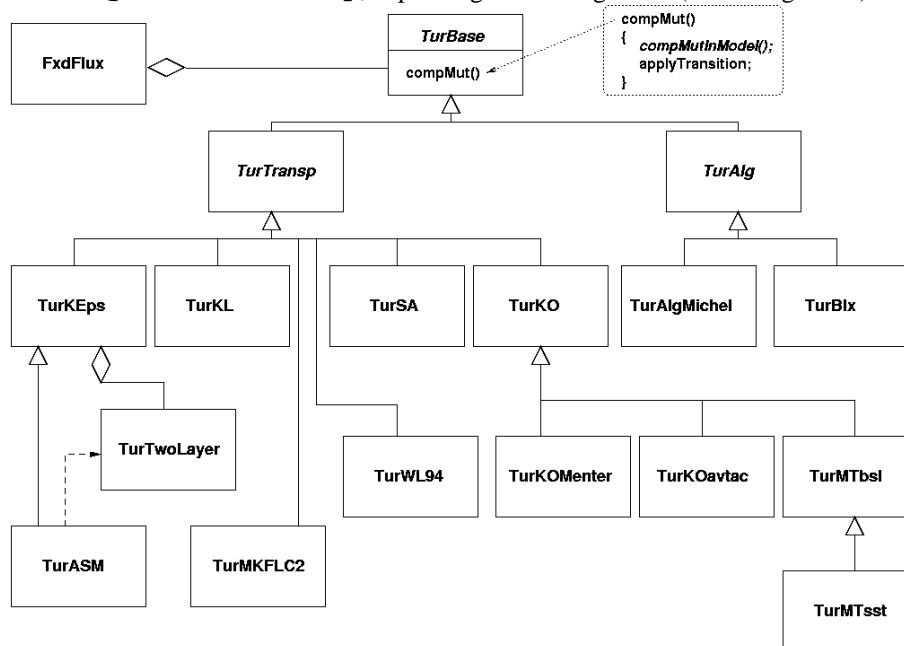
8.2 Class model

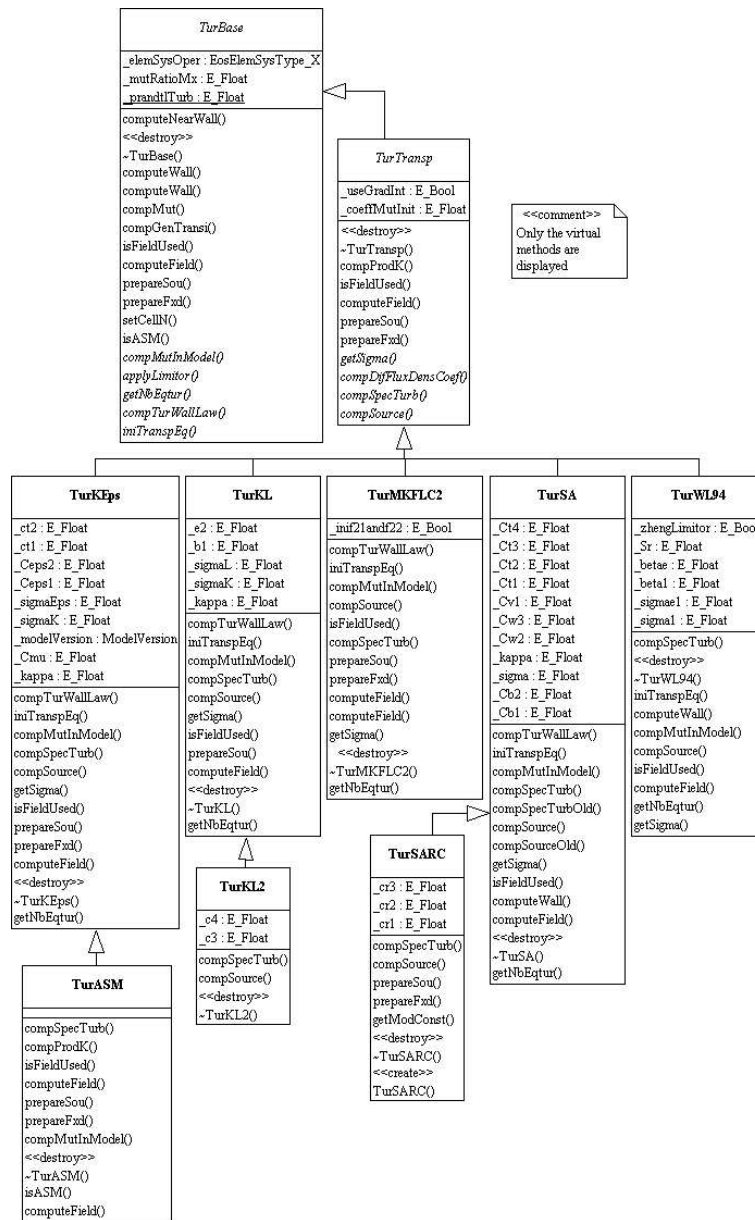
Finally, we obtain the following UML class diagram which presents a **tree hierarchical structure** organization:

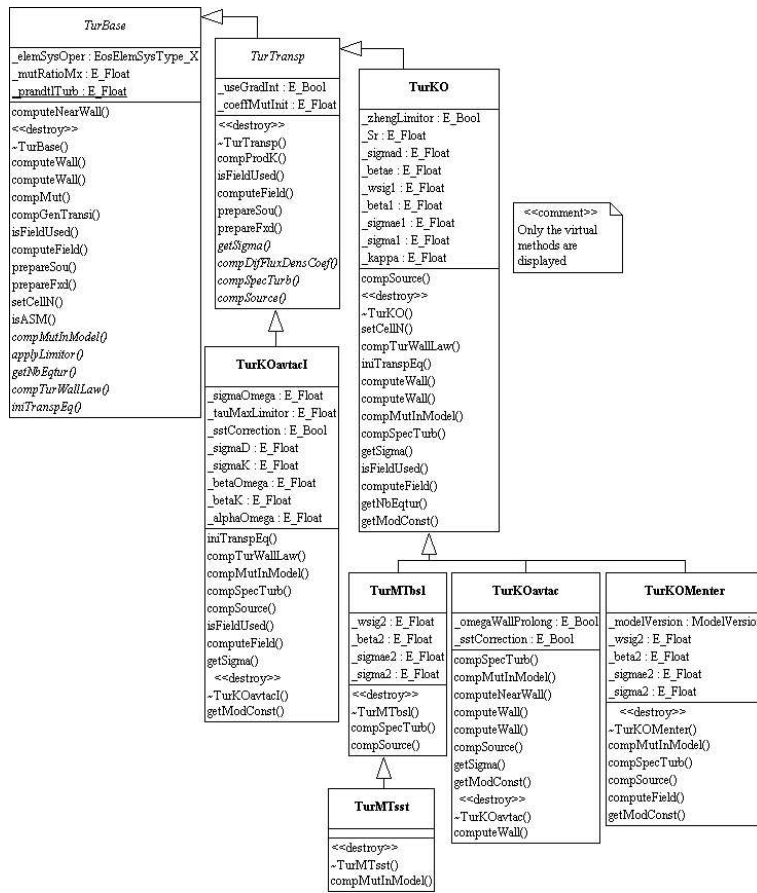
- TurBase is the base abstract class; its interface declares:
 - the **pure virtual** method `compMutInModel()`;

- the **concrete** (non virtual) method `compMut()`;
 - the **concrete** method `compDiffFluxDens_gradCen()`.
 - the **concrete** method `applyTransition()`;
- `TurAlg` is the base class for algebraic turbulence models; the derived classes provide the eddy viscosity computation (`compMutInModel()`);
 - `TurTransp` is the base class for transport equation turbulence models; the derived classes provide methods to compute the source terms (method `compSource()`), the coefficients needed to compute the turbulent diffusive fluxes (`compDiffFluxDensCoef()`) and the eddy viscosity (`compMutInModel()`).

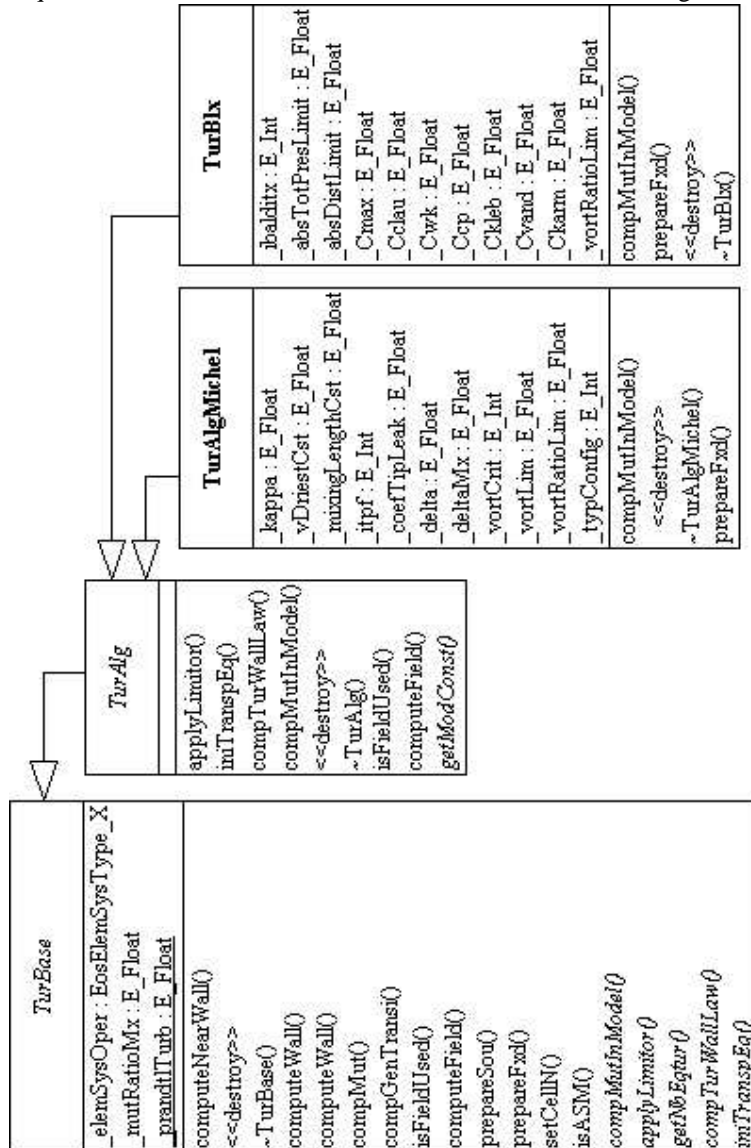
The actual turbulence models correspond to concrete classes. All the concrete classes belonging to the `Tur` component inherit either from `TurAlg` or from `TurTransp`, depending of their algebraic (or non algebraic) nature.







for the transport equations turbulence models, and for the algebraic turbulence models.



8.3 Polymorphism in turbulence modeling

All the classes deriving from the abstract class TurBase share its interface, which declares method compMut ().

In elsA, the client classes of the turbulence models are the diffusive fluxes (Fxd) and the time integration algorithm (Tmo); Tur (the provider) and Fxd (the client) interact using "messages" as for example:

```
_tur->compMut (...);
```

where _tur is an attribute of type TurBase* belonging to this Fxd object. TurBase::compMut () is a concrete method which consists of two stages:

```
TurBase::compMut ( )
{
```

```

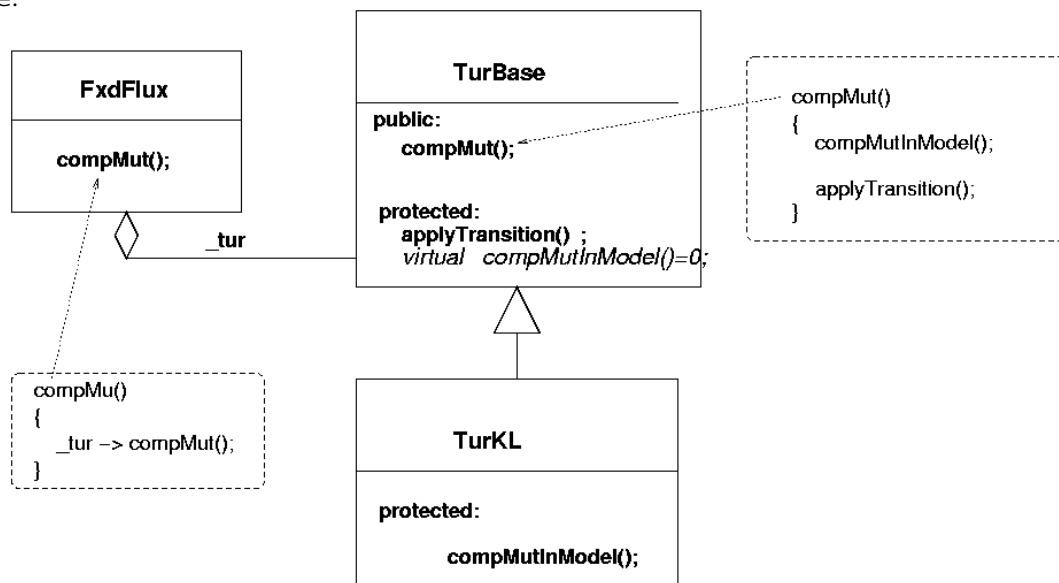
compMutInModel();
applyTransition();
}

```

If transition has to be taken into account, the method `applyTransition()` applies the intermittency function on the eddy viscosity, in a uniform way for all the models. The method `applyTransition()` is then a concrete method implemented in `TurBase`. Conversely, computation of the eddy viscosity depends on each particular turbulence model, and cannot be implemented in the `TurBase` abstract class.

When manipulated in term of this abstract interface defined by `TurBase`, the concrete classes have not to be known by the client classes. Client classes are only aware of abstract class.

Polymorphism allows the correct version of `compMutInModel()` to be called dynamically, without any explicit "switch" coding by the programmer. In the example discussed in the preceding sections of the `Fxd/Tur` interaction through the method `compMut()`, the client manipulates a pointer (or a reference) to an instance of a class derived from `TurBase`.



As a consequence, adding a new turbulence model will not modify the code of the client class.

8.4 How to introduce a new turbulent model?

8.4.1 Use of inheritance

Object-Oriented technology greatly facilitates the introduction of a new turbulence model. The developer does not have to have full knowledge of the whole `elsA` kernel. Instead, he can focus on a small number of well-defined tasks:

- introduce a new class in the turbulence hierarchy, deriving from a base class:
 - deriving from `TurTransp`, if it is a new transport equation model;
 - deriving from `TurAlg`, if it is an algebraic model;
 - or even deriving (specializing) from from an existing "leaf" concrete class, let's say `TurKL`, to test some *specialized* `TurKL` variant.
- implement a small number of virtual methods;
- additionally, to ease implementation, it may be useful to introduce new private methods and/or attributes.

Hence, OO programming provides a simple framework, allowing the programmer to work in a faster and safer way.

It remains to be seen how turbulent objects are created. This is fully discussed in section **Factory component**.

9. OPER COMPONENT

Operator classes are dedicated to the computation of space discretization terms. Every operator has to compute a `FldFieldF` object defined upon a specific geometric entity (cell or interface). This chapter is dedicated to all operators in *elsA*:

- `Oper`: Abstract classes;
- `Fxc`: Convective fluxes (centered scheme, upwind schemes and artificial dissipation);
- `Fxd`: Diffusive fluxes (laminar, mean flow or turbulent);
- `Sou`: Source terms (turbulence closure relations, moving frame, dual time stepping method).

9.1 Oper Module

9.1.1 *OperBase* abstract class

The general operator mechanism is defined inside `OperBase` class. Important attributes of `OperBase` are:

- `_geoEntity`: type of geometric entity where the computation has to be carried out;
- `_borderDepth`: width of the "border" region. The numerical treatment of an operator is performed on all cells or interfaces, using the same numerical scheme on all geometric entities. The "interior" region of the operator is the set of the geometric entities where this "current entity" treatment is directly correct. The "border" region is the set of geometric entities where a numerical adaptation (correction) has to be made because of the boundary neighborhood.
- `_elemSysOper`: identifier of the system of equations.

The other attributes of this abstract class are pointers:

- `EosSysEq* _sysEq`: current description of the problem;
- `EosIdealGas* _eos`: current equation of state;
- `GeoGridBase* _grid`: current working computational grid.

An operator has to work on different contexts (different grids, thermodynamic model, ...), so an `Oper` object cannot be fully configured at construction time. Instead, when context changes, it must be re-initialized in such a way that it can work correctly. This is precisely the job of `OperBase::prepare()`, whose signature is:

```
virtual void prepare(const EosSysEq&, EosElemSysType,  
                    EosIdealGas* eos, const GeoGridBase* grid);
```

The method implementation is very simple: it reduces to proper (re-)settings of the class pointer attributes.

We must clearly distinguish two different operator subtypes, both inheriting from `OperBase` class:

- `OperTerm` is responsible for the computation of one 'right hand side' term;
- Utility operators are used to perform auxiliary computations; they are usually called by `OperTerm` objects. Up to now, only two gradient operators have been implemented: `OperGrad` and `OperGradInt`.

9.1.2 OperGrad class

OperGrad and OperGradInt inherit from OperBase. OperGrad class provides with the implementation of the computation of gradients on cell centers, whereas OperGradInt provides with the implementation of the computation of gradients on interface centers. These operators do **not** own the result of their computation:

- They don't have more attributes than OperBase.
- They only compute gradients with two overloaded versions of `compute()`, whose signature are:

```
// compute the gradient of the conservative variables
void compute(      FldCellF&      fldOut,
                 const list<BndPhys*>& listBnd,
                 const list<JoinBase*>& listJoin,
                 AuxField          identOfField = MISC);
```

and:

```
// compute the gradient of non conservative variables (?)
virtual void compute(      FldCellF&      fldOut,
                          const list<BndPhys*>& listBnd,
                          const list<JoinBase*>& listJoin,
                          const FldCellF&      fldIn,
                          AuxField          identOfField);
```

The gradient or flux computation is performed on all cells or interfaces using the same numerical scheme, in the interior and the border region. The standard formula may give wrong results (or even produce arithmetic exception) for the border computation. So, operator objects must collaborate with boundary objects. This collaboration can take two different forms (called Strategy 1 and Strategy 2, see also 10.1):

- **Strategy 1:** computation in two stages: Gradient or flux computation is performed on all cells or interfaces, including those from the border region. Then, special formula are used to correct the computation on the border region, taking into account the boundary treatment. OperGrad uses this strategy.
- **Strategy 2:** computation in only one stage: Ghost cells are filled by boundary objects, before the gradient computation, such that the standard formula will give the correct result. Within this strategy, there is no need to use special formula to correct the computation on the border region. OperGradInt uses this strategy.

9.1.3 OperTerm abstract class

Most of the time, an operator needs to compute some auxiliary fields before the final computation of fluxes or source term (for example, the pressure field has to be computed to complete the centered convective flux computation). So, the stage "Computation of an OperTerm" is split into two sub-stages:

1. computation of all the required auxiliary fields (by means of the conservative variables),
2. computation of fluxes or source terms (using these auxiliary fields).

Auxiliary fields which have to be computed before flux or source term computation have to be identified. A specific attribute, `OperTerm::_setOfIdent`, of type `list<AuxField>`, is introduced to store auxiliary field identifiers. The method:

```
virtual
void computeAllField(const list<BndPhys*>* listBnd = E_NULLPTR,
                   const list<JoinBase*>* listJoin = E_NULLPTR);
```

calls the `computeField()` method for each auxiliary field registered by `_setOfIdent`. Operators compute each registered field through a call to `computeField()`:

```
virtual
void computeField(AuxField          identOfField,
                  const list<BndPhys*>* listBnd = E_NULLPTR,
                  const list<JoinBase*>* listJoin = E_NULLPTR);
```

`computeField()` is pure virtual and **must** be implemented by concrete operators.

Fluxes or source term computation are not implemented at this level. This is discussed in the next sections.

9.1.4 *OperFlux abstract class*

`OperFlux` inherits from `OperTerm`. It implements the major computational method `compute()` according to Strategy 1:

```
void OperFlux::compute(      FldIntF&          fldOut,
                             const list<BndPhys*>& listBnd,
                             const list<JoinBase*>* listJoin )
{
    compFlux(...);
    computeAllBorders(...);
}
```

This class defines the signature of one of the most important methods of every flux concrete operator:

```
virtual void compFlux(const FldCellF& fldIn,
                     FldIntF& fldOut) = 0;
```

Knowing the conservative variables on cell centers, this method provides with the flux values on the interfaces (interior and border region) of the operator.

The `OperFlux` class supplies also another important method: `computeAllBorders()`. The goal of this method is to compute flux values on all interfaces of the border region taking into account the boundary conditions. For every physical boundary, the following scenario is used:

1. the computation of the vector `wb1` of conservative variables defined on boundary interfaces is delegated to the `BndPhys*` object responsible for the boundary under consideration;
2. `wb1` is then used to correct the flux computation on the interfaces of the border of the operator. The implementation of this last stage is dependent on the concrete flux operator under consideration. Generally, it uses modified formulas issued from the standard treatment.

9.1.5 *OperSou abstract class*

`OperSou` is an abstract class for source terms. This class inherits from `OperTerm` class.

9.2 Fxc Module

The `Fxc` module gathers the concrete centered and upwind convective operators and the artificial dissipation operators.

9.2.1 Centered convective operators

In *elsA*, the centered convective discretization is written as the sum of a simple centered discretization and a numerical dissipation term. `FxcCenter` class inherits from `OperFlux` class, and provides with the implementation of the convective centered fluxes. The `compFlux()` method is implemented in `FxcCenter`, so that:

- `FxcCenter` is able to compute the convective centered flux for mean flow or turbulent system,
- `FxcCenter` is able to compute the convective centered flux according to divergence form or a skew-symmetric form.

However, since `computeOneBorder()` is not implemented in `FxcCenter`, `OperFlux::computeOneBorder()` is used.

To perform the flux computation on all interfaces, for the divergence form, flux density evaluated at cell centers is computed. In case of skew symmetric form, flux is computed directly on interfaces.

9.2.2 Dissipative operators

In the resolution of the mean flow system, one can choose between scalar artificial dissipation flux (class `FxcScaNumDiss`), or matrix artificial dissipation flux (class `FxcMatNumDiss`). `FxcScaNumDiss` class defines new implementations of both `compFlux()` and `computeOneBorder()`.

In the resolution of the turbulent system, *elsA* kernel provides two operators to implement the artificial dissipative term:

- `FxcRoeCorr`, based on `MinMod` limiter and Harten's entropy correction;
- `FxcScaNumDiss` is only available for the Spalart-Allmaras turbulent model.

9.2.3 Upwind convective operators

`FxcUpwind` inherits from `OperFlux` class, and has two important attributes:

- `FxcLimiter_limiter`: limiter function to complete MUSCL extrapolation for second order schemes;
- `FxcConvFunc*_convFunc`: the convective function which, given left and right states compute convective fluxes on interfaces.

The strategy used for the computation is close to Strategy 2. `FxcUpwind` defines a new implementation of the `compute()` method:

1. Primitive variables are computed from conservative variables,
2. Left and right values at the cell boundaries are evaluated, taking into account the boundary condition at each side of a boundary interface. If necessary (spatial second order accuracy calculations), a linear approximation of the solution on each cell is used in the projection stage, using slopes and non-linear limiters.
3. Finally, the upwind scheme is applied using the convective function.

9.3 Fxd Module

The `Fxd` is responsible for diffusive flux computations. All the classes of the `Fxd` module inherit from `OperFlux` class.

9.3.1 Diffusive flux operators for mean flow or turbulent system

The classes in charge of diffusive fluxes computation are:

- `FxdLaminar` or `FxdLaminarInt`: computes the dissipative fluxes for a Navier-Stokes laminar (no turbulence) problem;
- `FxdTurMeanFlow` or `FxdTurMeanFlowInt`: computes the dissipative fluxes of the mean flow system for a Navier-Stokes turbulent problem;
- `FxdTurTurbVar` or `FxdTurTurbVarInt`: computes the dissipative fluxes of the turbulent variable system for a Navier-Stokes turbulent problem.

For turbulent problems, the flux density evaluation is delegated to `Tur` objects. For this purpose, these operators own an attribute, `_tur`, of type `TurBase*`.

9.3.2 Diffusive flux operators with different kind of gradients

The flux density evaluation needs the computation of gradients. All operators of the `Fxd` module are direct users of the gradient operators presented above. Two kinds of gradient operators can be used to evaluate the flux density: `OperGrad` to compute gradients on cell centers, or `OperGradInt` object to compute gradients on interface centers. `FxdFlux` and `FxdFluxInt` are abstract classes which are respectively user of `OperGrad` and `OperGradInt` objects.

All of these operators use Strategy 1, and provides with an implementation of `compFlux()` and `computeOneBorder()`.

9.4 Sou Module

All the classes of the `Sou` Module inherit from the `OperSource` class.

- `SouDts` class is responsible for source terms associated with Dual Time Stepping (DTS) method. It gives a specific implementation of the `compute()` method. Here, no distinction is done between the interior and the border region.
- `SouTransp` class is responsible for source terms associated with transport equation of turbulence model. It gives a new implementation of the `compute` method, but delegates the computation to `TurTransp` objects.
- `SouRelFrameAbs` and `SouRelFrameRel` classes responsible for source term associated with relative frame and respectively absolute or relative velocity formulation.

9.5 How to introduce a new operator?

The developer does not have to know the whole *elsA* kernel. Instead, he can focus on a small number of well-defined tasks:

- Introduce a new class in the `Oper` hierarchy, deriving from a base class (for example deriving from `OperFlux`, if it is a new flux operator).
- Define the auxiliary field(s) required, and implement the method to compute it (them).
- Implement a small number of virtual methods:
 - `compute()`;
 - `compFlux()`;

- `computeOneBorder;`
- `computeField();`
- Additionally, it may be useful to introduce new private methods and/or attributes.

10. BND COMPONENT

The `Bnd` module is dedicated to the treatment of the physical boundary conditions.

The "join" boundaries, associated with the matching of two grids are not considered in this module, but in **Join component**.

This chapter is dedicated to two boundary types:

- "Simple" boundary: associated with a single window;
they can express physical properties imposed by underlying physical problem: adiabatic or isotherm wall, symmetry, inlet, outlet, etc...
- "Global" boundary: associated with a group of windows;
such an object must be able to express the coupling imposed on several grid objects through some constraints.
Presently, different types of global boundaries are implemented in *elsA* (imposed flow rate, multistage turbomachinery boundary,...).

Boundary objects are heavily used during the iterative loop to implement boundary conditions. They are also useful for post-processing.

10.1 Boundary treatments

10.1.1 Introduction

Thanks to ghost entities, flux objects compute flux values on all interfaces¹ using exactly the same numerical scheme, in the *interior* and the *border* region, and without any help of indirection. It could seem obvious that using ghost entities should allow to take into account boundary conditions without any need of a specific computation of the *border* region of a flux operator.

However precautions have to be taken; let us come back to the strategy in the case of a centered flux computation (Strategy 1). In that case, the strategy is made of the three following steps:

- Step 1: ghost cell values are filled by the boundary conditions:
 - (a) each boundary condition computes a state `wb1` in the center of the boundary interfaces of the considered boundary;
 - (b) this state `wb1` is extrapolated (zero-ordered) in the cells adjacent to the boundary.
- Step 2: operator performs flux computation in the cells including some ghost cells.
During this phase fluxes on border interfaces are computed, taking into account values in these ghost cells.
- Step 3: border fluxes are corrected; for that, the operator asks for the state `wb1` to each boundary condition; this state is then used in the border flux computation.

10.1.2 Discussion

The third step of this strategy could appear useless and time consuming.

In fact, for certain flux variant (skew-symmetric form convective term), it would be possible to avoid the specific border flux computation provided that the suitable extrapolation has been made during the ghost cells filling phase. In the case of skew-symmetric convective flux, such a suitable extrapolation should fill the ghost cells with:

¹except for a few ghost interfaces at the beginning and at the end

2. * $wb1 - w0$

where $w0$ is the conservative state in the real cell adjacent to the considered boundary.

But several problems could appear:

- values extrapolated in ghost cells are not necessary physically correct (ex: negative values of pressure or temperature);
- ghost cells filling would depend on the considered flux operator.

In conclusion, this third step allow to control the flux computation on border interfaces, what is fundamental in viscous computations.

In the following, we will note $wCons$ the object of type `FldCellF` storing the conservative variables in cell centers. We will discuss the two virtual methods `compBoundaryValues()` and `compBoundaryValuesInGhost()`.

10.1.3 Additional details

In order to perform Step 1, each boundary class has to implement the virtual method:

```
void compBoundaryValuesInGhost(FldCellF& wCons);
```

where $wCons$ is used both as input and output. This can be considered as a "preparation" stage to the flux computation.

Step 3 consists of two stages:

1. Knowing the conservative variables on all integration grid points (centers of cells), `compBoundaryValues()` computes $wb1$. Each boundary condition has to implement the following method:

```
void compBoundaryValues(const FldCellF& wCons,
                       FldIntF& wb1 )
```

2. Immediately after the computation of $wb1$, a second stage is performed in order to correct the flux values on the border interfaces:

```
void OperFlux::computeOneBorder(const FldCellF& wCons,
                                BndType bndType,
                                const GeoWindowStruct& window,
                                const FldIntF& wb1,
                                FldIntF& fldOut)
```

where:

- $wb1$ is given as input to compute "border" fluxes,
- the flux field: `fldOut` is corrected on the boundary interfaces using $wb1$.

So, whatever the flux values were on the "border" interfaces, these values are replaced by new ones.

10.2 Public interface, class model and polymorphism

This paragraph is quite similar to subsection **Class model** (in chapter **Tur component**) describing the design of turbulence models.

Both cases illustrate the subsection **Inheritance** (in chapter **What is Object-Oriented software?**) which introduces the concept of polymorphism and inheritance.

Following the previous section, Bnd concrete classes have the responsibility to implement the two methods declared in the abstract base class BndPhys by:

```
virtual void compBoundaryValues(const FldCellF& fld,  
                                FldIntF& wbl ) = 0;
```

corresponding to the treatment of Step 3, and

```
virtual void compBoundaryValuesInGhost(FldCellF& fld);
```

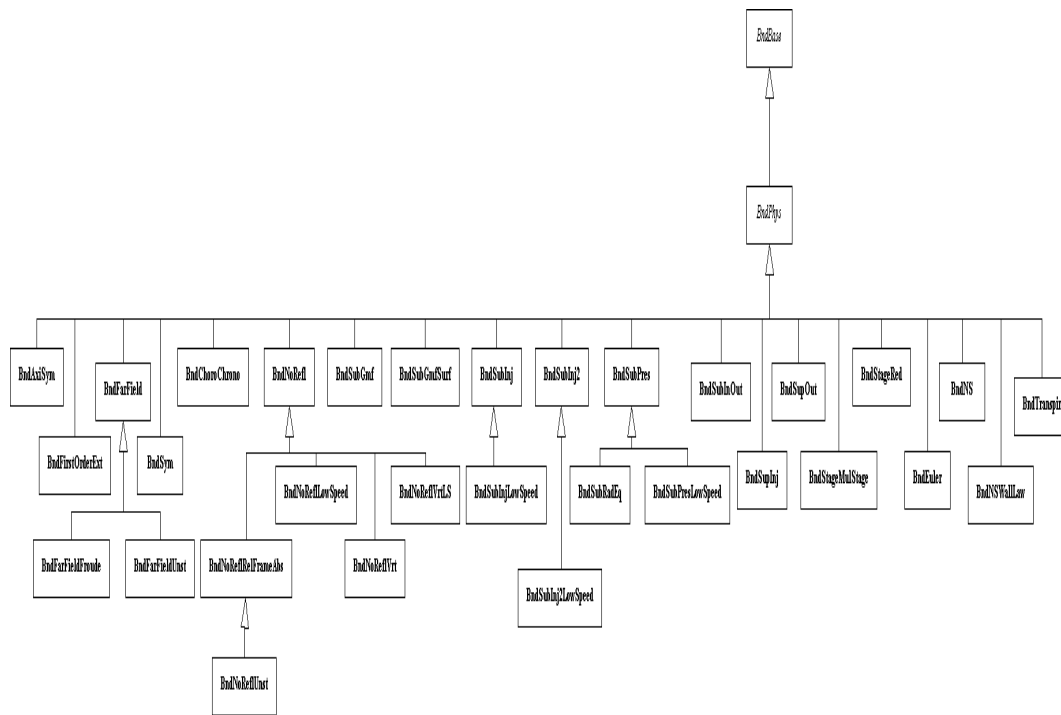
corresponding to the treatment of Step 1.

These two methods define the polymorphic behaviour of the abstract class BndPhys.

BndPhys proposes a default implementation for the second method, which consists of a simple 0-order extrapolation of wbl in the ghost layer cells.

All the classes deriving from BndPhys implement the first method and, if necessary, the second one.

Finally, we obtain the UML class diagram which presents the traditional tree hierarchical structure organization:



Bnd module contains a fairly important number of classes, each of one dedicated to a specific type of boundary condition.

Let us describe for example BndSubPres class, which deals with a " pressure downstream " subsonic boundary.

This type of boundary condition is associated with the resolution of a system of equations composed of four characteristic relations and of imposed pressure condition.

Therefore, the BndSubPres class includes a local implementation of the compBoundaryValues() method taking into account:

- the s-state (wbs) given by the method createSchemeValues() which computes predicted values (referenced by "scheme vales" or "s-state" in the Theoretical Manual) of conservative variables on the boundary;

in fact, vales on the interface are obtained by some kind of extrapolation from the interior of the domain;

- the 0-state (`wb0`) given by the method `compLinearisationValues()` which computes values of conservative variables (referenced by "0-state" in the Theoretical Manual) for linearization of characteristic relations; these values are often chosen as the scheme values, but the coding of this subroutine allows the use of an other set of values;
- the imposed boundary pressure: `_pres`.

The implementation is then:

```
void
BndSubPres::compBoundaryValues(const FldCellF& fld,
                               FldIntF&  wbl)
{
    E_Int intNbB    = _window.getNbInt();
    E_Int nint      = _grid.getNbInt();
    E_Int eqNb      = wbl.getNfld();

    FldIntF wbs(intNbB, eqNb);
    createSchemeValues(fld, wbs);
    FldIntF* wb0 = compLinearisationValues(&wbs);

    wbpres_(intNbB, nint,
            _window.getIndicBorder().begin(),
            eqNb,
            wb0->begin(), wbs.begin(), wbl.begin(),
            _pres->begin(),
            _grid.getSurf().begin(), _grid.getSurfNorm().begin(),
            _sens, _eos.getGamma());
    if (eqNb > 5)
    {
        for (E_Int eqInd = 6; eqInd <= eqNb; eqInd++)
        {
            E_Float* ptwbl = wbl.begin(eqInd);
            const E_Float* ptwbs = wbs.begin(eqInd);
            for (E_Int lint = 0; lint < intNbB; lint++)
                ptwbl[lint] = ptwbs[lint];
        }
    }
}
```

Boundary conditions have several client classes:

- the "right hand side" (`Rhs`) which calls the `compBoundaryValuesInGhost(FldCellF& fld)` method as a "preparation" stage to the flux computation;
- the "operators": fluxes (`OperFlux` class) and gradients which call the `compBoundaryValues(const FldCellF& fld, FldIntF& wbl)` method in order to apply the boundary condition on boundary interfaces before computing fluxes or gradients on "border" interfaces;
- the LUSSOR implicit method, time step computation and artificial dissipation which need the boundary values of the conservative variables to compute the convective spectral radius.

For example, OperFlux (the client) and Bnd (the provider) collaborate to compute fluxes on all the interfaces (see Step 3) in the following way:

```
void OperFlux::compute(      FldIntF&          fldOut,
                          const list<BndPhys*>& listBnd,
                          const list<JoinBase*>* listJoin )
{
  [...]
  // 1. Compute interior flux values:
  // fldIn : conservative variables (in cell centers)
  // fldOut: flux (cell interfaces)
  compFlux      (fldIn, fldOut);
  [...]
  list<BndPhys*>::const_iterator itr;
  for (itr=listBnd.begin();itr!=listBnd.end();itr++)
  {
    [...]
    // 2.a Compute border conservative variables:
    // (*itr) points to a boundary object
    // wbl stands for the conservative variables on boundary interfaces
    (*itr)->compBoundaryValues(fldIn, wbl);
    // 2.b Compute border flux values:
    computeOneBorder(fldIn, (*itr)->getBndType(),
                    window, wbl, fldOut);
    [...]
  }
}
```

OperFlux is here only aware of abstract class BndPhys.

But polymorphism allows the correct behaviour of the concrete boundary condition to be taken into account, calling dynamically the correct version of compBoundaryValues() for each concrete boundary condition pointed by the pointer (*itr) of the list listBnd.

10.3 How to introduce a new boundary condition?

10.3.1 Use of inheritance

It may happen that developers will have to add a new boundary treatment, say BndDev01, to Bnd module. This is basically a simple task:

- The definition of the new class must be written, say in the file Bnd/Phys/BndDev01.h.

Starting from an existing "similar" class, this stage should be relatively easy.

In most cases, we only have to adapt the specific attributes of the new class.

Examples of specific attributes:

```
BndNS::_tWall          // wall temperature
BndTranspir::_viw     // attribute for transpiration condition (Wall)
BndSubInj::_pa        // imposed boundary quantities
BndSubInj::_ha        // (total pressure, total enthalpy,
BndSubInj::_do[xyz]   // velocity directions)
```

- A constructor, `BndDev01::BndDev01` must also be coded.
The specific attributes of the class must be initialized by the constructor.
- A virtual destructor must be coded. In most cases, the new class will not call the new operator, and the destructor implementation reduces to:

```
BndDev01::~~BndDev01() {;
```

- `BndDev01::compBoundaryValues()` must be implemented.
Inside this method, it may be convenient to call a Fortran subroutine to perform the numerical computations for numerical efficiency.

It may also be useful to introduce private methods to help with the main method coding.

Example:

```
void BndSubRadEq::compBoundaryValues(...)
{...
  compAzimutalAverage(...);           // call of private methods
  compPressureDistribution();          // "
  wbpres_(...);                         // call of FORTRAN subroutine
  for (E_Int lint = 0; lint < intNbB; lint++)
  for (E_Int eqInd = 6; eqInd <= eqNb; eqInd++)
    wbl(lint,eqInd) = (*wbs)(lint,eqInd); // wbl computation
}
```

When the preceding steps have been completed, it is wise to write a unitary test to check the code correctness (see chapter **Unitary test cases** of /ELSA/MDEV-03036).

It remains to be seen how boundary condition objects can be instantiated when needed in integration tests.

This is fully discussed in section **Factory component**.

However, the new boundary treatment is still not accessible from the *elsA* interpreter.

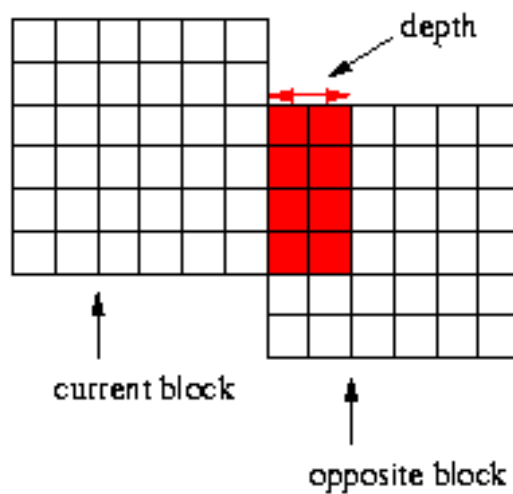
The procedure to add a new boundary treatment to the *elsA* interpreter is fully described in section 12.

11. JOIN COMPONENT

11.1 Definitions

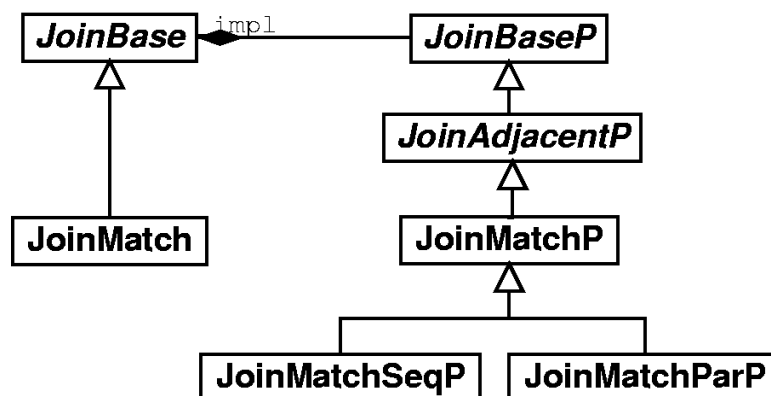
The `Join` package is responsible for the transfer of data between adjacent grids. Let us introduce some notations:

- the `current grid` is the grid receiving data;
- the `opposite grid` is the grid sending data;
- the `depth` is the number of rows of cells to retrieve.



11.2 Class diagram

11.2.1 Bridge design pattern



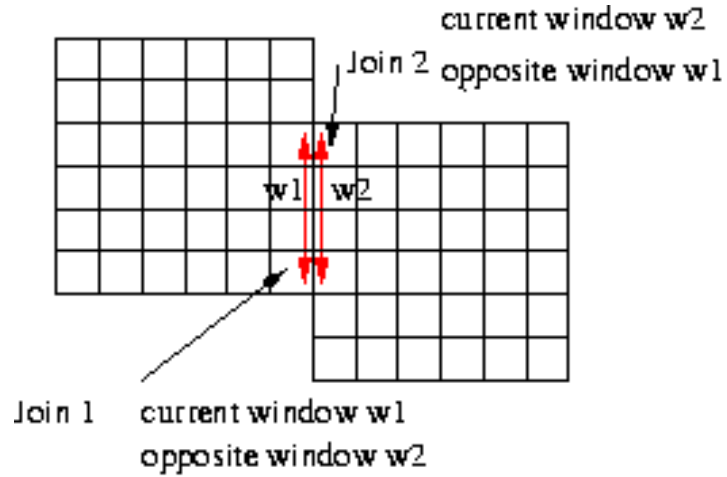
11.2.2 JoinBase

Abstract class : provides the interface for data transfer services implemented by derived concrete classes.

11.2.3 JoinAdjacent

Abstract class that provides common services for matching and near-matching join.

11.3 Characteristics



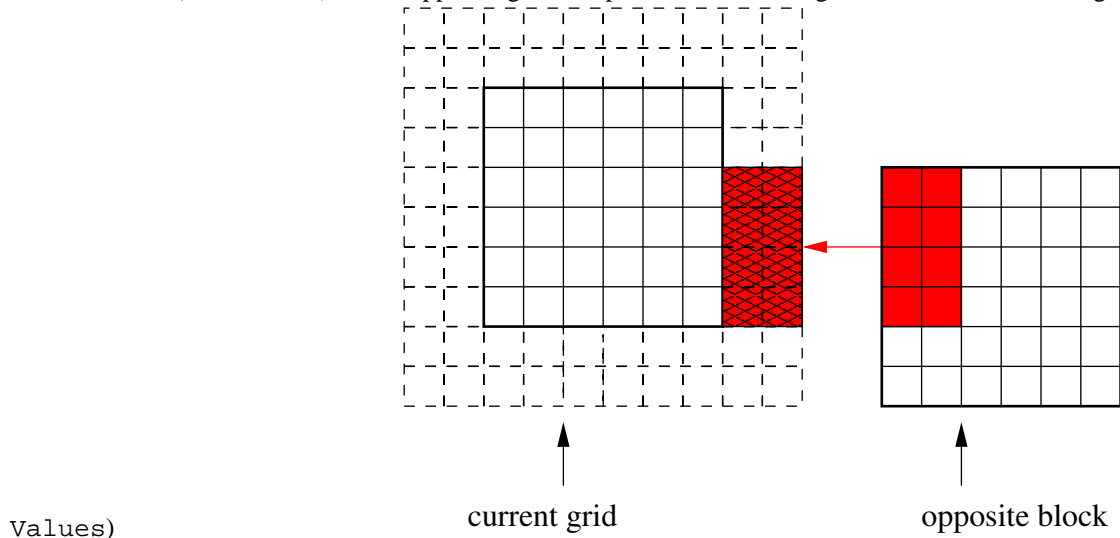
- a join per block face (or sub-face);
- sequential - multigrid - parallel;
- spatial periodicity through composition:



11.4 Interface

11.4.1 Main methods

- prepare objects before use (prepareJoin)
- retrieve values (cell,interface) of the opposite grid and put these values in ghost cells of the current grid (get -



Values)

11.5 Preparation of join for parallelism (JoinParBuffer)

11.5.1 singleton design pattern

- allocates memory for a buffer object (`JoinBufferP`);
- prepares the buffer object to send and receive data;
- holds received data until used.

11.5.2 Main methods

1. fill buffers with data to send (`pushCellField`);
2. send buffers to other processor (`sendBuffer`);
3. get received data (`getCellBuffer`);
4. delete buffers (`clearBuffer`).

11.6 Time progress

1. Send and receive conservative variables to and from other processors (`TmoSetOfSolver::fillInGhostCells()`).
2. Compute all fields (pressure, spectral radius, gradients,...) (`TmoSolverBase::prepareRhs()`).
3. Send and receive all fields to and from other processors (`TmoSetOfSolver::prepareOtherValues()`).
4. Compute fluxes (fluxes are computed using Strategy 2 *cf.* 10, since ghost cells are filled in). Each grid computes its own fluxes and conservation is ensured since values are equivalent in the two grids. (`TmoSolverBase::computeRhs()`).

11.7 Agt component (Affine Geometry Transformation)

Agt module Provides all services required to compute affine geometric transformation: permutation, translation and rotation:

- change of reference frame between current and opposite grids;
- periodicity application.

11.7.1 Change of reference frame

- **AgtIndice** is responsible for (integer) indices computations.
- **AgtFrame** deals with reference frames.

11.7.2 Example

```
AgtIndice translation(1,2,3);
```

```
AgtFrame(-2,3,1,translation);
```

```
(-2,3,1) --->  0  0  1  
               -1  0  0  
               0  1  0
```

e_i = -2 --> e_i corresponds to the -O_j axis

e_j = 3 --> e_j corresponds to the O_k axis

e_k = 1 --> e_k corresponds to the O_i axis

11.7.3 Geometric transformations

- **AgtCoord** manages coordinates (real).
- **AgtTransfo** provides a matrix transformation (rotation, translation,...).

11.7.4 Example

```
AgtCoord Point (1.1,2.2,3.3,0.0});
```

```
AgtCoord Vector (1.1,2.2,3.3,1.0});
```

12. FACTORY COMPONENT

12.1 Fact component : encapsulating object creation details

The `Fact` component is an important architectural component. It is responsible for the dynamic creation of all kernel objects involved in a CFD simulation. Starting from a description of the simulation expressed through `Descp` objects (coming from the Python script file), a small number of *factory* objects are responsible for the instantiation of all the objects required to run a CFD simulation. Basically, the work is made through simple test sequences based on attributes of specific description objects: depending upon the attribute values, a kernel object of a specific class is instantiated, and correctly initialized.

12.1.1 Factory concept

12.1.1.1 "Steady" state

A very significant advantage of OO software is that it is easy to extend through polymorphism: if client code interact with objects using only base (abstract) class interface, adding a new derived class does **not** require a modification of the existing code; the compiler takes care of the underlying switches (by calling the correct `virtual` method of the concrete `derived` class), and the client code has no knowledge of the actual object types (concrete classes).

12.1.1.2 Initialization stage

However, of course, there is no magic here: there must be somewhere in the code where specific derived class objects must be created based on some criteria. So, when the new derived class is introduced in the hierarchy, there must be some modifications. To keep the advantage of polymorphic extensibility, it is obvious that these modifications must be encapsulated in a single function (hopefully a small one), or, better, in a single class. If not, for example if clients were authorized to call derived class constructor directly, we would have simply moved the problem from the code *using* objects to the code *creating* them.

This class, the factory (`FactBase` or `FactTurb` in elsA), *knows* about all the different class of the hierarchy, and also has the information necessary to create the correct type of object. No other parts of the system need to have this information. A (usually unique) public class method defines the *interface*¹ for creating a family of polymorphic objects. Because of the unavoidable coupling between the factory and all the classes of the hierarchy, it has to be carefully designed.

This mechanism is used in elsA to instantiate objects corresponding to several important class hierarchies: `Bnd`, `Tur`, `Fxc`, `Fxd`, `Lhs` and `TmoStage`.

12.1.1.3 Creation of objects at runtime: "virtual" constructor

elsA kernel objects are created at runtime, depending of user inputs (through script files or interactive session). Information coming from the user must provide (among other things) a `type identifier`. This type identifier, which can itself be an object, helps the factory in creating the appropriate type of object. We may sum up the logic through the "object-type-object trade:

- the user information is coded in the type identifier object, which can be an integer, a string, ...
- this type identifier is exchanged (through an indirection) for the right type;

¹For example, `FactTurb::make()` for turbulent objects.

- finally, one can use this type information to call the correct constructor, and thus to get an object of the desired type.

In C++, creating objects of polymorphic types at runtime is sometimes called the "virtual constructor" technique. Note however that there is no virtual-ness here: each object creation is a block of statically bound, rigid (not virtual!) code.

12.1.1.4 A (too) simple example: choice of time integration algorithm

At runtime, depending upon the state description objects defining the simulation, the factory may choose to create either a TmoRKutta object, or a TmoFBEuler object:

```
// file Fact/Base/FactProblem.C
TmoStage*
FactBase::createAllTmoStage(TmoPbElem&    pbElem,
                           DesTimeInteg& desTimeInteg)
{ ...
  TmoStage* curStage;
  if (desTimeInteg->getS(KEY_ODE) == E_BACKWARDEULER)
    curStage = createTmoFBEuler();
  else if (desTimeInteg->getS(KEY_ODE) == E_RK4)
    curStage = createTmoRKutta(desTimeInteg);
  else
    DefError error(2115); error++; error.raiseError(); // Error

  pbElem.setTmoStage(*curStage);

  return curStage;
}
```

Here the type identifier is a string (E_BACKWARDEULER or E_RK4). To every concrete class (here TmoFBEuler and TmoRKutta) is associated a creation function (createTmoFBEuler and createTmoRKutta), whose main task is to call the corresponding constructor. Instead of calling directly class constructors, objects are created using these creation functions. Typically, the creation functions look like

```
Derived* createXXX(...)
{
  ...
  return new Derived(...);
}
```

Note:

This code assumes that covariant type return is supported by the compiler. We can encapsulate this:

```
#ifndef E_NO_COVARIANT_RETURN
Base* createXXX(...)
#else
Derived* createXXX(...)
#endif
{
  ...
  return new Derived(...);
}
```

12.1.1.5 Refinement of the Factory design

The previous example works perfectly well, and is probably well adapted when the class hierarchy does not change a lot. However, the design has some flaws:

- It performs a `switch` based on a type tag, with the associated drawbacks: to add a new class, we still have to *modify* code (here, implementation of method `createTmoStage()`), not just *add* new code.
- It introduces "magic" values directly inside compiled code (here two strings, `E_BACKWARDEULER` and `E_RK4`).

The following sections discuss several design improvements.

12.1.2 Factory design

To remove these disadvantages, we have implemented a more "advanced" design for the `Bnd`, `Oper` and `Tur` hierarchy. The basic idea is to use pointers to functions: the factory keeps a collection of pointers to (creation) functions (with identical signature), each function being responsible of the creation of objects of a single concrete type. Using free creation functions (instead of class methods) simplify the pointer to function management. The connexion between type identifier and pointer to function is implemented through an associative container object, that is, a `map`. The `map` object, which can be viewed as a dictionary, stores pairs of (`key`, `value`), where `key` is the type identifier and `value` is the pointer to creation function.

12.1.2.1 Choice of a unique type for type identifier

We decide to use `string` (`TbxString`) as the type of type identifier; the obvious value associated to the class `SomeClass` is of course the string object `string("SomeClass")`. With this choice, we solve the problem of finding a unique identifier; Using integers for type identifiers would lead to the difficult problem of finding a unused value for every new class.

12.1.2.2 Introduction of some typedefs

To simplify notations, we introduce some `typedef`; for exemple, for the `Tur` and `Bnd` hierarchies:

```
class FactBase
{
    ...
    /** Pointer on "Virtual" constructor of the Turbulence model */
    typedef TurBase* (*PtrVirtConsTur)(const DesNumSpaceDisc&,
                                       const DesModel&,
                                       const DesBlock&,
                                       GeoGrid& grid,
                                       vector<GeoWindowStruct*>&,
                                       vector<GeoWindowStruct*>&,
                                       vector<GeoWindowStruct*>&,
                                       vector<FldIntI>&,
                                       E_Float );

    /** Pointer on "Virtual" constructor of the BndPhys */
    typedef BndPhys* (*PtrVirtConsBnd)(const DesBoundary&,
                                       const DesBlock&,
                                       const DesNumerics&,
                                       const EosIdealGas&,
                                       TurBase*,
```

```
const GeoGrid&,
E_Int);

/** Type identifier */
typedef TbxString TurTypeId;
typedef TbxString BndTypeId;

/** map of Tur virtual constructors */
typedef map<TurTypeId, PtrVirtConsTur> DicoTur;
typedef map<BndTypeId, PtrVirtConsBnd> DicoBnd;
...
}
```

The factory owns dictionaries, `_allTurCtor`, `_allBndCtor`;

```
static DicoTur _allTurCtor;
static DicoBnd _allBndCtor;
```

Each entry is a pair resulting from the association of a name and a (pointer to) function. To every new turbulence class or new boundary condition class corresponds a new entry in this dictionary:

```
(ClassId, createClassName)
```

12.1.2.3 Register a new turbulence model class

The factory is *scalable* because you don't have to modify its code each time you add a new derived class to the system. `FactBase` divides responsibility: each new concrete class has to register itself with the factory by calling `registerTur()` and passing it its type identifier and a pointer to its creation function.

```
class FactTurb
{
...
/** Tur objects instantiation method
TurBase* make(const DesNumerics& desNumGlb, DesModel& desModGlb,
DesBlock& desBlock,
const list<DesBoundary*>& listDesBnd,
const list<DesInit*>& listInitBlock,
GeoGrid& grid);

/** registration */
E_Bool registerTur(TbxString name,
PtrVirtConsTur pvc);
}
```

```
FactBase::makeTurb(...) (File FactTurb.C):
{
...
E_Int turbMod = desModGlb.getI(KEY_TURBMOD);
TbxString trueName = _db.getTurClassName(turbMod);
turBase = (*(_allTurCtor[trueName]))
(desNSDGlb, desModGlb, desBlock, grid,
```



```

        vectorWindows, vecWakes, vecWalls, vecTurCriteriaFile,
        coeffMutInit);
    if (turBase == E_NULLPTR)
    {
        DefError error(2180); error++; error.raiseError();
    }
}
E_Bool FactTurb::registerTur(TbxString      name,
                             PtrVirtConstTur pvc)
{
    _allTurCtor[name] = pvc;
}

```

The registration itself is performed with startup code (code generated by the compiler to initialize global objects *before* entering `main()`):

```

namespace
{
    TurBase*
    createTurKL (...)
    {
        ...
        return new TurKL(cutvar1, cutvar2, muRatioMx, prandtlTurb, coeffMutInit,
                        turcriteria);
    }
    E_FactTurRegister(TurKL) // appel de la macro d'ebregistrement
}

```

where, to ease notation, we have used the macro:

```

#define E_FactTurRegister(className) \
    const E_Bool registered##className = \
    FactTurb::instance()->registerTur(TbxString(#className), \
                                     &create##className);

```

Let us stress again that nowhere in the elsA kernel should the constructor of `TurKL` be directly called, except inside method `createTurKL()`.

Note:

The only exception may arise in unitary test(s) written specially to test `TurKL` class.

12.1.2.4 Register a new boundary condition class

The same solution is applied to register a new boundary condition class: each new concrete class has to register itself with the factory by calling `registerBnd()` and passing it its type identifier and a pointer to its creation function.

```

class FactBase
{
    ...
    /** registration */
    E_Bool registerBnd(TbxString      name,
                      PtrVirtConsBnd pvc);
}

```

```
E_Bool FactBase::registerBnd(TbxString name,
                             PtrVirtConsBnd pvc)
{
    _allBndCtor[name] = pvc;
}
```

The registration itself is performed with startup code

```
namespace
{
    BndPhys*
    createBndSubPres(const DesBoundary& desBnd,
                    const DesBlock& desBlock,
                    const DesNumerics& desNumGlb,
                    const EosIdealGas& eos,
                    TurBase* tur,
                    const GeoGrid& grid,
                    E_Int level)
    {
        GeoWindowStruct windowFine = *desBnd.getDesWindow()->getWindow();
        GeoWindowStruct wind = windowFine.buildWindowAtLevel(level);
        E_Int intNbB = wind.getNbInt();
        FldIntF dataBnd(intNbB);
        [...]
        if (desBnd.queryF(KEY_PRESSURE))
        {
            dataBnd = desBnd.getF(KEY_PRESSURE);
        }
        bnd = new BndSubPres(grid, wind, dataBnd, eos);
        [...]
    }
    // Macro (register creation function)
    E_FactBndRegister(BndSubPres);
}
```

where, to ease notation, we have used the macro:

```
#define E_FactBndRegister(className) \
    const E_Bool registered##className = \
        FactBase::instance()->registerBnd(TbxString(#className), \
                                           &create##className);
```

12.1.2.5 Putting everything together

It remains only to specify how user input is translated into type identifier.

- The simplest solution would be to ask the user to give the class name directly.
- Presently, we use a more complex solution, using an indirection, implemented with Python dictionary objects. For example:

Python API:

```
DesModel my_model('my_model')
my_model.set("turb", SPALART)
```

Python User:

```
my_model = model()
my_model.turb = 'spalart'
```

Python dictionary ((file EpKernelClassName.py):

```
dict_tur = {
BALDWIN      : "TurBlx",
MICHEL       : "TurAlgMichel",
SPALART      : "TurSA",
...
}
```

Another example concerning the boundary conditions:

Python dictionary ((file EpKernelClassName.py):

```
dict_bnd = {
"ExcCenter+inactive"      : "BndSupOut",
"ExcCenter+outpres"       : "BndSubPres",
...}
```

Note:

User interface manage Tur hierarchy in a different way than Bnd or Oper hierarchies: in Python-API, it uses integer identifiers instead of strings. this non-uniformity should be removed.

13. DESCOP PACKAGE

13.1 Building Python interface with SWIG

The special module `Api` provides all the stuff needed to build the Python interface to *elsA*. `Api` is not a standard *elsA* module:

- there is no library (`libeApi.a` or `libeApi.so`).
- the local template `Makefile`, `Make_obj.mk`, deals with additional information to control SWIG operation;
- to build Python-elsA interface, SWIG needs special *interface* files, with `.i` extension, located in directory `Api/Wrapper`.

13.1.1 What is SWIG?

The output file created by SWIG contains everything that is needed to construct an extension module for the target scripting language. To build the final extension module, the SWIG output file is compiled and linked with the *elsA* libraries to create a shared library, or a statically linked executable (see also /ELSA/MDEV-3036).

13.1.2 *cpp-like syntax*

Like C, SWIG preprocesses all input files through an enhanced version of the C preprocessor. All standard preprocessor features are supported including file inclusion, conditional compilation and macros. SWIG is a very convenient special preprocessing symbol defined by SWIG when it is parsing an input file. SWIG (preprocessor symbol)

```
class DesBase
{
    ...
    /** */
    double    getF(const char* key) const;
    /** */
    int       getI(const char* key) const;
    /** */
    const char* getS(const char* key) const;

#ifdef SWIG
    /** */
    E_Float   getF(const TbxString& key) const;
    /** */
    E_Int     getI(const TbxString& key) const;
    /** */
    TbxString getS(const TbxString& key) const;
#endif
}
```

13.1.2.1 SWIG directives

Most of SWIG's operation is controlled by special directives that are always preceded by a "%" to distinguish them from normal C declarations. These directives are used to give SWIG hints or to alter SWIG's parsing behavior in some manner.

```
Wrapper/DesModel.i:
%constant int E_BALDWIN = DesModel::E_BALDWIN; /* = 0 */
```

13.1.2.2 SWIG parser limitations

Although SWIG can parse most common C/C++ declarations, it does not provide a complete C/C++ parser implementation. Most of these limitations pertain to very complicated type declarations and certain advanced C++ features.

In the event of a parsing error, conditional compilation can be used to skip offending code. For example: `#ifndef SWIG ... some bad declarations ... #endif`

Note:

Newer versions of SWIG are able to digest most C++ constructs. Workarounds that have been used in the past to build the swigged Python-elsA interface are probably useless, and should be removed.

13.2 elsA interface building strategy

This section describes the general approach for building elsA interface with SWIG.

- Identify the functions (i.e. class methods) that you want to wrap. It's probably not necessary to access every single function. A little forethought can dramatically simplify the resulting scripting language (presently, Python) interface.
- If you want to access a new C++ class from the scripting interface, create a new interface file (extension .i). Use SWIG's include directive to process an entire C++ source/header file.

```
File Api/Wrapper/DesCfdPb.i
%module DesCfdPb

%{
#include "DesCfdPb.g"
%}

/* DesCfdPb::Config */
%constant int E_1D = DesCfdPb::E_1D; /* = 0 */
%constant int E_2D = DesCfdPb::E_2D; /* = 1 */
%constant int E_3D = DesCfdPb::E_3D; /* = 2 */
%constant int E_AXI = DesCfdPb::E_AXI; /* = 3 */

/* DesCfdPb::Axis */
%constant int E_X = DesCfdPb::E_X; /* = 0 */
%constant int E_Y = DesCfdPb::E_Y; /* = 1 */
%constant int E_Z = DesCfdPb::E_Z; /* = 2 */

#include DesBase.g
#include DesCfdPb.g
```

- Make sure everything in the interface file uses ANSI C++ syntax.
- Eliminate unneeded members of C++ classes (using SWIG symbol).

13.2.1 Technical details

13.2.1.1 Static linking

With static linking, you rebuild the scripting language interpreter with extensions. The process involves compiling a short main program (file `Api/Wrapper/elsA_wrap.C`) that adds your customized commands to the language and starts the interpreter. You then link your program with a library to produce a new scripting language executable.

Although static linking is supported on all platforms, this is not the preferred technique for building scripting language extensions. In fact, there are very few practical reasons for doing this, we plan to switch to shared libraries instead.

Note:

We still have to take into account platforms that do not provide shared library: NEC SX, Fujitsu VPP.

13.2.1.2 *elsA* main()

elsA main() is located in file `Api/Wrapper/elsA_wrap.C`. To build `elsA_wrap.C`, SWIG uses the file `Api/Wrapper/elsAembed_template.i`.

```
...
int
main(int argc, char **argv)
{
    ...
    // print banner (general information)
    e_log << E_BANNERSTRING1;
    e_log << "Size of Float   : " << sizeof (E_Float) << " Bytes" << endl;
    e_log << "Size of Integer : " << sizeof (E_Int)   << " Bytes" << endl;
    e_log << endl;

    // call Python interpreter
    E_Int py_return = Py_Main(argc,argv);

#ifdef E_MPI
    MPI_Finalize();
#endif
    e_log << "# elsA : normal run termination (" << py_return << ")" << endl;
}
```

Modify `Api/Wrapper/elsAembed_template.i` with great care.

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