XenoView 3.4 User Manual

2008 Rensselaer Polytechnic Institute

Welcome to XenoView

Visualization for Atomistic Simulations

by Sergei Shenogin

This is not a real manual, but it will definitely help you to get started. Many features of XenoVIew are not documented yet. Sorry . I was surprised that writing a manual is even worse than reading a manual. So I never had patience to complete it.   But all appropriate procedures can be found in the menu. If you are familiar with simulation software and standard user interfaces, it will be easy for you to learn how to use XenoView.

Your questions and comments are welcome. Please write me to shenogin@mail.ru

Thank you for your attention

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1.2 Introduction

XenoView is software package for molecular simulations. It includes Graphical User Interface which allowes to create molecular structure, see it on the screen, run simulations, and easily monitor and analize the results on the screen. We tried to make the program as user friendly as possible. First of all, XenoView interface is made in compliance with Windows standards, and, second, many default simulation options usually work well from the beginning. This reduces learning time considerably, so you might be able to run your simulation right after reading this short introduction.

Standard configuration of XenoView includes modules for **energy minimization, molecular dynamics** and **normal modes analysis**, structure builder for **polymer chain packing**, and modules for data analysis.

Energy minimization and **molecular dynamics** modules are using DISCOVER/CERIUS force fields and data formats. When structure is saved, two text files are always created: *.car file with atomic positions and *.mdf file for the description of the covalent bonds between the atoms. The third file is required for molecular dynamics (**input file**, *.inp). You must save your structure in (*.car), (*.mdf) and (*.inp) files to run molecular dynamics simulation. Additional files with the initial **atomic velocities** (*.avf) , custom-defined force field parameters ("*.ff") and script file for special thermostat and external force settings (*.add) can be created as well.

Structure can be loaded from *.car and *.mdf files (see samples in DATA/Samples folder), converted from *.pdb format, converted from ASCII text file with atom coordinates, or just created from the scratch.

Within XenoView, **internal data format** (*.xvw) is supported. This is non-text format containing everything including the appearance of the graph and animation data. Default graph appearance is stored in '**default.xvw'** file which is located in program directory. This file may be modified to change graph appearance, i.e. hide covalent bonds by default. Use "Edit -> Preferences" command to change the presentation of your data on the screen.

Use "Edit -> Structure Editor" command to change something in the structure. The Structure Editor has tools for creating, deleting, copying, moving and rotating the objects. It could be more convenient to use keyboard shortcuts and 3D plot mouse procedures to work with the structure.

Clipboard procedures are implemented according to Windows standards (use Ctrl-C to copy, and Ctrl-V to paste selected structure). In the same time the whole 3D graph image will be copied to clipboard and can be retrieved from external program.

Use "Simulation -> Edit MD Parameters" command to change **MD settings**. The "Visualization" page of MD toolbox has a list of available data templates to plot simulation results. You may create your own data templates by using "Edit Data" option in the main program menu or data plot popup menu and save it to the template directory XTP;

Use "Simulation -> Molecular Dynamics" command to start MD, or "Simulation -> Energy Minimization" for run energy minimization. You may run several simulation processes with graph interface at a time. For each process, separate plot window will be open to control the simulation.

Several MD processes can be run simultaneously in **command-line mode**. The input file data format (*.inp) is associated with the command - line version of the MD program, so you may simply start command-line MD by double-clicking on the *.inp file. You may stop command-line MD process by pressing "Q" key. Pressing "ESC" key pops up simulation menu.

The results of MD simulation are stored in text and/or binary files in the "result" folder with the same name as your structure file. The "result" folder includes: (1) text file "current.car" with coordinates of all atoms at the end of simulation; (2) file "movie.anm" with atom trajectories (3) data files with recorded values such at temperature, pressure, and density; (4) file "FField.txt" with force field parameters used in the last simulation; and (5) log and error files. **MD results** can be viewed by "Simulation ->Show MD results" command at any time.

Two independent **control points** (files with system position) are stored in the same result folder in two unformatted "*.fi" files, so the simulation can continue from the point where it was interrupted. To start simulation from the beginning, delete the whole "result" folder.

Please send your comments, wishes and bug reports to shenogin@mail.ru

1.3 Creating New Molecular Structure

To create new molecular structure:

1. Open new 3D graphic window by '**File -> New**' command;

2. Insert new atom into the structure.
   - select '**Edit -> Create Atom**' option from main menu or press '*Ins*' key on keyboard;
- click on Graphic window with left mouse button;

3. Click on the atom you just created to select it. Atom will be highlighted;
Assign element, atom type and charge to new atom

4. Create another atom or copy already existing. **Clipboard** procedures are implemented according to Windows standards (use Ctrl-C to copy, and Ctrl-V to paste selected structure). See 3D plot mouse procedures and Editing Molecular Structure for more options.

5. To connect atoms with covalent bond:
- if you have previous selection, clear it by clicking on empty space on you plot (you need to select exactly two atoms which you want to connect with bond);
- click on the first atom to select it. Atom will be highlighted;
- press '*Ctrl*' key for multiple selection and click on the second atom ;
- run '**Edit -> Create Bond**' command or press 'Ctrl-B';

6. To change periodic cell parameters:
   - open *Graph Editor* by '**Edit -> Preferences**' command;
   - choose '*Cell'* tab and edit the parameters;
   - click '**OK**' to close *Graph Editor;*

7. To create polymer chain:
   - create one chain segment with all bonds and assigned charges;
   - select two atoms in the segment ("head" and "tail");
   - u*se* **Tools->Polymer Builder** command*;*
   - add terminal atoms (or select the chain and use **Edit->Auto Define->Hydrogens** command)*;*

9. To create amorphous polymer builder:
   - create one chain in the structure;
   - u*se* **Tools->Amorphous Builder** command*;*

10. To save you structure:
   - run '**File -> Save As'** command;
   - save structure as *Molecular Configuration (*.car and *.mdf) File*.

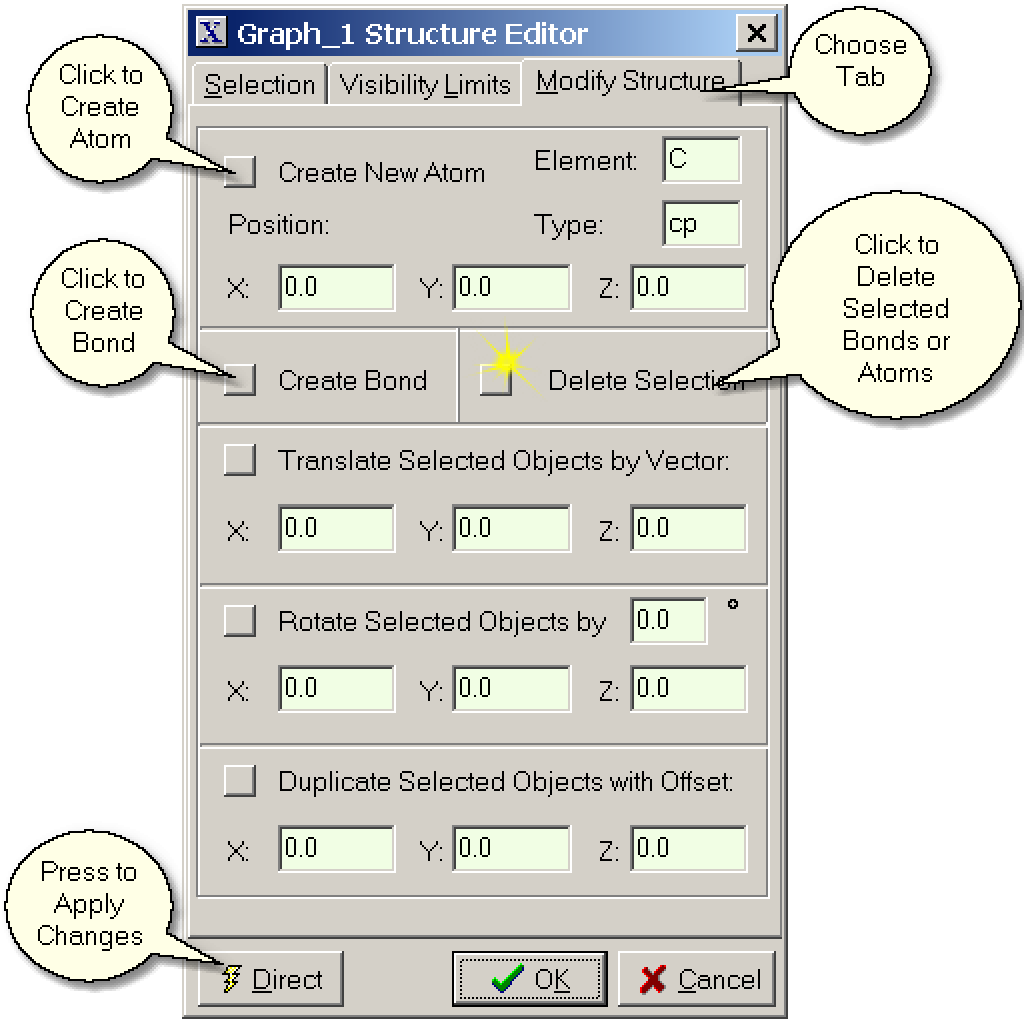
See also Editing Molecular Structure with structure editor.

1.4 Editing Molecular Structure

To modify molecular structure with structure editor:

1. open *Structure Editor* by '**Edit -> Structure Editor**' command;

2. choose 'Modify Structure' tab;



□ Create New Atom Element: C

Position: Type: cp

X: 0.0 Y: 0.0 Z: 0.0

□ Create Bond □ Delete Selection

□ Translate Selected Objects by Vector:

X: 0.0 Y: 0.0 Z: 0.0

□ Rotate Selected Objects by 0.0 °

X: 0.0 Y: 0.0 Z: 0.0

□ Duplicate Selected Objects with Offset:

X: 0.0 Y: 0.0 Z: 0.0

3. to create or delete atoms and bonds, click on the appropriate button;

4. to translate, rotate or duplicate selected parts of the structure, edit the parameters and click on the appropriate button;

5. to apply changes immediately, press 'Direct' button (not recommended for large structures and slow computers);

6. click '**OK**' button to apply changes and close dialog;

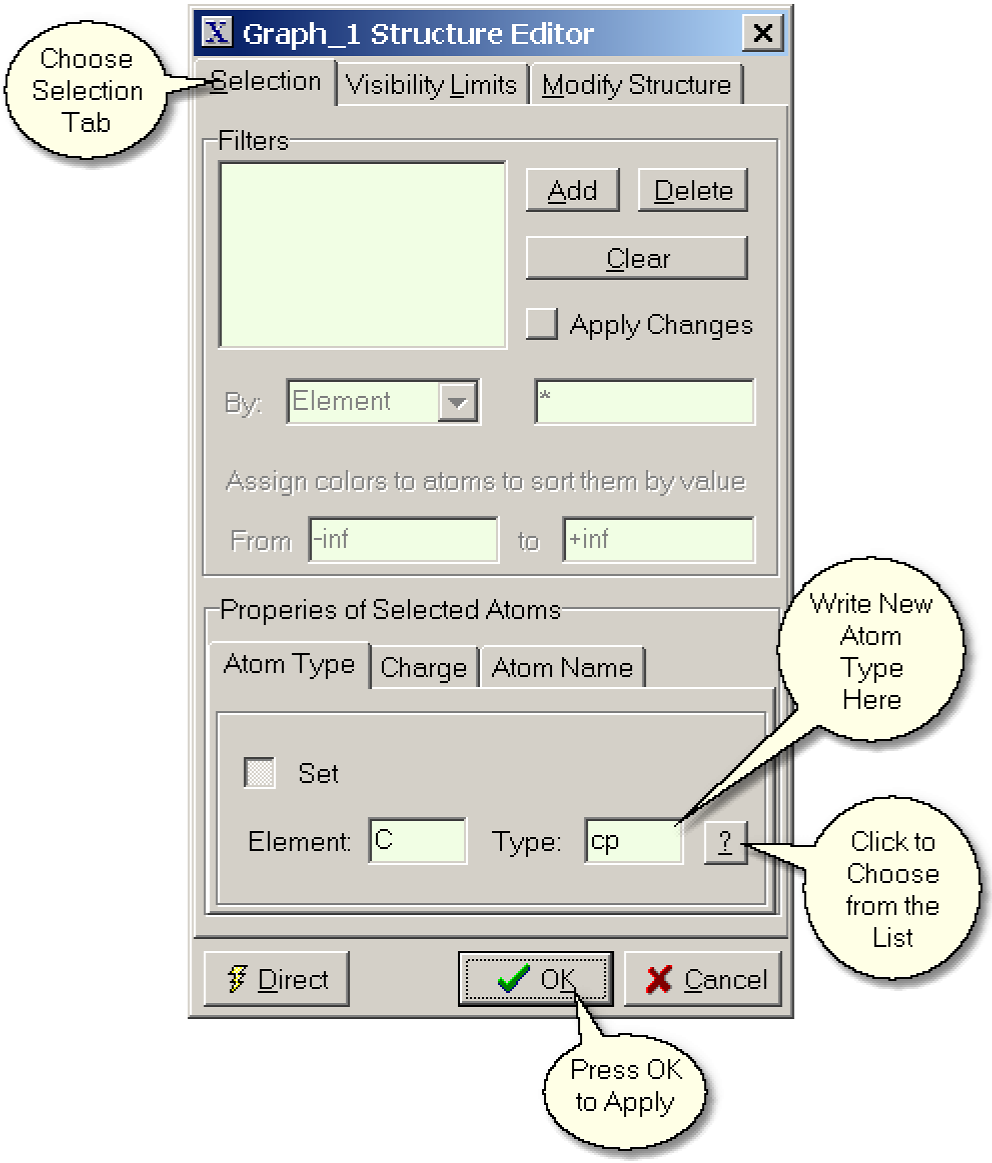
7. In the main menu ("Edit-AutoDefine") there are many options which do not present in data editor. For example, you may auto define covalent bonds using the connectivity information from the force field, or saturate structure with hydrogens.

1.5 Assigning Atom Type

To assign the same atom type to all selected atoms:

1. Open *Structure Editor* by '**Edit -> Structure Editor**' command;

2. Choose 'Selection' tab;



By: Element *

From -inf to +inf

Element: C Type: cp

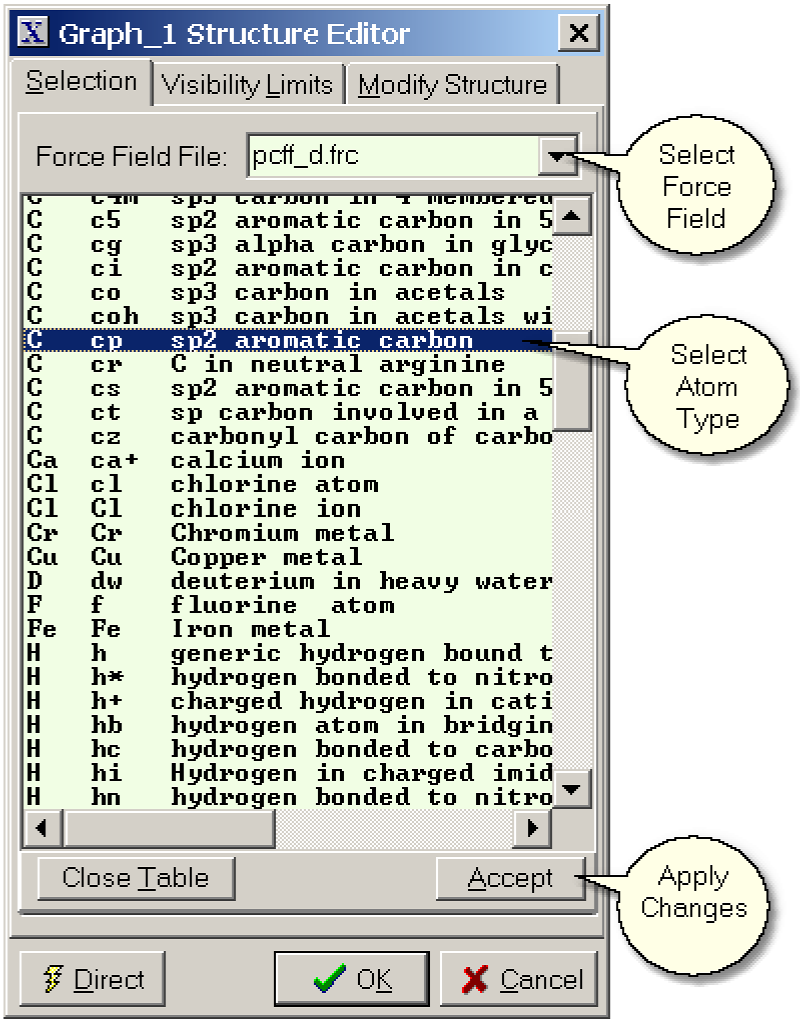
Choose Selection Tab

Write New Atom Type Here

Click to Choose from the List

Press OK to Apply

3. Press '?' button to see available atom types with descriptions, or type in desired Element and Type settings.



Force Field File: pcff_d.frc

C	c4m	sp3 carbon in 4 membered
C	c5	sp2 aromatic carbon in 5
C	cg	sp3 alpha carbon in glyc
C	ci	sp2 aromatic carbon in c
C	co	sp3 carbon in acetals
C	coh	sp3 carbon in acetals wi
C	cp	sp2 aromatic carbon
C	cr	C in neutral arginine
C	cs	sp2 aromatic carbon in 5
C	ct	sp carbon involved in a
C	cz	carbonyl carbon of carbo
Ca	ca+	calcium ion
Cl	cl	chlorine atom
Cl	Cl	chlorine ion
Cr	Cr	Chromium metal
Cu	Cu	Copper metal
D	dw	deuterium in heavy water
F	f	fluorine atom
Fe	Fe	Iron metal
H	h	generic hydrogen bound t
H	h*	hydrogen bonded to nitro
H	h+	charged hydrogen in cati
H	hb	hydrogen atom in bridgin
H	hc	hydrogen bonded to carbo
H	hi	Hydrogen in charged imid
H	hn	hydrogen bonded to nitro

4. When atom type is selected, close the table by pressing "Accept" button.

4. Make sure that 'Set' button is down to apply changes.

5. Press 'OK' button.

Read more about atom types and force fields.

1.6 Atom Types and Force Fields

Before running simulation (molecular dynamics or energy minimization), each atom must be assigned correct force field type. Because simulation program can read only one force field file, all atom types must exist within one force field. The default force field "PCFF_D.frc" works fine for most cases. To learn more about available force fields and select which force field file to use, go to XenoView program directory and read files with extension *.frc. Note that different force fields can use different expressions to calculate nonbonded interactions energy. After you have selected the force field, you may assign atom types to the atoms.

1. Select the atoms to which you want to assign the type. For example, click on the atom, use the frame (press 'Ctrl-F' for frame) or select all atoms by 'Ctrl-A'.

2. Assign atom type to the selected atoms.
After atom type was assigned, the color and size of the atom will change according to the type. If desired, you may change atom size and color by editing 'color.tbl' file in XenoView program directory. There is a special program - color editor, which may be used to edit 'color.tbl' file. Use **Edit->Atom Colors and Size** command to run it from XenoView.

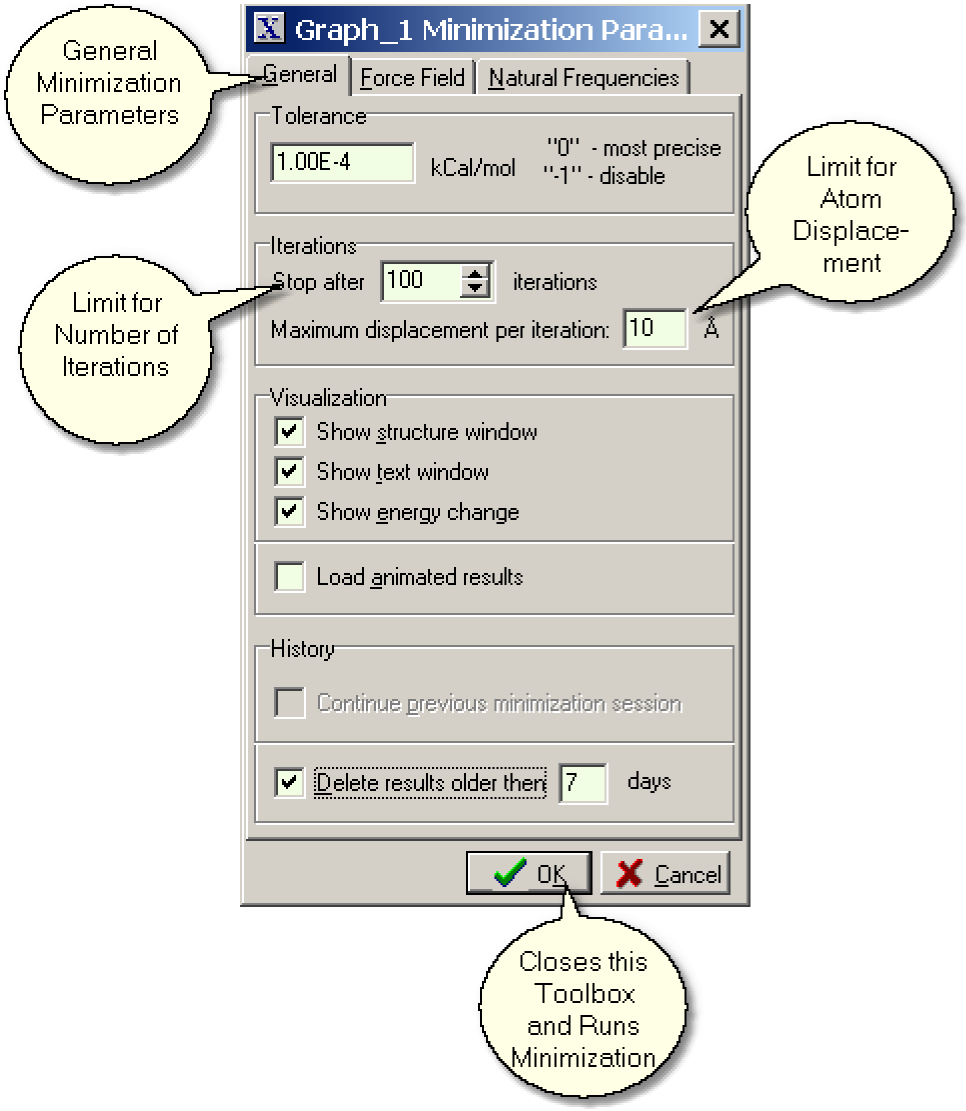
3.You may **read force field parameters** which are actually used in you simulation. Each simulation session (energy minimization or MD) creates the file "FField.txt" with complete set of actual force-field parameters used for this session. For energy minimization session, look for this file in the directory TEMP/%Sim_ID, located in the program directory (i.e. directory where executable files are installed). For MD session, look for this file in the directory with simulation results.

4. You may **specify force field parameters** for MD simulation explicitly. To do this, use **Simulation->Force Field->Modify** command and edit the script file with the parameters which you want to use. Make sure to keep the structure of the file intact, with all numbers in the same place with same format. Note that for non-bonded interactions the actual distance parameters are r^3 or r^6 (cube or the 6th power of zero-force distance), depending on the force field. If the script was modified, new parameters will be saved to the file with extension "*.ff" together with structure files "*.car" and "*.mdf". Parameters imported from file "*.ff" in the startup directory will override the parameters calculated from the source force field file "*.frc". File "FField.txt" in the results directory always contains actual parameters used in the simulation.

1.7 Energy Minimization

To run energy minimization, you must select force field and assign force field types to all atoms.

1. In main menu open **Tools -> Energy Minimization** dialog


Graph_1 Minimization Para...
General
Force Field
Natural Frequencies
OK
Cancel
General Minimization Parameters
Limit for Number of Iterations
Limit for Atom Displace-ment
Closes this Toolbox and Runs Minimization

Tolerance

1.00E-4 kCal/mol "0" - most precise "-1" - disable

Iterations

Stop after 100 iterations

Maximum displacement per iteration: 10 Å

Visualization

☑ Show structure window

☑ Show text window

☑ Show energy change

☐ Load animated results

History

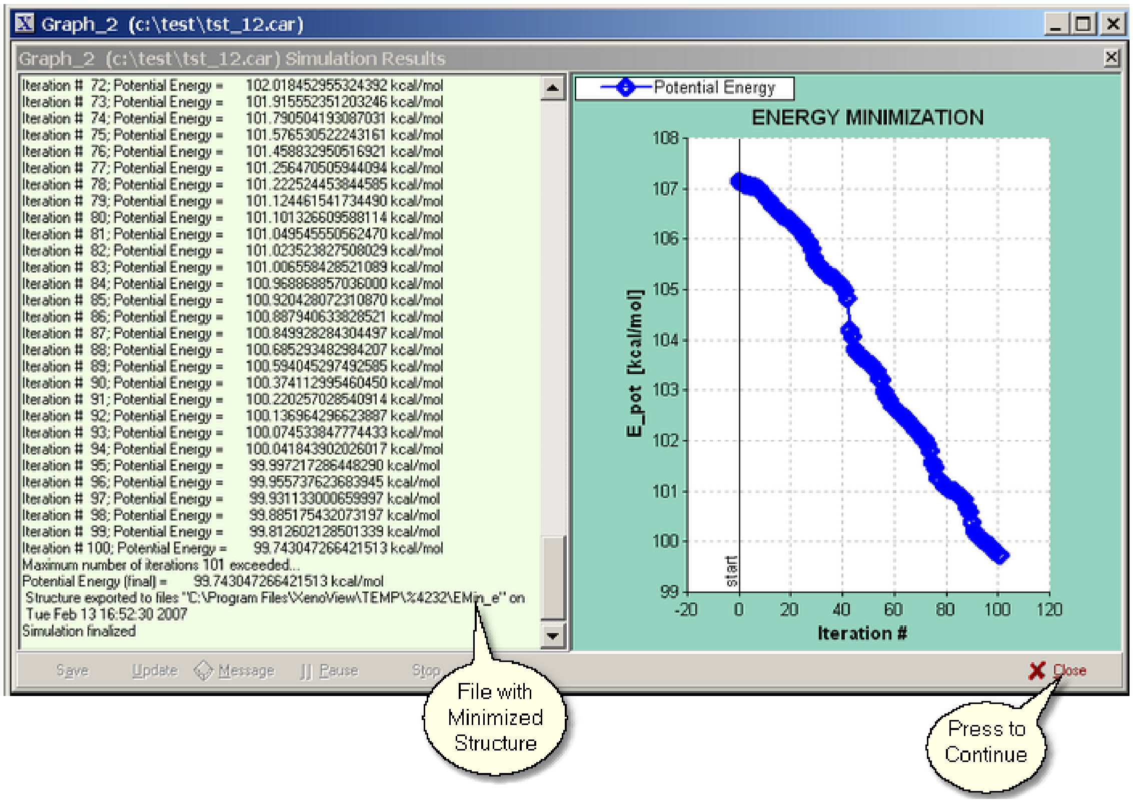
☐ Continue previous minimization session

☑ Delete results older then 7 days

2. Select desired minimization settings and press 'OK'. The plot window will

3. You may stop minimization at any moment by pressing 'Stop' button on the graphic window, or by **Simulation -> Stop** command. However, energy minimization program needs to finish iteration cycle to stop. To force simulation to stop immediately, just close the graphic window (with confirmation).

4. When minimization procedure is finished, close graphic window to see the minimized structure:



```
Iteration #  72; Potential Energy =     102.018452955324392 kcal/mol
Iteration #  73; Potential Energy =     101.915552351203246 kcal/mol
Iteration #  74; Potential Energy =     101.790504193087031 kcal/mol
Iteration #  75; Potential Energy =     101.576530522243161 kcal/mol
Iteration #  76; Potential Energy =     101.458832950516921 kcal/mol
Iteration #  77; Potential Energy =     101.256470505944094 kcal/mol
Iteration #  78; Potential Energy =     101.222524453844585 kcal/mol
Iteration #  79; Potential Energy =     101.124461541734490 kcal/mol
Iteration #  80; Potential Energy =     101.101326609588114 kcal/mol
Iteration #  81; Potential Energy =     101.049545550562470 kcal/mol
Iteration #  82; Potential Energy =     101.023523827508029 kcal/mol
Iteration #  83; Potential Energy =     101.006558428521089 kcal/mol
Iteration #  84; Potential Energy =     100.968868857036000 kcal/mol
Iteration #  85; Potential Energy =     100.920428072310870 kcal/mol
Iteration #  86; Potential Energy =     100.887940633828521 kcal/mol
Iteration #  87; Potential Energy =     100.849928284304497 kcal/mol
Iteration #  88; Potential Energy =     100.685293482984207 kcal/mol
Iteration #  89; Potential Energy =     100.594045297492585 kcal/mol
Iteration #  90; Potential Energy =     100.374112995460450 kcal/mol
Iteration #  91; Potential Energy =     100.220257028540914 kcal/mol
Iteration #  92; Potential Energy =     100.136964296623887 kcal/mol
Iteration #  93; Potential Energy =     100.074533847774433 kcal/mol
Iteration #  94; Potential Energy =     100.041843902026017 kcal/mol
Iteration #  95; Potential Energy =      99.997217286448290 kcal/mol
Iteration #  96; Potential Energy =      99.955737623683945 kcal/mol
Iteration #  97; Potential Energy =      99.931133000659997 kcal/mol
Iteration #  98; Potential Energy =      99.885175432073197 kcal/mol
Iteration #  99; Potential Energy =      99.812602128501339 kcal/mol
Iteration # 100; Potential Energy =      99.743047266421513 kcal/mol
Maximum number of iterations 101 exceeded...
Potential Energy (final) =      99.743047266421513 kcal/mol
 Structure exported to files "C:\Program Files\XenoView\TEMP\%4232\EMin_e" on
 Tue Feb 13 16:52:30 2007
Simulation finalized
```

5. Minimized structure and information about energy minimization can be retrieved from the folder "\TEMP\%Sim_ID" located in XenoView program directory, where "Sim_ID" stands for simulation ID which Minimization program reports in text window.

6. File "Errors.txt" in this directory contains information about errors occurred in the last energy minimization session.

7. File "FField.txt" contains complete set of actual force-field parameters used for this session.

1.8 MD Simulation

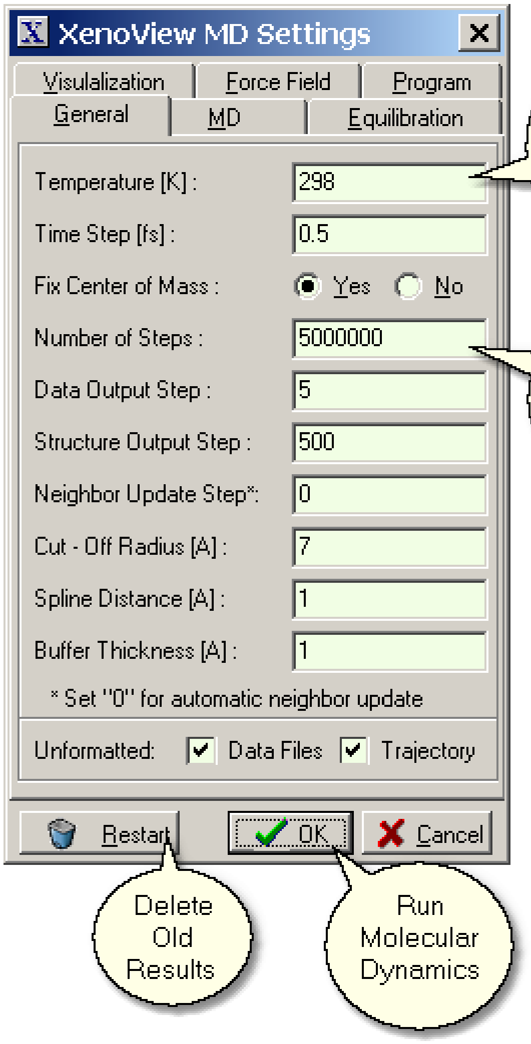
The easiest way to run MD simulations is to use the default program. However, if necessary, XenoView can be used with the **external simulation software** because:
- Atom positions can be imported from regular text files;
- **Animations** can be played from text files with some special formatting (see samples);
- Data are plotted from text files (comma separated columns is the only recommendation);

1. First Create your structure and save it on the disk. Three to six files must be saved in the same directory:
   a. "*.car" file with coordinates of all atoms.
   b. "*.mdf" file with covalent bonds information
   c. "*.inp" file with simulation settings

d. "*.avf" (*optional*) file with initial atomic velocities.
e. "*.add" (*optional*) file with additional script for advanced simulation options .
e. "*.ff" (*optional*) file with modified force-field parameters.

To run MD simulation with XenoView interface:

2. In main menu open **Simulation -> Molecular Dynamics** dialog. Select basic MD settings on the "General" and "MD" tabs:



Temperature [K] : 298

Time Step [fs] : 0.5

Fix Center of Mass : ● Yes ○ No

Number of Steps : 5000000

Data Output Step : 5

Structure Output Step : 500

Neighbor Update Step*: 0

Cut - Off Radius [A] : 7

Spline Distance [A] : 1

Buffer Thickness [A] : 1

* Set "0" for automatic neighbor update

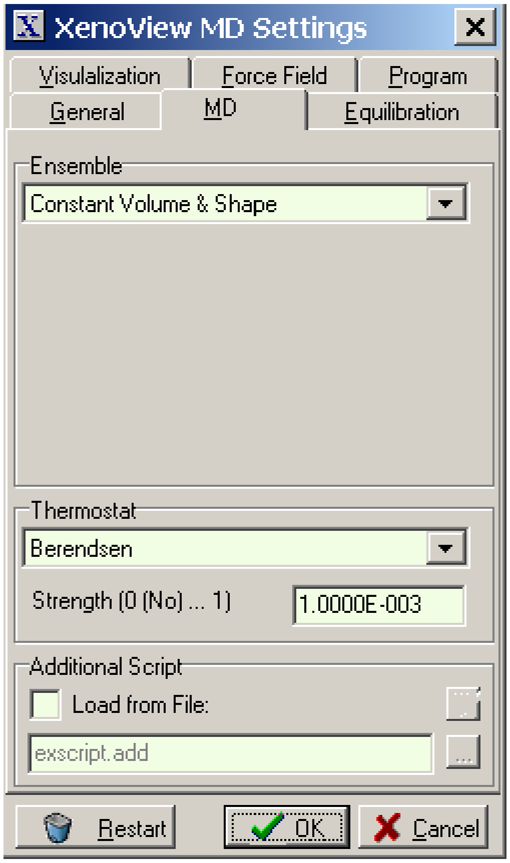
Unformatted: ☑ Data Files ☑ Trajectory

Temperature for Thermostat and Initial Velocities

Maximum Number of Steps

Delete Old Results

Run Molecular Dynamics



Ensemble

Constant Volume & Shape

Thermostat

Berendsen

Strength (0 (No) ... 1) 1.0000E-003

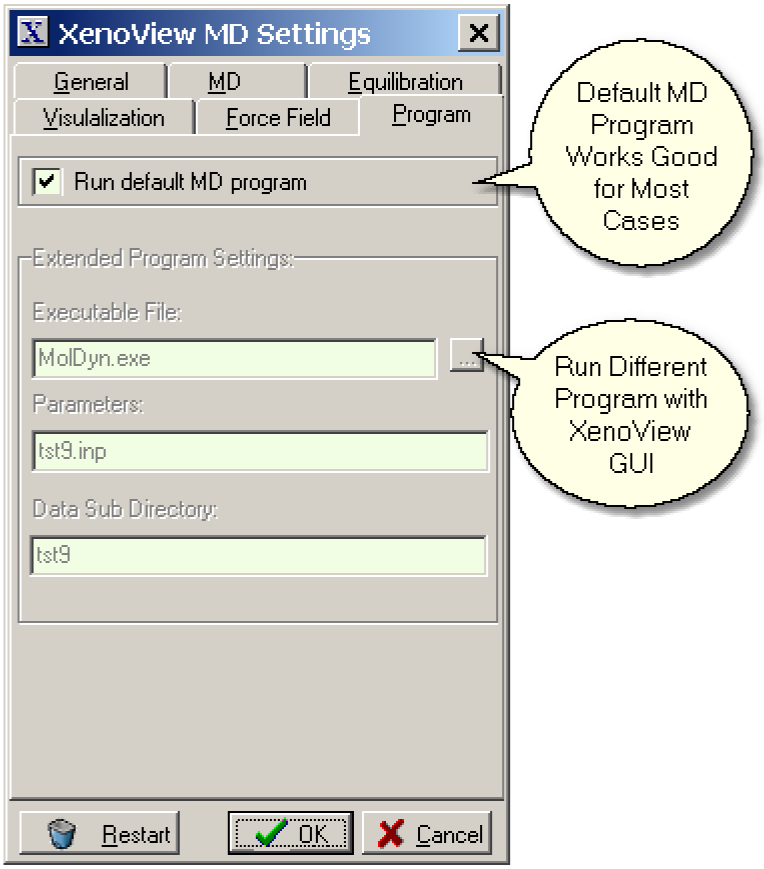
Additional Script

□ Load from File:

exscript.add

3. More advanced simulation settings can be performed using MD Script Langauge

4. Select the program for the simulation. In MD settings dialog open the **Program** tab:



☑ Run default MD program

Extended Program Settings:

Executable File: MolDyn.exe

Parameters: tst9.inp

Data Sub Directory: tst9

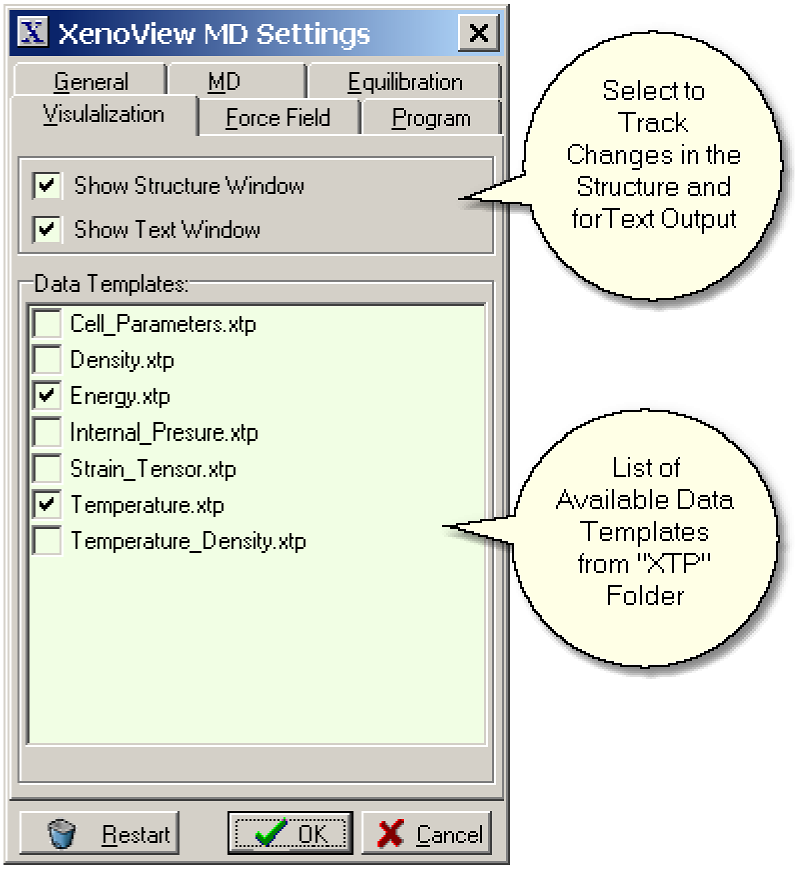
Default MD Program Works Good for Most Cases

Run Different Program with XenoView GUI

To run default MD program, check the "*Run default MD program*" checkbox.
To run your own simulation program, uncheck "*Run default MD program*" box and specify the parameters:

a. Executable file for your program (use '**...**' button to browse through directories);
b. Parameters (*optional*) for your program.
c. Data Sub Directory (*optional*). The working directory for your program will be the directory where the structure was saved. In this directory, you may create sub-directory and write you results in it. XenoView will look for your results in this directory and plot them.
Your program must use special commands for interaction with XenoView.

5. Select the data you want to plot during the simulation. In MD settings dialog open the **Visualization** tab:



☑ Show Structure Window
☑ Show Text Window

Data Templates:

☐ Cell_Parameters.xtp
☐ Density.xtp
☑ Energy.xtp
☐ Internal_Presure.xtp
☐ Strain_Tensor.xtp
☑ Temperature.xtp
☐ Temperature_Density.xtp

Select to Track Changes in the Structure and forText Output

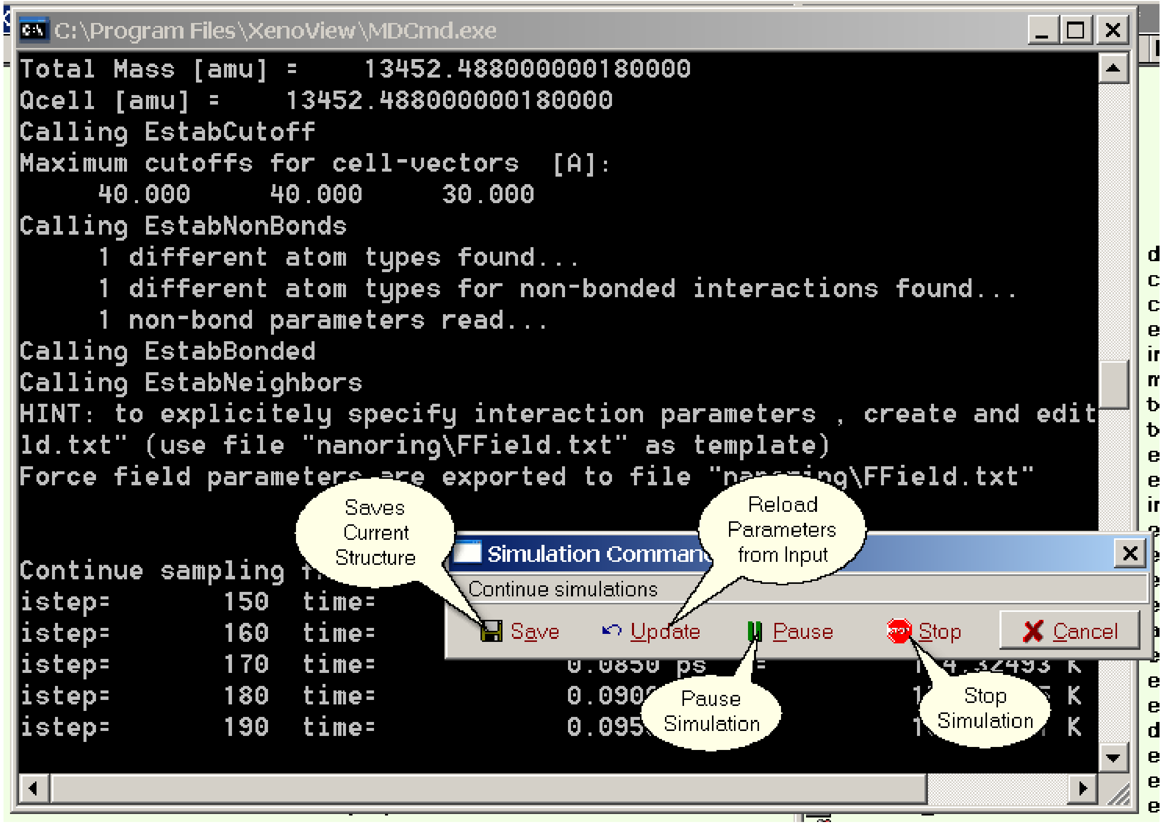
List of Available Data Templates from "XTP" Folder

If you want to read text messages from your program, check "Show Simulation Window" box.
Select required data templates from the list. The active templates will be used to plot the data from the text files created by simulation program.
You may create your own data template and save it to the "XTP" folder in XenoView working directory. For more details, see Creating Data Template.

To run MD simulation in command-line mode (without interface):

2. Double-click on the "*.inp" file in the startup directory. This will start "MDCmd.exe" program, which will re-direct the input to the MD executable specified in the file.

3. To stop command-line MD process, press ESC key. This pops up a menu.



```
Total Mass [amu] =     13452.488000000180000
Qcell [amu] =    13452.488000000180000
Calling EstabCutoff
Maximum cutoffs for cell-vectors  [A]:
     40.000     40.000     30.000
Calling EstabNonBonds
     1 different atom types found...
     1 different atom types for non-bonded interactions found...
     1 non-bond parameters read...
Calling EstabBonded
Calling EstabNeighbors
HINT: to explicitely specify interaction parameters , create and edit
ld.txt" (use file "nanoring\FField.txt" as template)
Force field parameters are exported to file "nanoring\FField.txt"


Continue sampling
istep=       150  time=
istep=       160  time=
istep=       170  time=          0.0850 ps   =        14.32493 K
istep=       180  time=          0.0900                        K
istep=       190  time=          0.095                         K
```

Continue simulations

1.9 MD Script Langauge

I. OVERVIEW

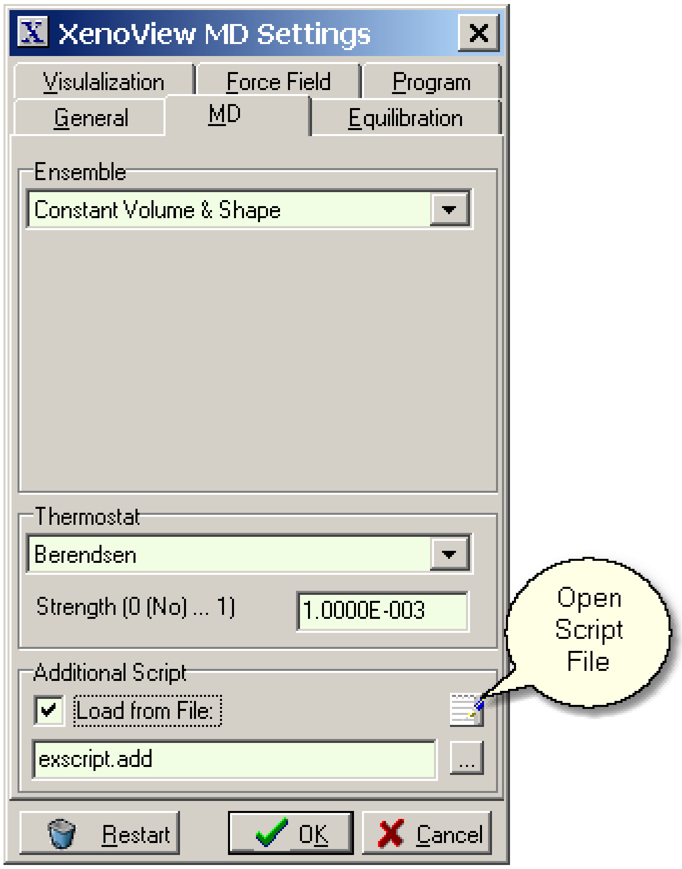
The script is used for:

- External forces applied to the specified atoms. Forces may change with time and/or atom parameters (coordinates, velocity etc.)
- Special thermostat options, for example:
  1. Temperature gradient or more complex temperature distributions
  2. Temperature changing with time

Although expression evaluation with script is only 3-5 times slower then with the compiled code, use this script only if necessary.
For example, do not the keep constant temperature with script like this:
"@all : Temp = 298.0;", use thermostat instead

II. EDITING THE SCRIPT

In main menu open **Simulation -> Molecular Dynamics** dialog. Select "MD" tab. Press the "Script Edit" button in the very bottom of the page:



Ensemble
Constant Volume & Shape

Thermostat
Berendsen
Strength (0 (No) ... 1) 1.0000E-003

Additional Script
☑ Load from File:
exscript.add

The use of script is straightforward. Here are some examples (to make the expression active, remove "!" sign):

```
#Forces
!
! @1   :  FX =  1.0E-2;    FY = 0;   FZ = 0;               ! Constant force is applied to atom #1
! @2   :  FX =  1.0*sin(10*Time);    FY = 0;   FZ = 0; ! Forced oscillations with frequency 10/2pi THz
! @2-4 :  FX =   -1.E0;    FY = 0;   FZ = 0;               ! Constant force is applied to atoms #2,3 and 4
! @5   :  FX =   1.E-2;   FY = 0;   FZ = 0;
! @10  :  FX =   2.E-2;    FY = 0;   FZ = 0;
! @all  : FX = -((SX<(-0.3))*(SX+0.3)+(SX>0.3)*(SX-0.3))*2.E1; FY = 0; FZ = 0;  ! Creates two soft walls in X-direction
!
#Temperature
!
! @all :  Temp = 2.0 + 600 * ABS(SX);          ! Constant temperature gradient
! @1   :  Temp = 200.0;                        ! Apply T=200.0 K only to atom # 1
! @10-20  :  Temp = 300.0;                     ! Apply thermostat T=300.0 K to atoms 10 through 20
! @all :  Temp = 200.0 + Time*10.0;             ! Heat all structure with constant temperature 10 deg/ps
! @all :  Temp=(Time<100)*(300+Time*1.0)+(Time>100)*(400-(Time-100)*1.0);  ! Heating+cooling cycle
! @all :  Temp = 200.0 + Index;                 ! For test. Temperature is defined by atom number in the structure
```

To write more complicated scripts for your own special case (i.e. for electric or magnetic field, radial temperature distribution, etc), read the following notes.

III. GENERAL NOTES:

1. Each section opens with "#" mark in first position
   Line "#Forces" opens external forces section
   Line "#Temperature" opens special thermostat section
2. Expression starts with "@" mark followed by the index of the atom
   to which it must be applied, then ":" mark, then expression itself
   closed by ";" sign. Examples:

```
 @1   :  FX =    1.E0;    FY = 0;   FZ = 0;  - to atom # 1
                                    apply constant force
                                    along X-axis


 @all :  Temp = 2.0 + 600 * ABS(SX);         - to all atoms
                                    apply constant
                                    temperature gradient
                                    along X-axis from
                                    2.0 K in the center to
                                    302.0 K in cell periphery
                                    (SX ranges from -0.5 to 0.5)
```

3. If atom appears in more then one active expression, the first expression takes precedence.
   For example, this script cools first 10 atoms, heats next 10 and keeps the rest of the structure
   at the middle temperature:

```
@1-10 : Temp = 200.0;
@11-20 : Temp = 400.0;
@all :  Temp = 300.0;
```

4. Mark "!" in the first position means comment line

IV. VARIABLES, OPERATORS AND FUNCTIONS DEFINED:

1. Variables:

"Time"	1. simulation time in [ps]
"Temp"	2. global temperature in [K]
"Press"	3. internal hydrostatic pressure in [kCal/Mol/A3]
"CellX"	4. cell size X in [A]
"CellY"	5. cell size Y in [A]
"CellZ"	6. cell size Z in [A]
"CellA"	7. cell angle Alpha in [degrees]
"CellB"	8. cell angle Beta in [degrees]
"CellG"	9. cell angle Gamma in [degrees]
"X"	10. atom coordinate X in [A]
"Y"	11. atom coordinate Y in [A]
"Z"	12. atom coordinate Z in [A]
"SX"	13. atom scaled coordinate X (ranges from -0.5 to 0.5)
"SY"	14. atom scaled coordinate Y (ranges from -0.5 to 0.5)
"SZ"	15. atom scaled coordinate Z (ranges from -0.5 to 0.5)
"VX"	16. atom velocity X-component in [A/ps]
"VY"	17. atom velocity Y-component in [A/ps]
"VZ"	18. atom velocity Z-component in [A/ps]
"FX"	19. X-component of the force actig on atom in [kCal/Mol/A]
"FY"	20. Y-component of the force actig on atom in [kCal/Mol/A]
"FZ"	21. Z-component of the force actig on atom in [kCal/Mol/A]
"Mass"	22. atom mass in [amu]
"Chrg"	23. atom charge in [e]
"Index"	24. atom number in the system

2. Operators - Fortran standard (power operator "**" works in addition to "^")
    "+"
    "-"
    "*"
    "/"
    "^"
    ">" - logical operator (returns 1 if A>=B, 0 otherwise)
    "<" - logical operator (returns 1 if A<B, 0 otherwise)
    "=" - logical operator (returns 1 if A=B, 0 otherwise)

3. Functions - Fortran standard
    "abs"
    "exp"
    "log10"
    "log"
    "sqrt"
    "sinh"
    "cosh"
    "tanh"
    "sin"
    "cos"
    "tan"
    "asin"
    "acos"
    "atan"

V. UNITS IN THIS SCRIPT:

Temperature units are [K]
Time units are [ps]
Energy terms are in [kCal/(mole)]
Explicit distances are in [A]
Atom partial charge is in electron charge units [e]
Atom masses are in [amu]
Velocity units are [A/ps]
Scaled coordinates are dimensionless (change from -0.5 to 0.5)
Cell angles here are in [degrees]
Forces are in [kCal/(mole A)]
Pressure and stress tensor components are in [kCal/(mole A^3)]

VI. SOME SAMPLE SCRIPTS:

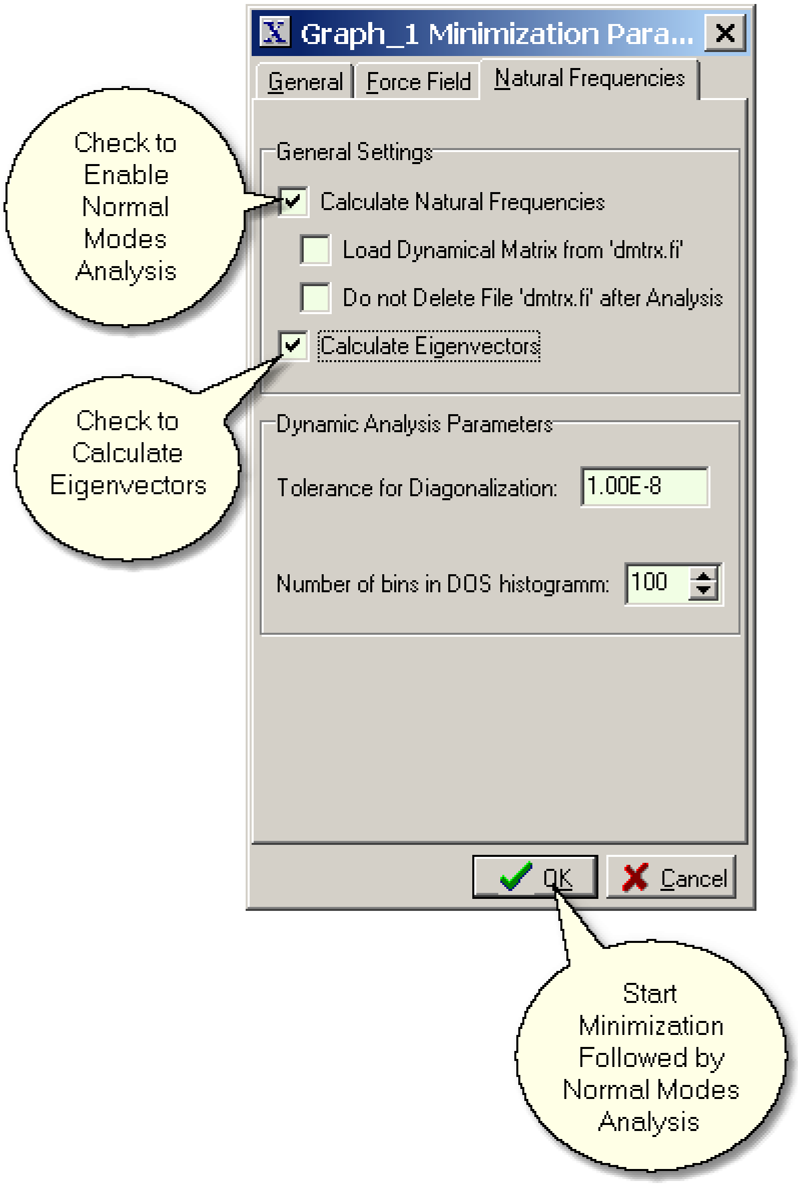
```
! To activate the line, remove "!" character from the first position.
! Identifiers "#Forces" and  "#Temperature" are required
! Each script line is terminated with ";" character
#Forces
! FX,FY,FZ - force vector components in [kCal/(mole A)]
!
! @1   :  FX =  1.0E-2;    FY = 0;   FZ = 0;             ! Constant force applied to atom #1
! @2   :  FX =  1.0*sin(10*Time);    FY = 0;   FZ = 0;   ! Forced oscillations with frequency 10/2pi THz
! @2-4 :  FX =   -1.E0;    FY = 0;   FZ = 0;             ! Same constant force applied to atoms #2,3 and 4
! @5   :  FX =   1.E-2;    FY = 0;   FZ = 0;
! @10  :  FX =   2.E-2;    FY = 0;   FZ = 0;
! @all  : FX = -((SX<(-0.3))*(SX+0.3)+(SX>0.3)*(SX-0.3))*2.E1; FY = 0; FZ = 0;  ! Create two soft walls in X-direction

#Temperature
! 1. Temp - required temperature in [K]
! 2. Berendsen-type thermostat with strength "thermOut" is used
! 3. This additional thermostat is applyed to the specified atoms
!    before the standard thermostat is applyed
! 4. If option "@all" was given, standard thermostat is forced to turn off
!
! @all :  Temp = 2.0 + 600 * ABS(SX);          ! Constant temperature gradient
! @1   :  Temp = 200.0;                        ! Apply only to atom # 1
! @10-20  :  Temp = 300.0;                     ! Apply thermostat to atoms 10 through 20
! @all :  Temp = 200.0 + Time*10.0;            ! Heating with constant temperature 10 deg/ps
!  Heating+cooling cycle beteen 300 and 400 K at 1 deg/ps:
! @all :  Temp=(Time<100)*(300+Time*1.0)+(Time>100)*(400-(Time-100)*1.0);
! @all :  Temp = 200.0 + Index;                ! For test. Temperature is defined by atom number in the structure
```

1.10 Normal Vibrational Modes

To calculate normal vibrational modes of the structure, use Energy Minimization procedure.

1. In main menu open **Tools -> Energy Minimization** dialog, choose the tab "Normal Frequencies" and check "Calculate natural Frequencies" box.



General Settings

☑ Calculate Natural Frequencies

□ Load Dynamical Matrix from 'dmtrx.fi'

□ Do not Delete File 'dmtrx.fi' after Analysis

☑ Calculate Eigenvectors

Dynamic Analysis Parameters

Tolerance for Diagonalization: 1.00E-8

Number of bins in DOS histogramm: 100

Check to Enable Normal Modes Analysis

Check to Calculate Eigenvectors

Start Minimization Followed by Normal Modes Analysis

2. It is always good to run careful energy minimization (with "zero" tolerance) before calculating normal vibrational modes. This will allow to create more symmetric dynamical matrix and calculate more accurate eigen frequencies. The reason is that "*.car" file stores atom coordinates with single precision, while the calculation of vibrational modes requires atom coordinates to be at energy minimum with double precision accuracy. Dynamical matric diagonalization is far more computationally extensive problem then energy minimization. Usually the structures with less then 1000 atoms can be analized within reasonable time frame (several hours).

3. The procedure will generate text file "eigValues.dat" in the program directory with frequency, density of states and participation ratio for each mode (the last parameter is calculated from the eigenvectors and shows the degree of localisation for each mode). The first several (three to six) modes with close to zero frequencies represent translational and rotational degrees of freedom. All other modes must have real frequencies.

4. If box "Calculate Eigenvectors" is checked, procedure will create file "EMin.eig" in the program directory. This is the text file with normalized eigen vectors. XenoView can load "*.eig" files along with the molecular structure and show the animated vibrations for each mode. To keep the results, move file "EMin.eig" to the folder where your structure "*.car* file is stored, and give it the same name (but with "eig" extension).

5. To animate vibrations:
   - Go to the next vibrational mode by **Normal Modes->Next Frequency** command
   - Start animation by **Animation->Start Movie** command
   - The animation can be saved in "*.avi" file format using external codec.

6. To unload vibrational modes, use **Normal Modes->Unload Modes** command

5. You may open "BBall.car" sample structure file to see how the results of normal modes analysis look.

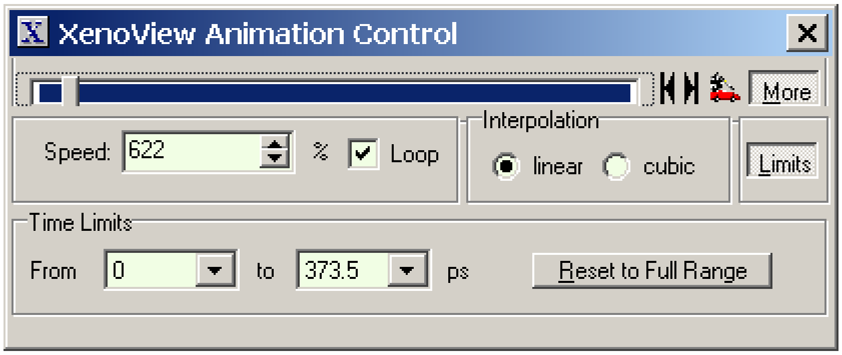
1.11 Animation Data Files

Animations can be loaded from the text files with extension '***.anm**'.

1. The animations can be exported to "*.avi" file by **Save As** command. You may select video codec from the list of codecs installed on your computer.

2. To play/pause animation use **Animation ->Start Movie** Command

3. Many settings for animation, including playback speed and time limits can be modified from animation control dialog. To open it, use **Animation->Show Animation Control** Command:



Speed: 622 % ☑ Loop

● linear ○ cubic

From 0 to 373.5 ps

4. Many additional procedures can be performed for animated structures loaded to XenoView. Some examples are:
   - Animation->Average Trajectories
   - Calculate->Atom Colors From->Atom Displacements
   - Calculate->Atom Colors From->Local Strain
   - Calculate->Diffusion Coefficient->From Random Walk

5. The XenoView animation files "*.anm" are usually created by MD or energy minimization program. It can be text file or binary file with text header (this option is preffered because of much smaller files and faster reading).

The text version of "*.anm" file may have different directives in addition to the coordinates.

-'**!**' - *comment* directive. Comment lines must be preceded by the '**!**' sign;

- '**@Connections=<filename.mdf>**' *optional* directive shows the filename with covalent bonds. If this directive is missing, connections will be loaded from file with the same name as *.anm file (but extension *.mdf).

- '**@NoColor**' *optional* directive means that the default atom colors and size will be used (i.e. defined in 'color.tbl' file) ;

- '**@Header**' *required* directive opens the header section. It defines atom numbers, types, radii and colors. This section must have 7 comma separated columns. First column is the number of each atom, second is the atom type in the force-field, third is atom radius for movie representation. The last 4 columns define atom color.

- '**@Coordinates**' *required* directive opens the coordinate section. It has several records, equal to the number of nodes that will be created in the trajectories. The movements between the nodes are defined by linear or cubic spline interpolation.

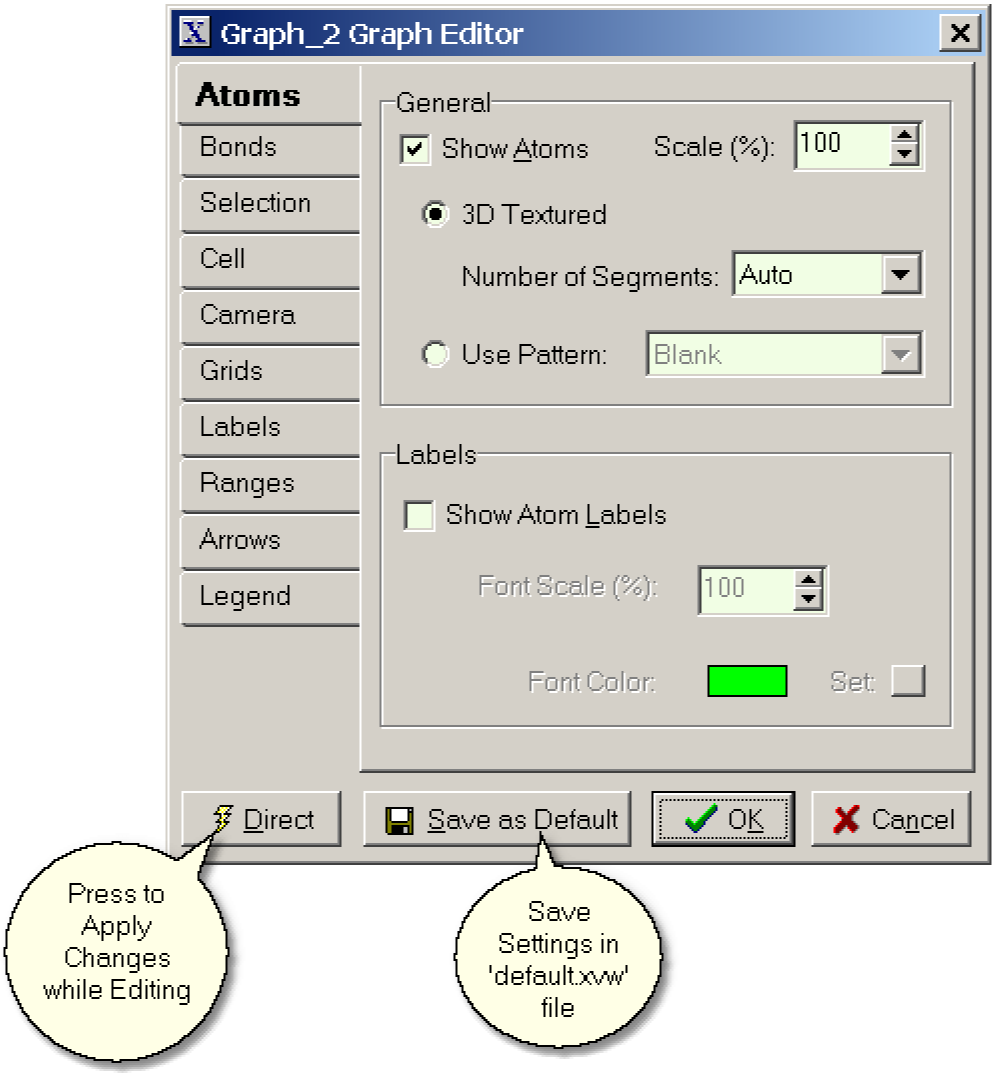
- '**@istep=<nnn> , time= <ttt> <units>**' directive opens the description of the node. **<nnn>** is the simulation time step for this node (not actually used), and **<ttt>** is the actual node time (*required*). Comma between them is required. **<units>** is the string representing time units to be shown on plot (*optional*).

- '**@cell= <X_Size>, <Y_Size>, <Z_Size>, <Alpha_Angle>, <Beta_Angle>, <Gamma_Angle>**' directive defines cell shape for current node.

- **Node description for atoms**: The following 5 columns define atom number, three coordinates and velocity value for each atom. All columns must be comma separated. For each atom one or two nodes can be defined at given time. Two nodes must be defined if atom jumps to a new position because of periodic boundaries. The velocity values are required only for additional calculations (like temperature calculations) and may be set to 0.

1.12 Appearance of 3D Structure

To change appearance of the graph (the way atoms and bonds are presented, size and shape of simulation cell, background color, legend size, camera perspective, sensitivity to mouse movements etc) use **Edit->Graph Editor** command:



General

☑ Show Atoms Scale (%): 100

● 3D Textured

Number of Segments: Auto

○ Use Pattern: Blank

Labels

□ Show Atom Labels

Font Scale (%): 100

Font Color: 🟩 Set: □

The default settings are stored in "default.xvw" file in the program directory. This file will be overwritten if you click "Save as Default" button in Graph Editor. Alternatively, you may open this file, edit it using Graph Editor and Structure Editor, and use "**Save As**" command to overwrite this file.

1.13 Save as a Picture

To export structure to a picture (Bitmap or JPG image), use **Save As** command and choose the required format. For JPG image file, you may select the resolution and compression quality of the file.

1.14 3D Plot Mouse Procedures

You may use the following mouse procedures in 3D structure window:

- To change view direction (**move camera around structure**), press mouse right button and drag. Arrows on the keyboard numeric pad work in the same way.

- **To translate viewpoint**, press mouse left button and move. Arrows on main keyboard do the same.

- To **ZOOM** in or out, rotate mouse wheel or press '+' or '-' on the numeric pad ;

- To **get centered view**, press mouse wheel or central button, or '*' on the numeric pad;

- To **select an object** (atom or bond), click on it with left mouse button;

- To **select several objects**, hold down Ctrl key (just like in Windows);

- To select objects with the **frame**, hold down Ctrl key, click on empty space and drag across the area (there is also a menu option for selection with frame);

- To **translate selected objects**, hold down Ctrl key and drag with left mouse button;

- To **rotate selected objects**, hold down Ctrl key and drag with right mouse button;

- To **translate selected objects** in the specified plane, hold down Shift key and press: left mouse button for X-Z plane, right button for X-Y plane and left+right buttons for Y-Z plane;

- To **duplicate selected objects**, hold down Shift and Ctrl keys at the same time and drag;

1.15 Data Plot Mouse Procedures

You may use the following mouse procedures in data plot window:

- To **MOVE** the individual GRAPH, drag it, holding it on the Upper Left angle;

- To **RESIZE** the individual GRAPH, drag the Bottom Right angle;

- To **ZOOM** the **FRAME**, hold the Shift key down and drag cursor across the area you want to enlarge (press Left Mouse button while dragging);

- To **UNDO FRAME ZOOM**, hold the Shift key down and click Left Mouse Button (or click Central Mouse Button);

- To **ZOOM** IN or OUT, rotate mouse wheel (use "Auto zoom all" option in pop-up menu to return back);

- To **OFFSET** plot area, hold the Ctrl key down and drag the plot area (use "Auto zoom all" option in pop-up menu to return back);

- To **MOVE** the **LEGEND**, hold the Ctrl key down and drag the legend, holding it on the Upper Left angle;

- To **RESIZE** the **LEGEND**, hold the Ctrl key down and drag the legend border;

- To **MOVE** the **MARK**, hold the Ctrl key down and drag;

- To **DRAW** the temporary **TRACE**, hold the Alt key down and drag**.** These traces are erased after redraw;

- To **TOGGLE** the **MARKS** ON/OFF use Left mouse button dbl click;

- To open **POPUP menu** click Right mouse button;

- To check **MOUSE POSITION** and POINT POSITION in the current DataSet press Left mouse button;

1.16 Interaction Between XenoView and Simulation Program

All functions and procedures for interacting between your software and XenoView are residing in '**mssgs.dll**' file which must be present in the program directory.

Here are the examples:

C/C++:

1. File "interface.h"

```
// This unit is responsible for interaction with XenoView

#include <windows.h>

class XVInterface
{
     private:
       signed char res;
       HINSTANCE dllp;
       int (__stdcall *SH)(void);
       int (__stdcall *XVH)(void);
       signed char (__stdcall *CHCK)(int*,int*);
       signed char (__stdcall *PS)(int*,int*);
       signed char (__stdcall *RP)(int*,int*);
       signed char (__stdcall *PF)(int*,int*);
      public:
       int XenoView_HANDLE;
       int SELF_HANDLE;
       bool xenoViewFound;
       bool exitRequested();
       void MDInitialized();
       void dataReady();
       void  MDFinished();
       void initialize(char* dllFileName);
       void clear();
             };
```

2. File "Interface.cpp"

```
#include <stdio.h>
#include <windows.h>
#include "interface.h"

      void XVInterface :: initialize(char* dllFileName)
     {
      xenoViewFound = false;
      dllp=LoadLibrary(dllFileName);
      if (dllp)
      {
       SH=(int(__stdcall *) (void))GetProcAddress(dllp,"giveMeMyID");
       XVH=(int(__stdcall *) (void))GetProcAddress(dllp,"findViewer");
       CHCK=(signed char(__stdcall *) (int*,int*))GetProcAddress(dllp,"_StopSimulation");
       PS=(signed char(__stdcall *) (int*,int*))GetProcAddress(dllp,"_SimulationInitialized");
       RP=(signed char(__stdcall *) (int*,int*))GetProcAddress(dllp,"_MDDataReady");
       PF=(signed char(__stdcall *) (int*,int*))GetProcAddress(dllp,"_MDFinished");
       if ((!SH)||(!XVH)||(!CHCK)||(!RP)||(!PS)||(!PF)) printf("XenoView interface not found...\n");
        else xenoViewFound = true;
      }
    if (xenoViewFound)
      {
       if (SH) SELF_HANDLE = SH();
       if (XVH) XenoView_HANDLE = XVH();
      }
    }

    void XVInterface :: clear()
    {
     if (dllp) FreeLibrary(dllp);
    }

    bool XVInterface :: exitRequested()
    {
     if (xenoViewFound)
      {
       // printf("exitRequested\n");
       // exit(-1);
       res = CHCK(&SELF_HANDLE,&XenoView_HANDLE);
       return (res==1);
      }
     else return false;
    }

    void XVInterface :: dataReady()
    {
     if (xenoViewFound) res = RP(&SELF_HANDLE,&XenoView_HANDLE);
    }

    void XVInterface :: MDInitialized()
    {
     if (xenoViewFound) res = PS(&SELF_HANDLE,&XenoView_HANDLE);
    }

    void XVInterface :: MDFinished()
    {
     if (xenoViewFound) res = PF(&SELF_HANDLE,&XenoView_HANDLE);
    }
```

// 3. Main program

```
#include "interface.h"
static XVInterface     XVInt;

main(int argc, char *argv[])
{
 XVInt.initialize("mssgs.dll");

// .... prepare the simulation...

 XVInt.MDInitialized();    // Signal to XenoView that simulation is initialized

// .. run simulation ...

XVInt.dataReady()

// Check for interrupts
```

```
 if (XVInt.exitRequested())
   {
    printf("Interrupt from XenoView\n");
    XVInt.clear();
    exit(1);
   }

// ... finish simulation

XVInt.MDFinished();
XVInt.clear();
}
```

Fortran:

1. File "interface.inc"

```
!=============================================================================
!  Parameter responsible for interaction with  XenoView
!   ------------------------------------------------------------------------------

      INTEGER*4        XenoView_HANDLE        ! External viewer handle (signed 32-bit)
      INTEGER*4        SELF_HANDLE            ! Self window handle (signed 32-bit)
      INTEGER*1        RUN_FLAG               ! Common variable showing simulation status
      LOGICAL          WITH_GUI,NO_DLL

      COMMON /viewer_handle/  XenoView_HANDLE,SELF_HANDLE,RUN_FLAG
      SAVE   /viewer_handle/

      COMMON /run_mode/  WITH_GUI,NO_DLL
      SAVE   /run_mode/


      INTERFACE

        INTEGER*4 FUNCTION giveMeMyID
        END FUNCTION

        INTEGER*4 FUNCTION giveMeMyHandle
                END FUNCTION

        INTEGER*4 FUNCTION findViewer
        END FUNCTION

        INTEGER*4 FUNCTION initKBDialog
                        !DEC$ ATTRIBUTES STDCALL :: initKBDialog
                END FUNCTION

                CHARACTER*8 FUNCTION XenoViewVersion
                        !DEC$ ATTRIBUTES STDCALL :: XenoViewVersion
        END FUNCTION

        INTEGER*1 FUNCTION MDDataReady(hProcess,hViewer)
                         !DEC$ ATTRIBUTES STDCALL :: MDDataReady
                         !DEC$ ATTRIBUTES REFERENCE :: hViewer
                         !DEC$ ATTRIBUTES REFERENCE :: hProcess
                         INTEGER*4 hViewer
```

```
           INTEGER*4 hProcess
 END FUNCTION

 INTEGER*1 FUNCTION MDStructureReady(hProcess,hViewer)
           !DEC$ ATTRIBUTES STDCALL :: MDStructureReady
           !DEC$ ATTRIBUTES REFERENCE :: hViewer
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hViewer
           INTEGER*4 hProcess
 END FUNCTION

 INTEGER*1 FUNCTION MDFinished(hProcess)
           !DEC$ ATTRIBUTES STDCALL :: MDFinished
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hProcess
 END FUNCTION

 INTEGER*1 FUNCTION SimulationInitialized(hProcess)
           !DEC$ ATTRIBUTES STDCALL :: SimulationInitialized
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hProcess
 END FUNCTION

 INTEGER*1 FUNCTION MD_EquilStep(hProcess,hViewer)
           !DEC$ ATTRIBUTES STDCALL :: MD_EquilStep
           !DEC$ ATTRIBUTES REFERENCE :: hViewer
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hViewer
           INTEGER*4 hProcess
 END FUNCTION

          INTEGER*1 FUNCTION SimulationStopped(hProcess)
           !DEC$ ATTRIBUTES STDCALL :: SimulationStopped
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hProcess
 END FUNCTION

      INTEGER*1 FUNCTION StopSimulation(hProcess,hViewer)
           !DEC$ ATTRIBUTES STDCALL :: StopSimulation
           !DEC$ ATTRIBUTES REFERENCE :: hViewer
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hViewer
           INTEGER*4 hProcess
 END FUNCTION

INTEGER*1 FUNCTION SimulationError(hProcess)
           !DEC$ ATTRIBUTES STDCALL :: SimulationError
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hProcess
END FUNCTION

INTEGER*1 FUNCTION MD_EMinStep(hProcess,hViewer)
           !DEC$ ATTRIBUTES STDCALL :: MD_EMinStep
           !DEC$ ATTRIBUTES REFERENCE :: hViewer
           !DEC$ ATTRIBUTES REFERENCE :: hProcess
           INTEGER*4 hViewer
           INTEGER*4 hProcess
 END FUNCTION
```

```
  INTEGER*1 FUNCTION simDialog(hProcess)
            !DEC$ ATTRIBUTES STDCALL :: simDialog
            !DEC$ ATTRIBUTES REFERENCE :: hProcess
            INTEGER*4 hProcess
  END FUNCTION

       INTEGER*1 FUNCTION EMinFinished(hProcess)
            !DEC$ ATTRIBUTES STDCALL :: simDialog
            !DEC$ ATTRIBUTES REFERENCE :: hProcess
            INTEGER*4 hProcess
  END FUNCTION

      END INTERFACE

      pointer (p_giveMeMyID,giveMeMyID)
      pointer (p_giveMeMyHandle,giveMeMyHandle)
      pointer (p_findViewer,findViewer)
      pointer (p_initKBDialog,initKBDialog)
      pointer (p_XenoViewVersion,XenoViewVersion)
      pointer (p_MDDataReady,MDDataReady)
      pointer (p_MDStructureReady,MDStructureReady)
      pointer (p_MDFinished,MDFinished)
      pointer (p_SimulationInitialized,SimulationInitialized)
      pointer (p_MD_EquilStep,MD_EquilStep)
      pointer (p_SimulationStopped,SimulationStopped)
      pointer (p_StopSimulation,StopSimulation)
      pointer (p_SimulationError,SimulationError)
      pointer (p_MD_EMinStep,MD_EMinStep)
      pointer (p_simDialog,simDialog)
      pointer (p_EMinFinished,EMinFinished)

      integer iDll
     pointer (pDll,iDll)

 COMMON /ext_proc/  p_giveMeMyID,
&            p_giveMeMyHandle,
&            p_findViewer,
&            p_initKBDialog,
&            p_XenoViewVersion,
&            p_MDDataReady,
&            p_MDStructureReady,
&            p_MDFinished,
&            p_SimulationInitialized,
&            p_MD_EquilStep,
&            p_SimulationStopped,
&            p_StopSimulation,
&            p_SimulationError,
&            p_MD_EMinStep,
&            p_simDialog,
&            p_EMinFinished,
&            pDll
 SAVE   /ext_proc/
```

2. File "initInter.for"

```
  LOGICAL FUNCTION initInterface
      USE kernel32
      IMPLICIT        NONE

      INCLUDE 'define.inc'
      INCLUDE 'interface.inc'

      INTEGER i

      NO_DLL = .true.
           initInterface = .false.

! Locate the dll and load it into memory

      pDll = loadlibrary("mssgs.dll"C)
           if (pDll.EQ.0) return
           NO_DLL = .false.
          initInterface = .true.

! "giveMeMyHandle" - returns WINDOW handle, has a meaning only if special WINDOW was
! created for simulation, i.e. only in command-line mode
! (otherwise returns the same as "findViewer")
!
! "giveMeMyID" returns PROCESS (not window) ID


          p_giveMeMyID= getprocaddress(pDll, "giveMeMyID"C)
          if (p_giveMeMyID.NE.0) then
           SELF_HANDLE = giveMeMyID()
!DEC$ IF DEFINED (_DEBUG_)
           write(*,*) "Loaded procedure : giveMeMyID"
!          write(*,*) "SELF_HANDLE = ",SELF_HANDLE
!DEC$ ENDIF
          else
           SELF_HANDLE = 0
           initInterface = .false.
          endif

          p_findViewer= getprocaddress(pDll, "findViewer"C)
          if (p_findViewer.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : findViewer"
!DEC$ ENDIF
          else
      write(*,*) "Can not load procedure : findViewer"
           initInterface = .false.
          endif

     p_giveMeMyHandle = getprocaddress(pDll, "giveMeMyHandle"C)
          if (p_giveMeMyHandle.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : giveMeMyHandle"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : giveMeMyHandle"
           initInterface = .false.
          endif

          p_initKBDialog = getprocaddress(pDll, "initKBDialog"C)
           if (p_initKBDialog.NE.0) then
```

```
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : initKBDialog"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : initKBDialog"
           initInterface = .false.
          endif

          p_XenoViewVersion = getprocaddress(pDll, "XenoViewVersion"C)
           if (p_XenoViewVersion.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : XenoViewVersion"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : XenoViewVersion"
           initInterface = .false.
          endif


          p_MDDataReady= getprocaddress(pDll, "_MDDataReady"C)
          if (p_MDDataReady.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : MDDataReady"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : MDDataReady"
           initInterface = .false.
          endif

          p_MDStructureReady= getprocaddress(pDll, "_MDStructureReady"C)
          if (p_MDStructureReady.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : MDStructureReady"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : MDStructureReady"
           initInterface = .false.
          endif

          p_MDFinished= getprocaddress(pDll, "_MDFinished"C)
          if (p_MDFinished.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : MDFinished"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : MDFinished"
           initInterface = .false.
          endif

          p_SimulationInitialized =
    &      getprocaddress(pDll, "_SimulationInitialized"C)
          if (p_SimulationInitialized.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : SimulationInitialized"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : SimulationInitialized"
           initInterface = .false.
          endif

          p_MD_EquilStep= getprocaddress(pDll, "_MD_EquilStep"C)
          if (p_MD_EquilStep.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : MD_EquilStep"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : MD_EquilStep"
           initInterface = .false.
          endif

          p_SimulationStopped= getprocaddress(pDll, "_SimulationStopped"C)
          if (p_SimulationStopped.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : SimulationStopped"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : SimulationStopped"
           initInterface = .false.
          endif

          p_StopSimulation= getprocaddress(pDll, "_StopSimulation"C)
          if (p_StopSimulation.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : StopSimulation"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : StopSimulation"
           initInterface = .false.
          endif




          p_SimulationError= getprocaddress(pDll, "_SimulationError"C)
          if (p_SimulationError.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : SimulationError"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : SimulationError"
           initInterface = .false.
          endif

          p_MD_EMinStep= getprocaddress(pDll, "_MD_EMinStep"C)
          if (p_MD_EMinStep.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
           write(*,*) "Loaded procedure : MD_EMinStep"
!DEC$ ENDIF
          else
           write(*,*) "Can not load procedure : MD_EMinStep"
           initInterface = .false.
          endif

          p_simDialog= getprocaddress(pDll, "_simDialog"C)
          if (p_simDialog.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
```

```
       write(*,*) "Loaded procedure : simDialog"
!DEC$ ENDIF
      else
       write(*,*) "Can not load procedure : simDialog"
       initInterface = .false.
      endif

      p_EMinFinished= getprocaddress(pDll, "_EMinFinished"C)
      if (p_EMinFinished.NE.0) then
!DEC$ IF DEFINED(_DEBUG_)
       write(*,*) "Loaded procedure : EMinFinished"
!DEC$ ENDIF
      else
       write(*,*) "Can not load procedure : EMinFinished"
       initInterface = .false.
      endif



!DEC$ IF DEFINED(_DEBUG_)
       write(*,*) "Finished loading interface"
!DEC$ ENDIF

   END

   SUBROUTINE freeInterface
       USE kernel32

   IMPLICIT     NONE

   INCLUDE 'define.inc'
   INCLUDE 'interface.inc'

   LOGICAL status


   status = freelibrary(pDll)

       END
```

3. File "interface.for"

```
   SUBROUTINE checkKeyboardEvents

   IMPLICIT     NONE

   INCLUDE 'define.inc'
   INCLUDE 'interface.inc'

   LOGICAL PEEKCHARQQ !function
       CHARACTER(1) GETCHARQQ

   INTEGER*1 j

       CHARACTER(1) key /'A'/
       INTEGER    ESC
   PARAMETER (ESC = 27)
    if(PEEKCHARQQ()) then   ! Keyboard key pressed
```

```
      key = GETCHARQQ()
      IF ((key.EQ.'q').OR.(key.EQ.'Q')) THEN
                RUN_FLAG = 1 ! EXIT
      ELSEIF (ICHAR (key).EQ.ESC) THEN
       RUN_FLAG = simDialog(SELF_HANDLE)
      ELSE
       RUN_FLAG = -1
      ENDIF
        if (RUN_FLAG.EQ.1) then
         write(*,*) 'Interrupt from keyboard'
         write(*,*) 'Saving current configuration...'
         IF  (WITH_GUI) THEN
         j = SimulationStopped(SELF_HANDLE)            ! signal to XenoView that stop signal
received
         ENDIF
        endif
     else
      IF  (WITH_GUI) THEN
       CALL checkExternalExit
      ELSE
       RUN_FLAG = -1
      ENDIF
     endif
    END



    SUBROUTINE checkExternalExit

    IMPLICIT       NONE

    INCLUDE      'define.inc'
    INCLUDE      'interface.inc'
    INTEGER*1  i,j

    RUN_FLAG = StopSimulation(SELF_HANDLE,XenoView_HANDLE)
    if (RUN_FLAG.EQ.1) then
     write(*,*) 'Interrupt from XenoView'
     write(*,*) 'Saving current configuration...'
     j = SimulationStopped(SELF_HANDLE)          ! signal to XenoView that stop signal received
    endif
    END


! This procedure stops the program because of critical error

    SUBROUTINE criticalError(ErrMsg)

    IMPLICIT       NONE
    INCLUDE      'define.inc'
    INCLUDE      'const.inc'
    INCLUDE      'interface.inc'

    CHARACTER*(*)     ErrMsg
    INTEGER*1        i
    CHARACTER       CONCAT*maxP                ! Function
    INTEGER         LENSTR_Last          ! function
    WRITE(*,*)
    WRITE(*,'(A,$)') 'ERROR: '
    WRITE(*,*)  ErrMsg
    WRITE(*,*) 'Simulation stopped.'


   open(unit=100,file=errMsgFile)
   write(100,*) ErrMsg(1:LENSTR_Last(ErrMsg))
   close(unit=100)

   IF  (WITH_GUI) THEN
   i = SimulationError(SELF_HANDLE)              ! signal to XenoView that stop signal received
   ELSE
       i = SimulationError(-1)
   ENDIF

   STOP

   END
```

4. Main program (for Molecular Dynamics):

```
      LOGICAL          initInterface          ! Function
      LOGICAL          interfaceError,WITH_GUI

! Initialize interface and load functions
   IF (initInterface()) THEN
       interfaceError = .false.
       WITH_GUI = .true.
   ELSE
       interfaceError = .true.
   ENDIF

! findViewer() function will find XenoView
  IF (WITH_GUI) THEN
     XenoView_HANDLE=findViewer()
    ! SELF_HANDLE=giveMeMyID() is defined already
  ELSE
     SELF_HANDLE = giveMeMyHandle() !Re-define SELF_HANDLE as handle to simulation
Window, not process
     XenoView_HANDLE = 0
     i = initKBDialog()              ! So that it will automatically get focus in the future
   ENDIF

! Signal to XenoView that simulation is initialized
   IF  (WITH_GUI) THEN
   if (SimulationInitialized(SELF_HANDLE).EQ.1) then
    write(*,*) 'Connection with XenoView was established...'
   else
    write(*,*) 'No external data viewer detected...'
   endif
  ENDIF

! Signal to XenoView that data are ready
     if (MDDataReady(SELF_HANDLE,XenoView_HANDLE).EQ.1) then
       write(*,*) 'Data exported to XenoView...'
     else
```

```
      write(*,*) 'External viewer not detected...'
    endif

! Signal to XenoView that structure is ready
    if (MDStructureReady(SELF_HANDLE,XenoView_HANDLE).EQ.1) then
      write(*,*) 'Structure successfully exported to XenoView...'
    else
      write(*,*) 'External viewer not detected...'
    endif

! Check for interrupts:

   CALL checkKeyboardEvents
   IF (RUN_FLAG.EQ.1) then
     write(*,*) 'Warning: equilibration cancelled'
     write(*,*) 'Configuration can not be saved. Exiting...'
     dateLine = CurrentDATE()
     write(fs(19)%ch,*) 'EQUILIBRATION CANCELLED ON ',dateLine
     GOTO 1000           ! EXIT
   else
    RUN_FLAG=-1
   endif


! Signal to XenoView that simulation is finished
  if (MDFinished(SELF_HANDLE).EQ.1) then
    write(*,*) 'Structure successfully exported to XenoView...'
  else
    write(*,*) 'Connection with XenoView was not established...'
  endif
```

Note that ***stdcall*** calling convention is used for passing parameters .
The list of main functions is here:

- **giveMeMyHandle** : Integer
  Used for command-line mode programs. Returns *simWindowHandle* parameter to be passed to **_checkKBEvents** function. Must be called once in the beginning of simulation.

- **initKBDialog** : Integer
  Initializes pop up dialog menu for command-line mode. Must be called once in the beginning of simulation. Result is always 0.

- **_checkKBEvents(*simWindowHandle* : Integer)** : Integer
  Used in command-line mode only. Checks, if ESC key was down at the moment of the call. If it was, pops up a menu with "*Save"*, "*Reload"*, "*Pause"*, "*Stop"* and "*Cancel"* buttons. Returns:
  -1 if ESC button was not down;
  0 if "*Cancel*" button was pressed;
  1 if "*Stop*" button was pressed;
  2 if "*Reload"* button was pressed;
  3 if "*Save"* button was pressed;

- **findViewer** : Integer
  Used for interaction with XenoView. Returns *XenoViewHandle* parameter which is the handle of XenoView program. Must be called once in the beginning of simulation.

- **_MDDataReady(*XenoViewHandle* : Integer)** : Integer
  Sends XenoView a message that data files are updated. XenoView will reload new points and plot them. To get *XenoViewHandle* value, use **findViewer** function.

- **SimulationInitialized** : Integer
  Sends a signal to XenoView that simulation initialized. Returns 0 if XenoView was not found, 1 otherwise. Required to activate "*Pause*" and other options in XenoView menu.

- **_StopSimulation(*XenoViewHandle* : Integer)** : Integer
  Checks if XenoView wants to stop simulation. XenoView handle must be known already (this saves a lot of time). To get XenoView handle, use **findViewer** function. Result won't be received if XenoView wants to pause simulation (until simulation is unpaused).
  Returns:
  0 if XenoView was not found
  0 if XenoView does not want to stop simulation;
  1 if XenoView wants to stop simulation;

- **SimulationStopped**: Integer
  Sends message to XenoView that stop signal was received. Returns 0 if XenoView was not found, 1 otherwise.

- **SimulationError**: Integer
  Sends message to XenoView that simulation finished with error. Returns 0 if XenoView was not found, 1 otherwise. XenoView will show error message from "cmdLine.err" file located in program directory.

1.17 Data Plot Format

XenoView program supports **XenoPlot graphic format** for 2D data plotting. For more information about this format, see Plot Drawing

The default graphic settings are stored in the template file with name **default.xtp**. If this file does not exists in XenoView directory, it will be created with the default values assigned.

2D Graph may be copied to the *clipboard* as a graph and pasted to another graph window or XenoPlot graph window, or copied as an image to be retrieved by external program.

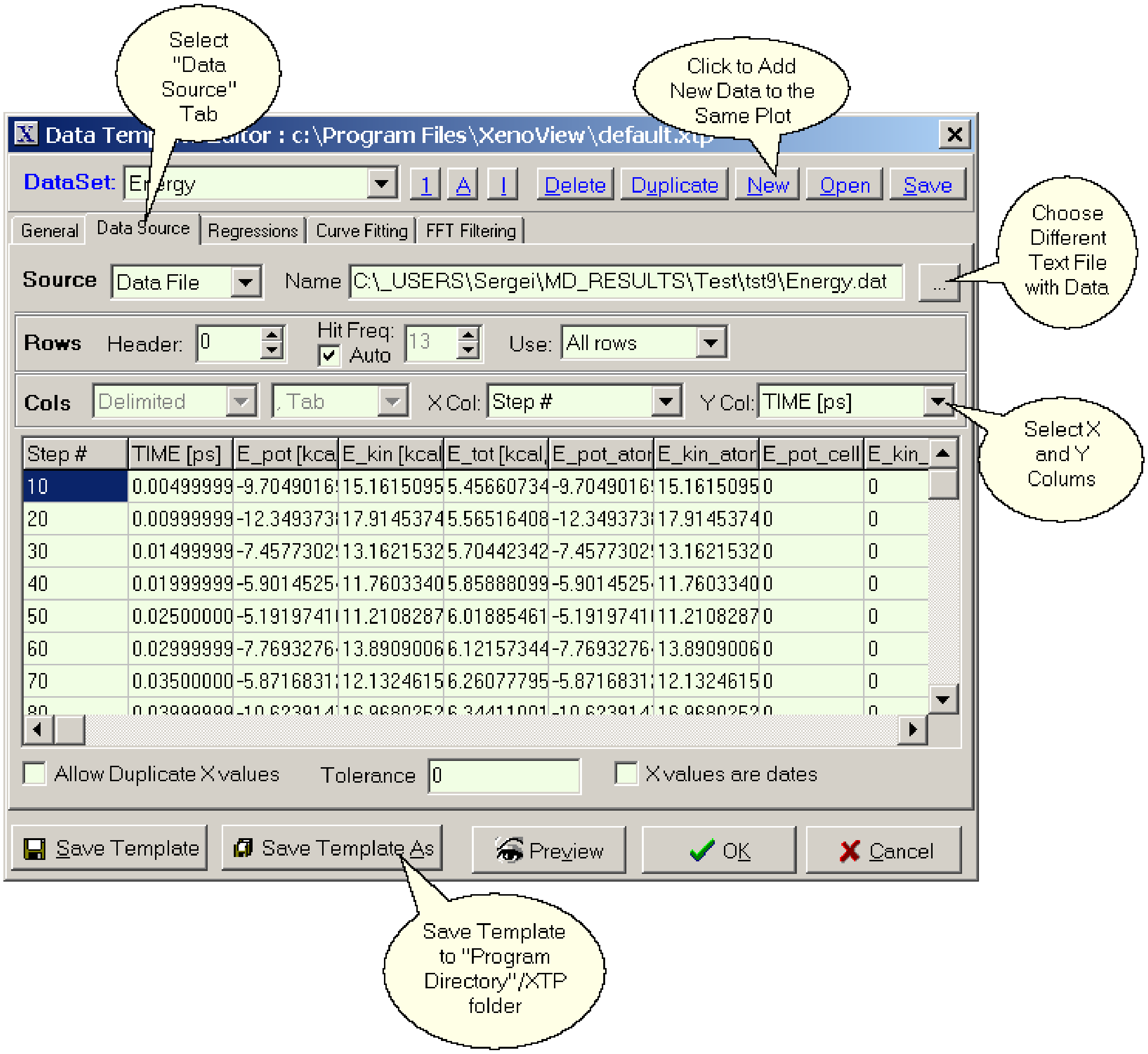
1.18 Creating Data Template

You may create your own data template to store your DataSet settings (names of DataSets, data source information, regression settings, colors etc.) and Graph appearance (legend, axes, colors, fonts etc.). The easiest way to do this is to *plot data from your text file*.

1. Open plot window for your structure by **Simulation -> Show Results** command;

2. Open you text file by **File -> Open** command (select 'ASCII data file' type in the open dialog);

3. If data columns in the file are TAB or comma - separated, simply select X and Y columns your want to plot. Otherwise first specify column width:



Select "Data Source" Tab

Click to Add New Data to the Same Plot

Choose Different Text File with Data

Select X and Y Colums

Save Template to "Program Directory"/XTP folder

Data Template Editor : c:\Program Files\XenoView\default.xtp

DataSet: Energy

Source: Data File Name: C:_USERS\Sergei\MD_RESULTS\Test\tst9\Energy.dat

Rows Header: 0 Hit Freq: 13 ☑ Auto Use: All rows

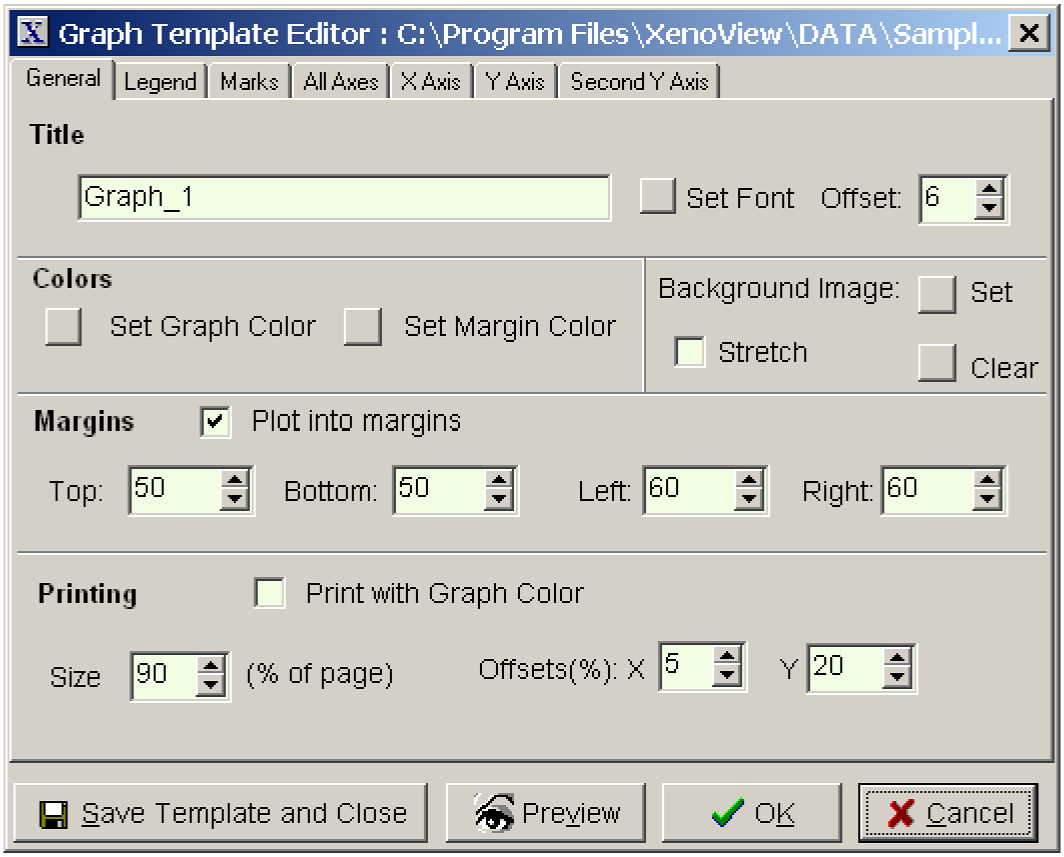
Cols Delimited , Tab X Col: Step # Y Col: TIME [ps]

Step #	TIME [ps]	E_pot [kca	E_kin [kcal	E_tot [kcal,	E_pot_ator	E_kin_ator	E_pot_cell	E_kin_
10	0.00499999	-9.7049016	15.1615095	5.45660734	-9.7049016	15.1615095	0	0
20	0.00999999	-12.349373	17.9145374	5.56516408	-12.349373	17.9145374	0	0
30	0.01499999	-7.4577302	13.1621532	5.70442342	-7.4577302	13.1621532	0	0
40	0.01999999	-5.9014525	11.7603340	5.85888099	-5.9014525	11.7603340	0	0
50	0.02500000	-5.1919741	11.2108287	6.01885461	-5.1919741	11.2108287	0	0
60	0.02999999	-7.7693276	13.8909006	6.12157344	-7.7693276	13.8909006	0	0
70	0.03500000	-5.8716831	12.1324615	6.26077795	-5.8716831	12.1324615	0	0
80	0.03999999	-10.623914	16.9680252	6.34411001	-10.623914	16.9680252	0	0

☐ Allow Duplicate X values Tolerance: 0 ☐ X values are dates

4. Click '*Save Template As'* button. To make template available for automatic loading, save it to the "XTP" folder in XenoView working directory.

5. You may edit your template using two dialogs: *Data Template Editor* and *Graph Template Editor* which may be open by **Graph -> Edit Graph** command:



Graph Template Editor : C:\Program Files\XenoView\DATA\Sampl...

Title

Graph_1 ☐ Set Font Offset: 6

Colors

☐ Set Graph Color ☐ Set Margin Color

Background Image: ☐ Set

☐ Stretch ☐ Clear

Margins ☑ Plot into margins

Top: 50 Bottom: 50 Left: 60 Right: 60

Printing ☐ Print with Graph Color

Size 90 (% of page) Offsets(%): X 5 Y 20

2 XenoPlot Help

2.1 Content

2.2 Introduction

XenoPlot is the program for importing, plotting, and analysis of experimental data. The major part of it's code was taken from free old version of **xyGraph** component from © Kestral Computing. **XenoPlot**

is used to plot simulation results from XenoView program.

Main features of XenoPlot:

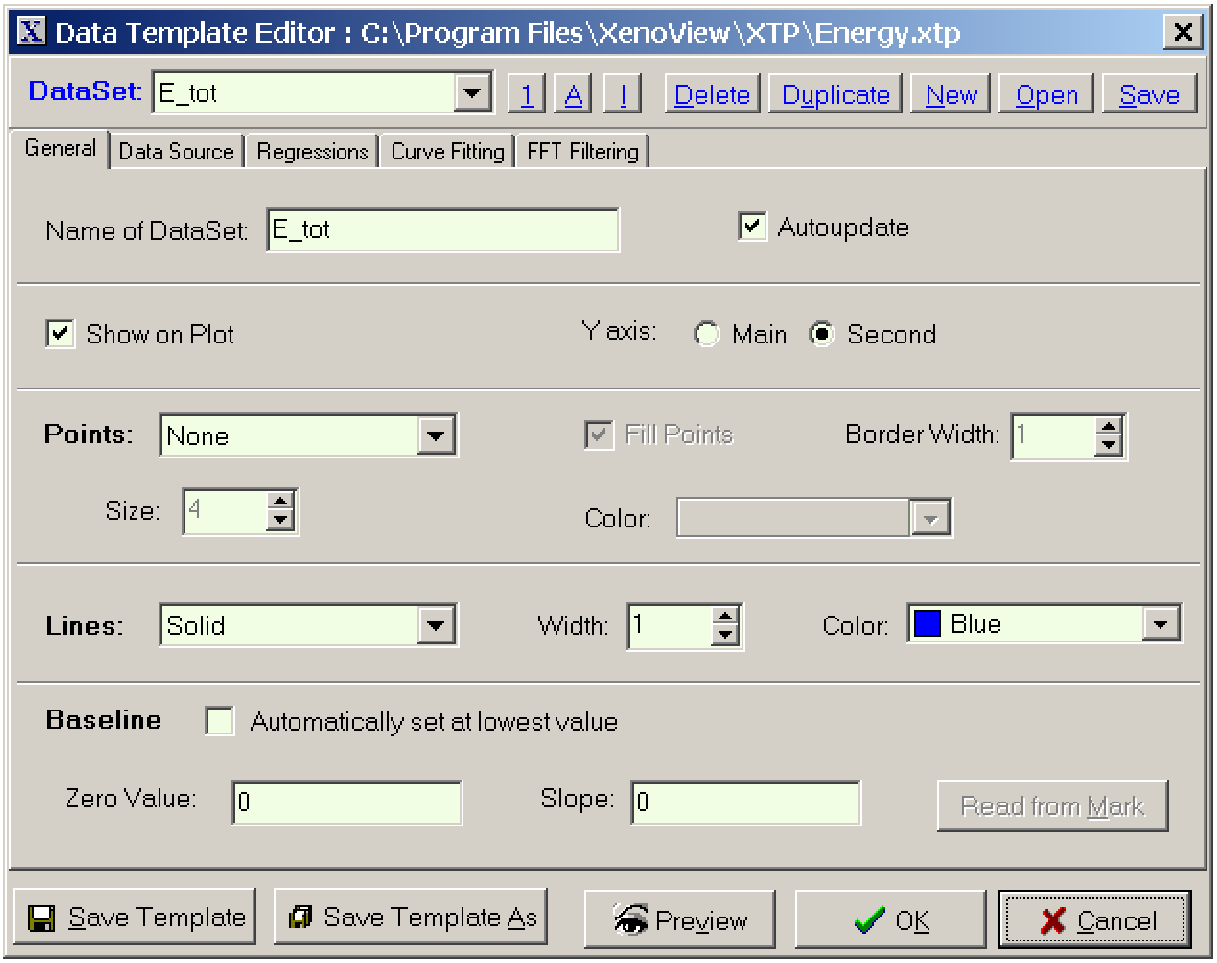
- Data may be imported from text files or databases;
- Selective filtering may be applied to the data using fast Fourier transform;
- Data curves may be smoothed with different types of regressions;
- Fitting of the results with custom functions using Curve Fitting procedures;
- Printing of the drawing;

2.3 Drawing Format

The Drawing Contains the following Data:
Graph Appearance (color, size, marks etc.);
Dimensions;
All Axes ;
Legend;
All DataSets with data points, references to the data files etc...
DataSet appearance (points, lines, colors etc.);
Curve fitting settings;
Regression settings;

The graph may be stored in the file with ***.xgr** extension. You may print it, make some analysis or export data from it to the text file.

The **graph data template** stores all graph settings except for the data points. However, if the source data file associated with the DataSet exists, these points will be automatically loaded. To make DataSet independent from its data source (text files etc.), you may convert it to **Manual** format. To do this, open **Data Template Editor** by *Graph->Edit Data* command from main menu (or by *Edit Data* command in pop-up menu), go to '**Data Source**' page and change '*Source*' setting to '*Manual*'.



Data Template Editor : C:\Program Files\XenoView\XTP\Energy.xtp

DataSet: E_tot

Name of DataSet: E_tot

☑ Autoupdate

☑ Show on Plot

Y axis: ○ Main ● Second

Points: None

☑ Fill Points

Border Width: 1

Size: 4

Color:

Lines: Solid

Width: 1

Color: 🟦 Blue

Baseline □ Automatically set at lowest value

Zero Value: 0

Slope: 0

2D Graph may be copied to the *clipboard* as a graph and pasted to another graph window or XenoPlot graph window, or copied as an image to be retrieved by external program.

2.4 XenoPlot Mouse Procedures

You may use the following mouse procedures in the XenoPlot graphic window:

- To **ZOOM** the **FRAME**, hold the Shift key down and drag cursor across the area you want to enlarge (press Left Mouse button while dragging);

- To **UNDO FRAME ZOOM**, hold the Shift key down and click Left Mouse Button (or click central mouse button);

- To **ZOOM** IN or OUT, rotate mouse wheel (use "Auto zoom all" option in pop-up menu to return back);

- To **OFFSET** plot area, hold the Ctrl key down and drag the plot area (use "Auto zoom all" option in pop-up menu to return back);

- To **MOVE** the **LEGEND**, hold the Ctrl key down and drag the legend, holding it on the Upper Left angle;

- To **RESIZE** the **LEGEND**, hold the Ctrl key down and drag the legend border;

- To **MOVE** the **MARK**, hold the Ctrl key down and drag;

- To **MOVE** the **BORDER**, of the margin hold the Ctrl key down and drag;

- To **DRAW** the temporary **TRACE**, hold the Alt key down and drag. These traces are erased after redraw;

- To **TOGGLE** the **MARKS** ON/OFF use Left mouse button dbl click;

- To open **POPUP menu** click Right mouse button;

- To check **MOUSE POSITION** and **POINT POSITION** in the current DataSet press Left mouse button;

- To **MOVE** the inserted GRAPH, drag it, holding it on the *upper left* corner;

- To **RESIZE** the inserted GRAPH, select it and drag the *bottom right* corner;

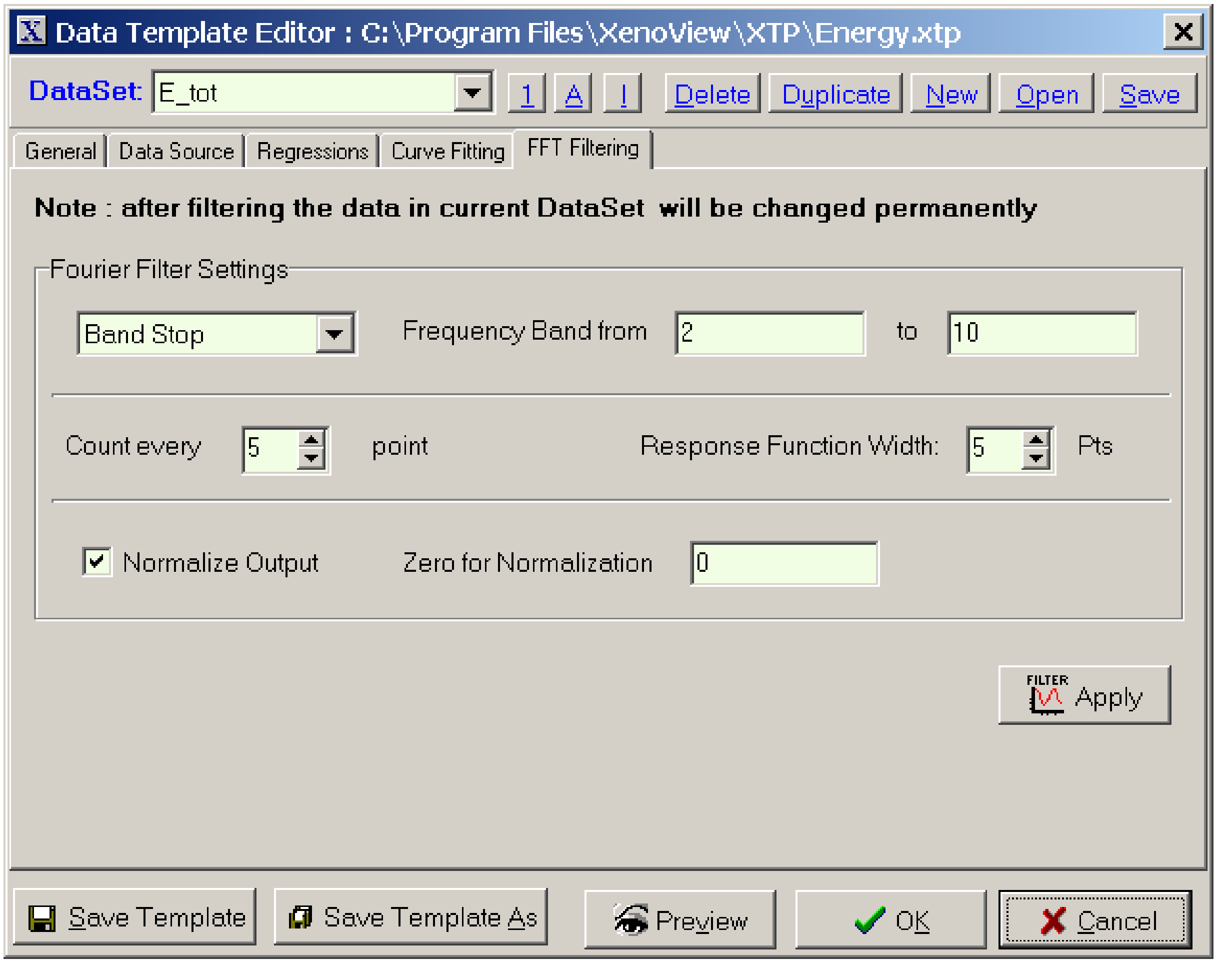
2.5 FFT Filtering

The selective filtering procedure is based on the **Finite Impulse Response Digital Filter (FIRDF)** adapted from:

Okan K. Ersoy "*Fourier-Related Transforms, Fast Algorithms and Applications*"// Prentice Hall PTR, NJ, 1997

Filtering can be applied only permanently. To smooth the calculated data on the reversible basis, use regressions instead.

Filter parameters can be verified and changed through the Edit Data|FFT filtering dialogue:



Data Template Editor : C:\Program Files\XenoView\XTP\Energy.xtp

DataSet: E_tot

Note : after filtering the data in current DataSet will be changed permanently

Fourier Filter Settings

Band Stop

Frequency Band from 2 to 10

Count every 5 point

Response Function Width: 5 Pts

☑ Normalize Output

Zero for Normalization 0

Filter parameters are:
- Band Stop or Band Pass - cut off or pass the frequencies specified;
- Frequency Band : the frequency range to be passed or filtered out;
- Count Every "given number" Point : skip ("given number" - 1) of points and pass one to the filter (the original number of data points will be restored after filtering);
- Response Function Width : the width of filter response function, points;
- Normalize Output : normalize the resulting data to keep the same area under the curve;
- Zero for Normalization : the baseline for normalization (0 by default);
- Apply button : apply filter to the data loaded to Data Editor permanently. To discard this changes, close the editor with "Cancel" button;

Note : it is recommended to use "Preview" option of the Edit Data dialogue to check the results of filtering and cancel them, if necessary.

2.6 Regressions

Regressions are procedures for smoothing of experimental points. Original data points may be not shown on the plot. If the original data points are hidden, the "*export ASCII*" procedure takes only smoothed data points and writes it to the data file.

Different types of the regressions may be chosen from the "*Edit* | *Edit Data*" Dialogue Menu:

1. Linear Least Squares - fits data with the line;

2. **Quadratic Least Squares** - fits data with parabola;

3. **Passing Bablok** - from Bablok W, and Passing, H.: "Application of Statistical Procedures in Analytical instrument testing", J. Auto. Chem. v7, 1985, pp74-79. (no parameters required)

4. Running Average - simple averaging between data points. Parameter **1/**α gives the approximate number of points to be averaged.

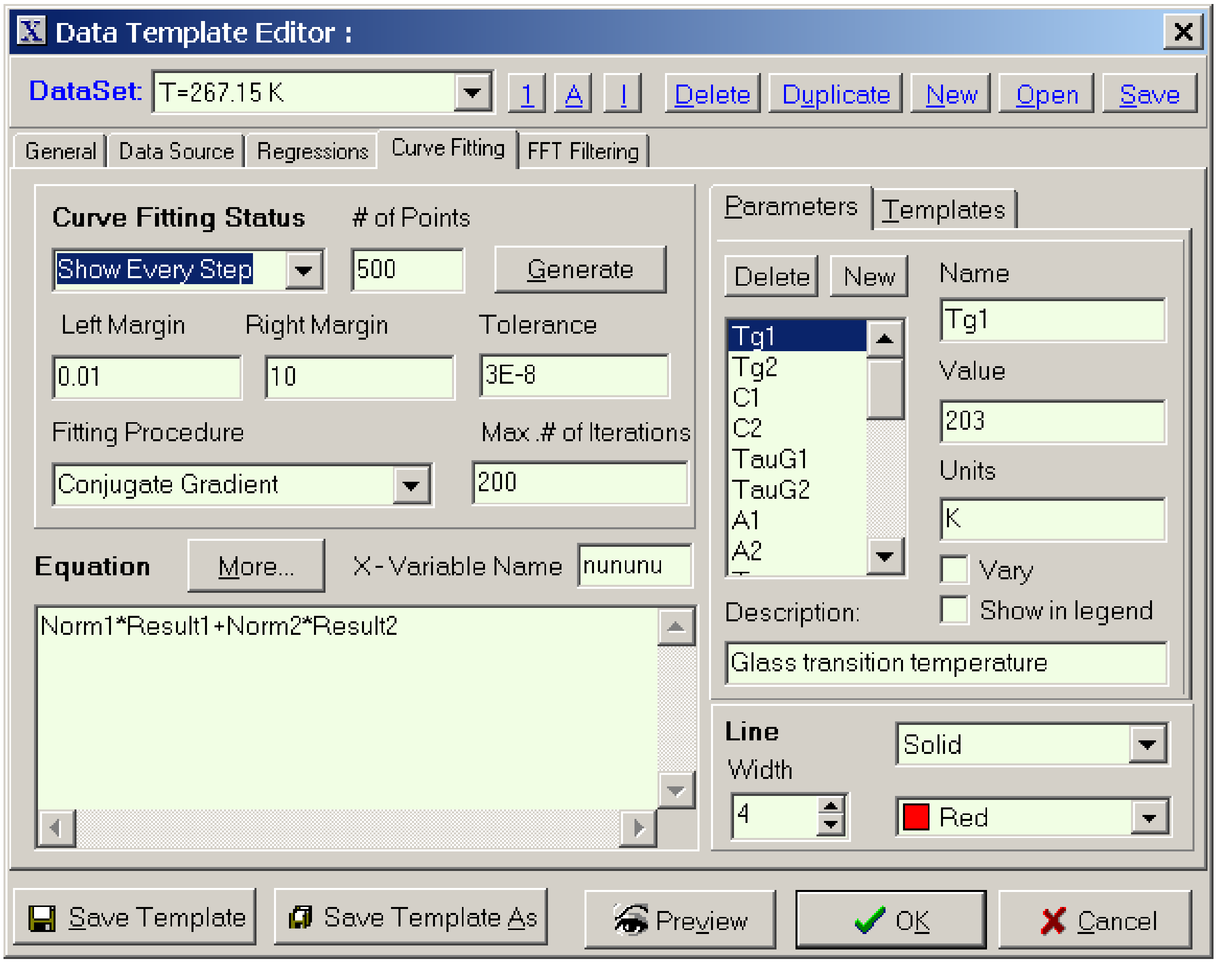
5. Spline - algorythm from the "Numerical Recipes in Pascal" toolkit. Takes gradient at the end as a parameter.

6. Nonlinear least squares - usually gives the best result. For more details, see *Distance Weighted Least Squares* algorythm in McLain DH.: "Drawing Contours from arbitrary data points." *Comp. J.,* v17, 1973? pp 318 **-** 324; **Fitting tension** parameter is used to control smoothing quality.

To fit data points with special type of equation and find fitting parameters, use Curve Fitting procedures.

2.7 Curve Fitting

Curve fitting procedures allow you to write explicit equation that you want to use for fitting of the datapoints.
To perform curve fitting, open the Data Editor by "Edit -> Edit Data" command from the main menu and go to the *Curve Fitting Page*:



DataSet: T=267.15 K

Curve Fitting Status: Show Every Step

# of Points: 500

Left Margin: 0.01

Right Margin: 10

Tolerance: 3E-8

Fitting Procedure: Conjugate Gradient

Max.# of Iterations: 200

Equation

X-Variable Name: nununu

```
Norm1*Result1+Norm2*Result2
```

Tg1
Tg2
C1
C2
TauG1
TauG2
A1
A2

Name: Tg1

Value: 203

Units: K

☐ Vary

☐ Show in legend

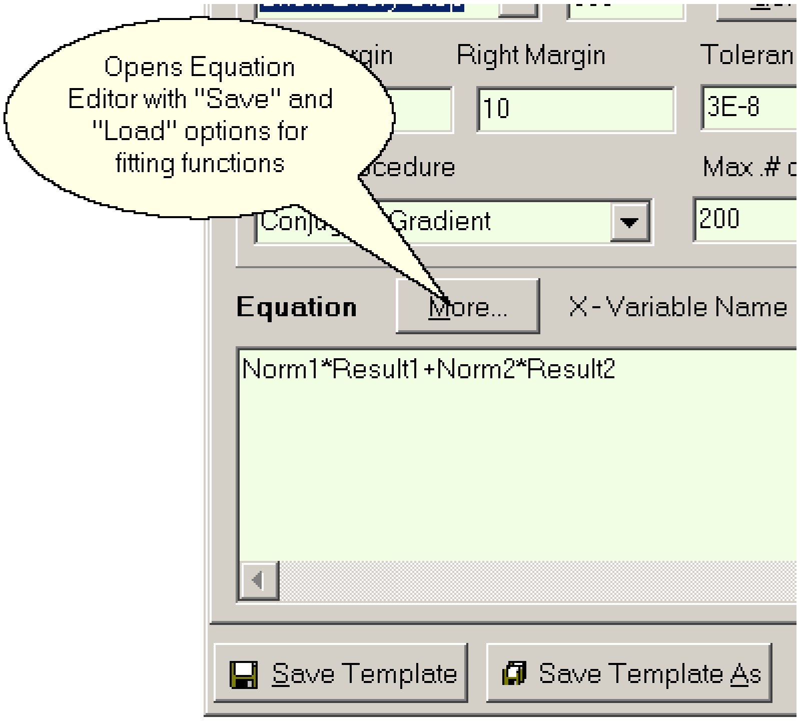
Description: Glass transition temperature

Line: Solid

Width: 4

🟥 Red

You may save your custom fitting functions to the file with ***.xfn** extension. This option is available from **Equation Editor** dialogue. Use *Data -> Curve Fitting -> Edit* option from the main menu:



Norm1*Result1+Norm2*Result2

2.8 Printing

- You may print the drawings both in Landscape or Portrait orientations. This option may be changed from Printer Setup dialogue.
- The scaling / offset printing options may be adjusted from the *Edit -> Edit Plot* dialogue menu.
- To suppress Color background everywhere except for the Legend, uncheck "Print with Graph Color" option from the *Plot Editor* dialogue:

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Endnotes 2... (after index)

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