Guide to Kalypso 1.0

Contents

Introduction

Kalypso is one of 3 programs which constitute the core of the Kalypso package (the other major programs are Spider and Winnow). Kalypso is the 'engine' which actually performs the numeric computations required for the simulation. (Spider prepares the input files used by Kalypso, while Winnow processes the output files.)

This document is derived from the Kalypso online Help file (with minor omissions and changes). The Help file focusses on the commands needed to run simulations, but does not discuss the details of creating simulation projects. For this, you should consult the documentation which accompanies the Kalypso package (in the `docs` directory).

Getting Started

For a step-by-step guide to running a simulation, see next section.

To see the function of a speed button, hold the mouse cursor over it until a hint box appears. You will normally use the Run speedbutton (or File|Run menu command) to start a simulation, and the Abort speedbutton (or Ctrl-C) to stop it prematurely.

The best way to get started with Kalypso is to load the tutorial project and some of the example projects (found under the examples directory) into Kalypso. Once you have sucessfully achieved this, you can begin loading some of the example files into Spider for modifications. You may be able to use some of these files (after modification) as templates for your own projects. Begin cautiously with simple changes such as the projectile type and/or energy. As you make each change, click the help button on the dialog box (or hit the F1 key) to get information about the associated parameter. View the readme.txt file in the \examples directory before you attempt to run any example projects.

Before you commit yourself to running a huge simulation with a 'realistic' target, it is always a good idea to carry out some test runs using a 'toy' target. This will help you to fine tune some of the simulation parameters, including the time step.

The Options|Simulation command gives you an opportunity to run the simulation in the most efficient way.

Step-by-Step Guide

These instructions are mainly intended for new users of Kalypso. Previous users of the Simulation Kit will have no trouble running the new program version.

- Click on the yellow folder icon, or select 'Specify input files' on the File menu. A dialog box comes up.
- Click on the topmost button labelled 'Select' (for projectile data).
- Select a file of extension 'prj' (e.g. under the \kalypso\examples directory), and close the dialog box (the 'Open' button). Notice that all the other files needed by the project were found at the same time (you can select individual files one by one if you need to override this behaviour). See the file `readme.txt` in the examples directories for information about the various example projects distributed with this version of Kalypso, before you attempt to run them. You have now specified your input files.
- You can start the simulation by clicking the Run button or by selecting Run from the File menu.
- A message box comes up, asking whether you want to proceed. You may drag the message box to one side and inspect the messages in the editor to see that all parameters are correct. Click the Yes button.
- The simulation now runs. The status line at the bottom of the window tells you how many timesteps have elapsed, and reassures you that something is happening.

- If you want to see a visual representation of the collision cascade, open the graphing window by clicking on the Graphing button (blue sphere). Explore the effect of the various options in the menu.
- The simulation will now run to termination without need for intervention by the user. If you want to stop the simulation, click on the Halt/Abort button. You can start the simulation from the beginning by clicking the Run button again.

The Options|Simulation command lets you set up the simulation for running in the most efficient way.

If you want to explore the program's capabilities beyond the example projects, the next step is to examine the program Spider, and work through its documentation. Spider will allow you to create simulation projects according to your own specifications.

Specify Input Files

Summary

Kalypso needs information from 5 or 6 input files in order to run a simulation. These files will be used to load data specifying the projectile and target characteristics, and the details of the simulation model. The designations of these input files, and their default extensions, are as follows:

- projectile file (.prj)
- target file (.trg)
- model file (.mdl)
- run file (.run)
- impact file (.imp)
- inelastic file (.inl) - this file is optional

Use the 'Select' buttons to open up a file dialog box where you select the input file(s) which you want to use. If the Inelastic file option is disabled (dimmed), it means that you have not chosen to incorporate inelastic effects in your simulation. If you wish to do so, you need to select one or more inelastic loss models from the Simulation Options dialog box. The inelastic file is only needed for simulations that include inelastic effects.

Tips

Specify the .prj file first. When you specify the .prj file, Kalypso by default looks for other input files with the same stem name, and loads them into the dialog box. You can overwrite any of these default file names if you choose by clicking the appropriate Select button.

Note: Input files are created using the Spider program.

Specify Output Files

Summary

Use this option to specify names for the output files generated by Kalypso. These are called inivars.snk, dynvars.snk and inelastic.dat by default. The first file, which simply records the initialised state of the system, will only be created if you enable the corresponding option in the Options|Simulation dialog box. For most applications you don't need this file.

The type of data which are written to dynvars.snk is determined by the options specified in the simulation's .run input file (see the Spider Help for details). This file will normally contain the information generated by your simulation.

The last file (inelastic.dat) is an ascii text file which contains information about any discrete

inelastic energy processes which occurred in the course of the simulation. The Options|Simulation checkbox "Record Inelastic Events" must first be selected, otherwise the events are not stored. You will only need this file if your interest is in inelastic processes in themselves. The file format is described here. If you are not including inelastic effects in your simulation, you can ignore this parameter.

Tip

It is a good idea to save your output files in the directory which contains your input files. (By default, the output files will be written to the directory where Kalypso resides.)

Inelastic Data File

File Format

The inelastic data file (*.dat) is an ascii file consisting of 1 line per recorded inelastic event with the following format:

```
RC, i, j, dE,rlast, rcurr, zapsis, ti, Erel, idx, mod, Ne
```

where:

- RC = run counter (1, 2, 3 ...): the simulation run in which the event occurred
- i, j = the 'row numbers' (in the TRG file) which label the atoms involved (NB. this number is zero for the projectile)
- dE = inelastic energy loss
- rlast = separation of atoms i and j before the inelastic algorithm was applied (in A)
- rcurr = separation of atoms i and j after the inelastic algorithm was applied (in A)
- zapsis = depth at which the inelastic event took place (in A)
- ti: time elapsed at the moment of the event(fs)
- Erel = relative energy of the collision responsible for the event
- mod = label for the inelastic model (= 0 for Oen-Robinson, = 1 for Shapiro-Tombrello)
- Ne = Number of electrons promoted (only Shapiro-Tombrello has non-zero values)

No special support is provided for further analysis of inelastic data files. If you need to analyse them, you will have to write your own routines.

Run

Summary

This option starts a simulation, based on the specifications contained in the input files which you selected previously. After data have been read from the input files, you will be prompted for confirmation: at this point you should check the overview of simulation conditions which is presented on the screen.

Tips

To abort a running simulation you can use the speed-buttons, or hit the Ctrl-Break key combination.

Step (and Abandon Current Run)

Summary

This command is only available as a speed-button short cut.

It causes the current run to be abandoned. The simulation then proceeds with the next run (if any). To use this option, you must have the "Enable Stepping" button in the checked state before

the simulation run begins. This is a safety feature, to prevent accidental stepping during an important series of runs.

Abort

Summary

This command is only available as a speed-button short cut, or as a hot-key short-cut (Ctrl-Break). It causes the current simulation to be aborted.

Clear Page

Summary

This command is only available as a speed-button short cut. It causes the edit window page to be cleared. The contents of the edit window are lost.

Batch Run

Summary

This command executes a sequence of runs, based on input files specified in a user-supplied definition file. You can run batch jobs in the background while you work on other programs, or you can run them over the weekend. All you need to do is specify the name of the definition file which defines your batch jobs.

To run Kalypso in batch mode, you need to prepare a definition file which contains the names of your 5 input files and 2 output files for every simulation. You can name the file however you like. Lines 1, 11,... of the file are comment lines (which may be left empty if you choose). The comments will be displayed as the simulations run (so that you can gauge the progress). The example below shows the format for 2 simulations.

```
Your comment here (line 1)
c:\kalypso\copper\copper.prj
c:\kalypso\copper\copper.trg
c:\kalypso\copper\copper.mdl
c:\kalypso\copper\copper.run
c:\kalypso\copper\copper1.imp
c:\kalypso\copper\copper.inl
c:\kalypso\copper\inivars1.snk
c:\kalypso\copper\dynvars1.snk
c:\kalypso\copper\inelast1.dat
Your comment here (line 11)
c:\kalypso\copper\copper.prj
c:\kalypso\copper\copper.trg
c:\kalypso\copper\copper.mdl
c:\kalypso\copper\copper.run
c:\kalypso\copper\copper2.imp
c:\kalypso\copper\copper.inl
c:\kalypso\copper\inivars2.snk
c:\kalypso\copper\dynvars2.snk
c:\kalypso\copper\ielast2.dat
```

In this case, Kalypso will execute both sets of simulation data in succession, unless interrupted by the user. Note the order in which the various files are specified (prj,trg,mdl,run,imp,inl,snk,snk,dat): it is the responsibility of the user to ensure that this order is maintained, and that all necessary file names are listed (9 per simulation). (Even if your project does not use the "inivars" and inelastic data output files you must still specify something on the

appropriate lines.)

The Utilities menu of Spider has an option that will allow you to generate batch file templates far more efficiently than you can do by hand.

Save Log to File

Summary

This command writes the contents of the log editor window to a disk file. The disk file has a "rich-text" (rather than plain text) format.

Load File into Log

Summary

This command allows you to load a plain text or "rich-text" file into the log editor window. The current contents of the edit window will be lost.

Print Log

Summary

This command initiates printing of the current contents of the log editor window.

Graph Window

Summary

This command opens the graph window, which displays a plot of particle positions or velocities as the simulation runs. The plotting mode (particle positions or velocities) is determined by the selection made in the Options|Simulation dialog box (default is positions).

The graph window is only available after the input files for the simulation have been specified. The window can also be opened by clicking on the graph speedbutton.

The window display is only updated when a simulation is running. If you resize the window at other times, its graphical display is lost. The graphing window projects the coordinates or velocities of atoms onto a selected plane (xz, xy or yz). The display is very simple, and consists either of sphere-like 'icons', circles or dots plotted at the coordinate positions. The time in fs (10^{-15} s) is indicated at the top corner for each frame plotted. The graphing options are selected via the menu on the window itself.

The screen display is updated at intervals determined by the 'Update Time' parameter in the Run file (typically set at about 10 timesteps). Graphing coordinates takes a lot of time, so always keep the graphing window closed when you want to run the simulation at full speed (i.e. for intensive computations).

Bear in mind that the timestep intervals tend to increase towards the end of the simulation (see Spider Help for more about this). Although the particles are slowing down (by orders of magnitude) this is not evident in the motion seen on the screen, which begins to look almost 'explosive' after 100-200 fs, contrary to reality. You can eliminate this effect by selecting a 'fixed timestep' option in the Options|Simulation dialog box.

Graph: Perspective

Specifies onto which plane coordinates are projected. In Kalypso, the z-axis is parallel to the

surface perpendicular; the xz-plane is shown by default, which represents a 'side view' of the system; the xy-plane is the 'view from above.'

Graph: Copy Image

Copies the graphical display as a bitmap to the Windows clipboard. You can then paste it into a document or image processing program.

Graph: Zoom

The Zoom In option enlarges the graphical display, while the Zoom Out option reduces it.

Graph: Symbols

The Symbols sub-menu offers options to plot icons, circles or 'points' at atomic positions. Different displays will probably appeal to different users. Unless the Highlight option is active, the projectile position is distinguished from the target by plotting as a different colour (using either red circles/dots or blue icons).

If the Draw Small option is selected, icons and circles will be displayed at a smaller size when either of these symbol selections is active (no effect on point plots).

Graph: Refresh Each Step

If this option is selected, the image will be redrawn after every timestep; otherwise, the old image will be overwritten (giving a 'bubble chamber track' effect in the display).

Graph: Reset Defaults

This option sets the display parameters to their default values.

Graph: Highlight

This option provides some depth information in icon plots. For example, consider an icon display plotted from the xy perspective. Then the z-axis represents the dimension of depth perpendicular to the screen. The highlight option plots in blue any particle for which z is greater than 1 Å (1.0E-10 m). You may find this useful, for instance, for identifying ejected atoms.

Graph: Toggle Background

This option toggles the background colour of the graph window image between black and white. (The black background option is only active when the plot Refresh option is enabled.)

Graph: Hot Keys

The hot keys for the graphing window are:
arrow keys: shift image on screen (small shift)
Shift+arrow keys: shift image on screen (large shift)
Short-cut keys for the menu options are displayed on the menu, as well as on the status line at the bottom of the window. In most cases, they take the form Ctrl+Letter.
You can double-click the graphics screen to pause the display.

Spider

Summary

This command allows you to run the program Spider (spider.exe). This routine first assumes that spider.exe is located in the default installation directory (\kalypso\bin); failing that, it attempts to launch spider.exe from the directories on your PATH statement specified (in autoexec.bat). If that also fails, then you are prompted for the location with a file dialog box.

Tips

It is often useful to run Spider when you are setting up a simulation project, so that you can quickly see the effects of modifying simulation parameters such as the timestep.

Winnow

Summary

This command allows you to run the program Winnow (winnow.exe). This routine first assumes that winnow.exe is located in the default installation directory (\kalypso\bin); failing that, it attempts to launch winnow.exe from the directories on your PATH statement specified (in autoexec.bat). If that also fails, then you are prompted for the location with a file dialog box.

Edit Menu

Summary

The Edit menu interacts with the edit window which records the progress of, and error messages from, simulations. You can select, copy, cut and paste text and images to/from the Windows clipboard. No Help topics are provided for these operations, which are similar to those used by ordinary word processor applications.

Edit menu commands are available even while a simulation runs. However, some (not all) image pasting operations may fail if you execute them while a simulation is running. (This is a low-level problem which can only be "fixed" by disabling all pasting operations during a run.) Text pasting operations can be safely carried out even during a simulation.

The editor buffer can be emptied by clicking on the white page speedbutton. The edit buffer is emptied periodically as simulations are run. This is to avoid wasting CPU and memory resources. The default buffer is 500 lines, but this can be modified in the Options|Simulation dialog box.

Options Menu

Summary

The Options menu offers options to specify the computational details of your simulation (the Simulation command), and to specify the font and colour used by Kalypso's edit window (the Font and Colour commands respectively).

Simulation Options

Summary

The Simulation Options dialog box gives you the opportunity to fine-tune the way the simulation runs.

Here is the normal selection of options used to perform the simulation at maximum speed on a large (500+ atoms), elemental target:

- Integration Algorithm: Verlet
- Verbose Reporting: No
- Report energy: No
- Report inelastic loss: No
- Assume elemental target: Yes (only if elemental target)
- Fixed Timestep: No
- Neighbour list search: Box method
- No y-vibration: Yes [ICISS simulations only]

Note: for very fast simulations, like those used for ICISS, the time required for screen updates will become the limiting factor. You should shrink the program window to a bar (or minimise the application) if you don't need to monitor it.

The check-boxes at the bottom of the dialog box allow you to save the options to disk, and/or reload them when Kalypso next starts. The name of the options file is kalypso.cfg. You can delete this file later if you do not need it, but it is better to archive it with your project..

Integration Algorithm

[This option is not used currently by Kalypso, so disregard the following]

Summary

Kalypso offers a choice of 4 different integration algorithms. The default option is the Verlet algorithm, which is suitable for virtually all purposes. The other options were originally included for testing purposes by the author.

You can read about the different algorithms in: R. Smith and D.E. Harrison, Jr., Computers in Physics, 3 (1989) 68-73, as well as in the Simulation Primer which ships with the Kalypso package.

The Verlet algorithm is fast, as well as being economical with resources, and seems to be the favourite choice of the particle-surface community. The Beeman algorithm should be used with a fixed timestep, and is slow for that reason in normal applications. The Two Step A algorithm was reported to be more accurate than Verlet in the above paper, but my own experience does not bear this out (possibly because of the way Kalypso handles timestep variations). Usually, you will find that the Two Step and Verlet energy errors are of a different sign. Verlet tends to overestimate scattering angles, while Two Step underestimates them.

The HGE B algorithm is the most time- and memory-intensive of these algorithms, without being noticeably better than the Two Step algorithm, so its use is not recommended.
The inelastic loss models are only implemented for the Verlet algorithm (Kalypso will remind you of this, so you don't need to remember it).

Screen Output

Summary

There are 3 options which control screen output from a simulation.

- Verbose: Maximum possible screen output is generated. Useful when setting up a simulation.
- Report Energy: Reports energy conservation and, if Verbose mode is active, momentum and angular momentum conservation. The energies reported by this routine take into consideration inelastic losses (other than cooling) and cut-off effects, and therefore differ from true thermodynamic energies (see Lattice and Cohesive energy topic below). The purpose of the calculation is to detect energy leaks which are not accounted for by conversion processes. These leaks are either due to integration errors or to precision errors associated with the OR and ST inelastic models. Integration errors are usually caused by timesteps which are too large, or by non-optimal specification of the r0 parameter(s) in the attractive potentials.
- Report Inelastic Loss: Reports the energy lost due to inelastic processes (if any). You can write this information to disk using the 'Inelastic events to disk' option.
- Lattice and Cohesive Energy: Reports the true (thermodynamic) lattice energy, and the cohesive energy for the specified lattice site index in the Target file before the simulation commences. The calculations use the potential parameters read in from the Model file, including the potential cut-off. Neither of these quantities is relevant to simulations, but may be

useful for studying the properties of potentials.

You may like to use the lattice energy calculation to estimate the surface relaxation predicted by the potential. The method involves plotting the total lattice energy as a function of the surface interplanar spacing in a series of different Target files.

The cohesive energy calculation is only useful when the index refers to a bulk atom in an elemental target - the result should be similar to the experimental value of the cohesive energy, assuming the potential is correctly described in the MDL file. Note: the cohesive energy calculation has no simple interpretation for a binary target (in some cases it is related to the alloy heat of solution). The lattice and cohesive energy are normally calculated with the lattice vibration option disabled in the Model file (to ensure that atoms are at lattice sites). These calculations assume that all atoms are in locations covered by the attractive many-body potentials (i.e., that r > high spline node).

- Edit Buffer: Specifies the number of lines to keep in the edit window: the window is emptied if the size of the edit buffer is exceeded.

Screen updates take a lot of time, and can slow your simulations down considerably. When you are satisfied that the simulations are running correctly, you can disable the first three options to increase running speed.

Miscellaneous Options

Summary

These are options which you may need from time to time.

Assume elemental target

Kalypso can determine automatically whether your target is 'elemental' (homonuclear) or 'complex' (heteronuclear). (This information is needed because the force and potential calculations execute differently for the two cases.) This option allows you to "short-circuit" the detection method for an elemental target, which may result in time savings (particularly if the target is large). For a complex (binary) target you should always leave this option unchecked, otherwise an erroneous potential will be applied in the energy conservation and (if appropriate) spline force calculations (what happens in such cases is that the mass and atomic number of the anchor atom are assumed to hold good for all target atoms in certain parts of the calculation, but not all). For an elemental target you ought to check this option: but note that in the current version of the program this option has virtually no effect on running speed (so there is no great time loss if you ignore it).

Initial Conditions to disk

If this option is selected, the initial conditions of your dynamical system will be written to a disk file (named inivars.snk by default). For a multi-run simulation, this option should be disabled, since only data for the last run will be saved (the other data will be overwritten by the succeeding run). In practice, there is little reason to store this information.

Inelastic Events to disk

Writes information about discrete inelastic events to the inelastic data file (*.dat). Individual inelastic losses associated with the continuous LSS model are not recorded (because they take up too much space), but a summary is provided (see preceding link for file format).

Fixed Timestep

Normally you will not need to use this option, since the integration algorithms used by Kalypso (with the exception of Beeman) can run much more efficiently with variable timesteps. However,

you may find the fixed timestep is useful if you run a simulation for presentation purposes (giving a more realistic representation of the motion in the system) rather than for its numeric output.

Hot Target

This option initialises the target atom kinetic energies according to a Maxwellian distribution which has a mean value 3/2kT (T is read from the Model file data). There is a discussion about this procedure in the Simulation Primer (see chapter 8). The option only has an effect if the Model file specifies that thermal vibration effects are to be used. If the Hot Target option is not selected, the static thermal displacements will still be applied to lattice atoms. For most purposes you can ignore this option.

No y-vibration

The option only has an effect if the Model file specifies that thermal vibration effects are to be used. What it does is to suppress the application of thermal displacements in the y-direction; i.e. the lattice y-coordinates retain their value of the Target file (the ideal lattice). The option is useful (almost essential) in conjunction with simulations of Impact Collision Ion Scattering Spectrometry (ICISS) measurements, (see the Simulation Primer) but can otherwise be ignored.

Ignore Inter-Target Forces

This option ignores all target-target interactions (forces and potential energies), thereby speeding up the calculations. Projectile-target interactions are calculated as usual. Target atom velocities are updated after collisions with the projectile. The option is useful for processes like ion backscattering (ICISS), where target-target interactions play no significant role. The resulting simulation is somewhere intermediate between a 'BCA' and an 'MD' simulation, because multiple interactions of the projectile are taken into account as usual. **You must use the 'Brute Force' neighbour list method to realise these time savings, otherwise a normal, full-interaction. calculation will proceed.**

Self-Bombardment

Normally Kalypso treats the projectile-target interaction differently from the target-target interaction, in that the former always uses a screened Coulombic potential. You can override that behaviour by checking this option. This makes physical sense if your projectile species (atomic number) is the same as that of the target e.g. Cu projectiles bombarding a Cu target, or (for a binary target) the same as one of the elements in the target. The projectile-target potential parameters specified in the Model file will then be ignored. Instead, the target-target composite potentials will be used, with the assumption that the projectile atom is of the "A" type as specified in the Model file. In other circumstances you should not use this option (e.g. for the Ar-Cu system), because it is not physically sensible, and will lead to meaningless calculations.

Graph Window (Mode)

Summary

The graph window can display either:

- Particle positions (on a default scale of 10 pixels = 1 Angstrom)
- Particle velocities (on a default scale of 1 pixel = 100 m/s)
-

Note: the default scales can be modified via the graph window Zoom options.

Neighbour List Search

Summary

This option determines which algorithm is used for the range-search which is carried out each

time the neighbour lists are updated.

- For large lattices, the cell-index (or box) search method is the fastest (but not necessarily for small lattices), and can reduce simulation time by about 10%.
- For lattices with less than 500 particles, the brute-force method (described in the Simulation Primer, chapter 3) will probably be faster than the box method (you should check this for yourself).

Note

The cell-index search method is restricted to lattice zones (i.e. the particle initial positions + the potential cut-off distance) which can fit into a box whose x- and y-coordinates fall within the range -48 to +48 Angstrom, and whose z-coordinates fall in the range -48 to + 16 A. This corresponds to a very large lattice, and should not restrict you, but in any case, Kalypso checks that this condition is met.

Show Memory Use

Summary

This command shows a display the total dynamic memory (in bytes) allocated to variables in your program. This allocation will increase considerably while Kalypso is running a simulation. The information is mainly useful for debugging purposes.

Notes

You may notice that there is a small "memory leak" associated with the opening and closing of file dialog boxes. This is due to a known minor bug in the libraries of the compiler manufacturer. While undesirable, it is not cause for alarm.

It is also normal that the memory display may flicker and oscillate in an irritating way: this restless behaviour is characteristic of the Windows 95 memory management system.

Inelastic Loss Models

Overview

Select the inelastic loss models (if any) that you wish to incorporate into your simulation. The relevant parameters will be extracted from the *.INL (Inelastic) file of your simulation project. Note that the inclusion of inelastic effects is optional. Only the options you select here will be incorporated into your simulation.

Kalypso treats cooling effects as a form of inelastic energy loss. The energy loss associated with cooling is not tracked explicitly, so you can expect energy conservation to be violated when you use this option. To make sure that this energy loss is really due to cooling (and not integration errors or other causes), you should also run some simulations with the cooling option disabled. (This will show the energy loss from other causes.)

See the Simulation Primer for more information about inelastic loss models used by Kalypso.

Run Counter Offset

Summary

The Run Counter Offset allows you to start a simulation from the middle of the Impact file. The default value of zero (0) starts the simulation from line 1 of the impact file. A value of 2 would instruct Kalypso to ignore the first 2 lines of the Impact file,and to start from the third line. In this

case, the run number would take values 3, 4, 5... instead of the usual values 1, 2, 3.

Font Options

Summary

This command brings up a standard font dialog box which allows you to change the font used by the edit window (the selected font will be applied to the entire body of text in the editor).

Page Colour Options

Summary

This command brings up a standard colour dialog which allows you to specify the background colour of the edit window.