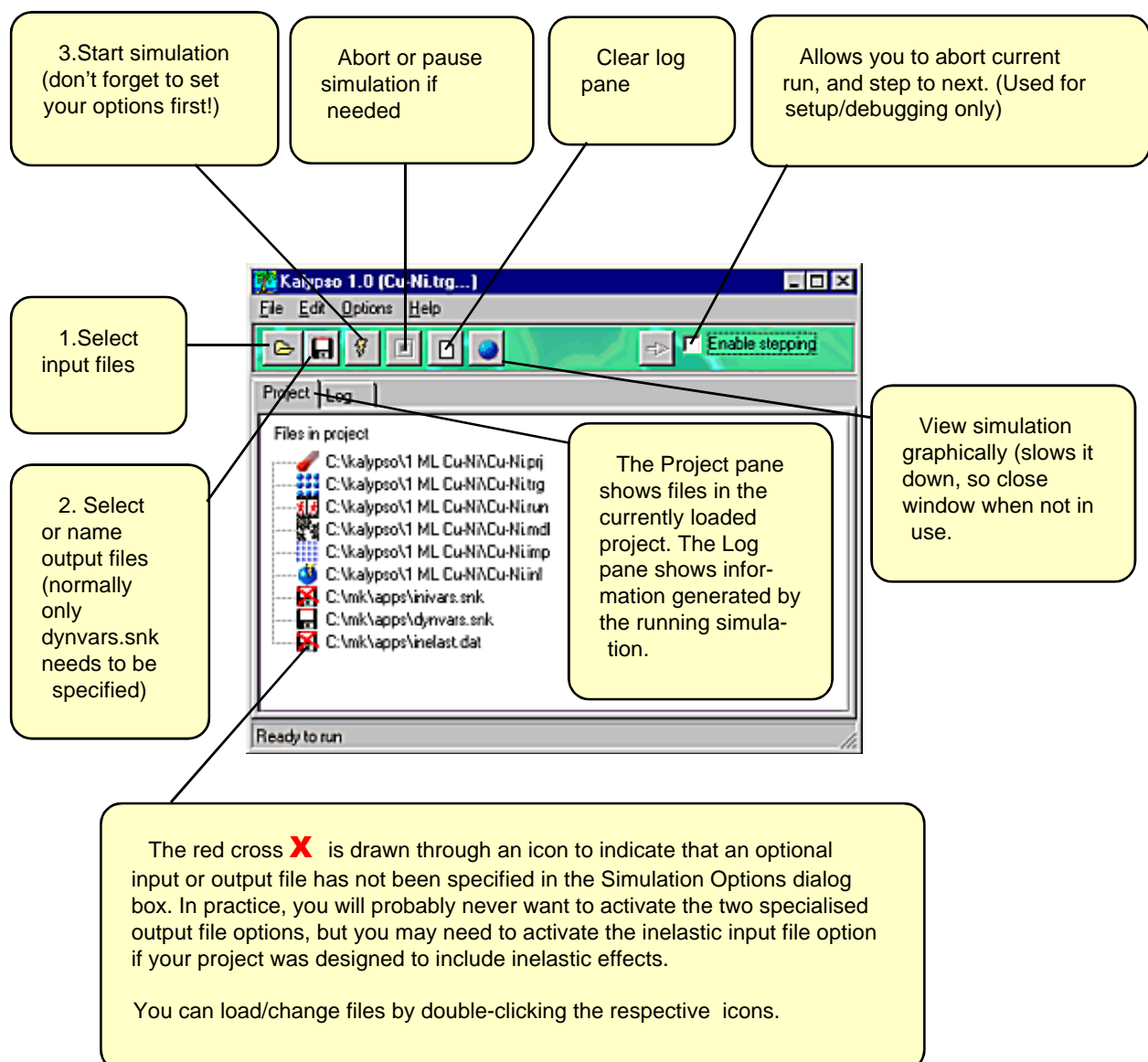# KALYPSO'S USER INTERFACE

The Kalypso program is the 'simulation engine' of the Kalypso package (which includes other programs like Spider and Winnow). Kaypso itself is relatively easy to use. You can run a simulation singly or as part of a batch job.

(a) Running a single simulation: You specify the names of your input and output files (File menu), select simulation options you require (Options menu), and click the Run button to start the simulation.

(a) Running one or more simulations as batch jobs: Select the simulation options that you require (Options menu), then execute the Batch Run command (File menu), which will load your batch job definition file (create these via Spider's Utilities menu).

To abort or pause a simulation, hit Ctrl-C or click the Abort button. Other buttons on the toolbar provide shortcuts to commonly used commands from the File menu. A number of commands are disabled while a simulation is running.

3.Start simulation (don't forget to set your options first!)

Abort or pause simulation if needed

Clear log pane

Allows you to abort current run, and step to next. (Used for setup/debugging only)

1.Select input files

2. Select or name output files (normally only dynvars.snk needs to be specified)

Kalypso 1.0 [Cu-Ni.trg...]

File Edit Options Help

Enable stepping

Project Log

Files in project

    C:\kalypso\1 ML Cu-Ni\Cu-Ni.prj
    C:\kalypso\1 ML Cu-Ni\Cu-Ni.trg
    C:\kalypso\1 ML Cu-Ni\Cu-Ni.run
    C:\kalypso\1 ML Cu-Ni\Cu-Ni.mdl
    C:\kalypso\1 ML Cu-Ni\Cu-Ni.imp
    C:\kalypso\1 ML Cu-Ni\Cu-Ni.inl
    C:\mk\apps\inivars.snk
    C:\mk\apps\dynvars.snk
    C:\mk\apps\inelast.dat

The Project pane shows files in the currently loaded project. The Log pane shows information generated by the running simulation.

View simulation graphically (slows it down, so close window when not in use.

Ready to run

The red cross **X** is drawn through an icon to indicate that an optional input or output file has not been specified in the Simulation Options dialog box. In practice, you will probably never want to activate the two specialised output file options, but you may need to activate the inelastic input file option if your project was designed to include inelastic effects.

You can load/change files by double-clicking the respective icons.

(Obsolete)

The first 3 options control the amount of information reported to the user while the simulation runs. The Lattice/Cohesive energy option reports the total lattice energy and the cohesive energy at the specified lattice site (a useful check on the potential).The log (history) buffer should not be too large (200-500 lines), but its exact value is not important.

In general, you should leave these miscellaneous options unselected unless you have a good reason to do otherwise. The only exception to this is the 'self-bombardment' option, which should be selected if the 'projectile' species is of the same atomic type as one of the atoms in the target. See the documentation for a description of the other options, which are intended for various specialised purposes.

Simulation Options

Integration algorithm
- ○ HGE B
- ○ Two-Step A
- ○ Beeman
- ● Verlet

Neighbour search
- ○ Brute force
- ● Cell-index (box)

Screen output options
- Verbose reporting ☐
- Report energy etc. ☐
- Report inelastic loss ☐
- Lattice & cohesive energy ☐
- Lattice site index [1]
- Log buffer (lines) [500]

Miscellaneous options
- Assume elemental target ☐
- Initial conditions to disk ☐
- Inelastic events to disk ☐
- Fixed timestep ☐
- Hot target: <KE> = 3/2kT ☐
- No y-vibrations (ICISS expt) ☐
- Ignore inter-target forces ☐
- Self-bombardment expt ☐

Inelastic loss models in use
- ☑ Lindhard-Scharff-Schiott model
- ☑ Oen-Robinson model
- ☐ Shapiro-Tombrello model
- ☐ Cooling model

Graph window plot type
- ● Spatial plot (1 px = 0.1 A)
- ○ Velocity plot (1 px = 100 m/s)

- ☐ Save options to disk
- ☑ Load options at start-up

Random seed [1]   Run counter offset [0]

[Load options]   [✓ OK]   [✗ Cancel]   [? Help]

Leave at the default value (cell-index), unless your target contains less than ~500 atoms, when the brute force method might produce a faster calculation (you will have to confirm this by testing it yourself).

Leave at the default value (spatial), unless you want to plot velocities.

It is a good practice to save options to disk, for archival purposes.

Leave at the default value of 1 (initialises random number generator). Use a seed of 0 if you want to seed the randomizer via the system clock.

Leave at the default value (0), normally. If you aborted a simulation mid-way, you can continue it from run (N+1), if N is the value entered here. Note: in this case, you must write output to a new file, and combine it later with the previous output. In DOS:

copy /b f1.snk + f2.snk both.snk

In order to include inelastic effects in your simulation, you must select the applicaple models here. If you do not select them, they will not be used, even if parameters for them are defined in the inelastic file.

After hitting the run button, you will see output on the log pane as the input data loads, and then you will be prompted to continue ('Proceed with simulation?'). It is a good idea to check the summary of the simulation which is written to the log pane, to make sure that it is what you expected. If you are satisfied you can click the Yes button or hit the Enter key. Kalypso will then run the simulation. Typically a serious simulation will entail many runs, and will last for 1-3 days.
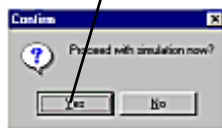
Abort/pause

Graphical view
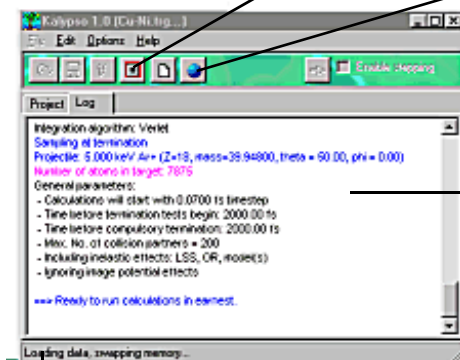
Any error messages will be written in red. Warnings may be issued if the input data seem anomalous. The amount of information reported by a running simulation depends on the options which you selected. In general, choose verbose output only when setting up the simulation.

Reports progress on the current run (time elapsed and number of timesteps calculated).