

kMC-Vis Walkthrough

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Website: <http://www.cis.ksu.edu/~clt3955/research.php>

All sample files are in “sample_data.zip” provided on the above website.

Overview

KMC simulations require:

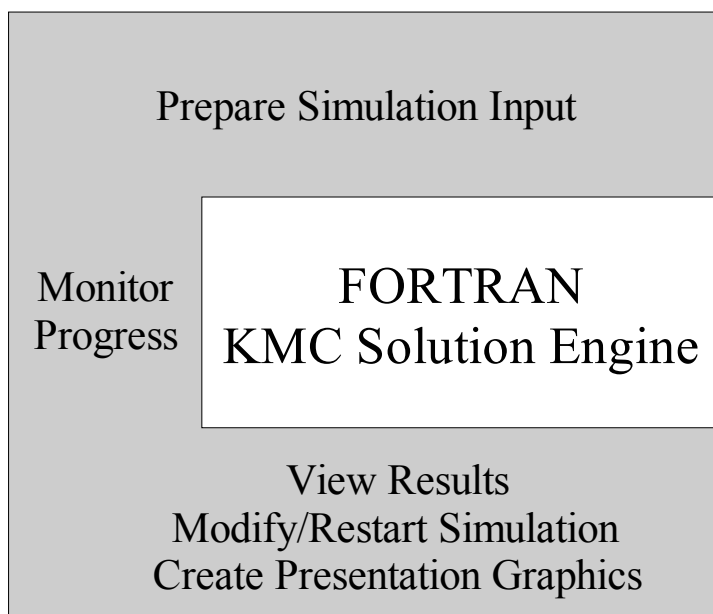
- A database of atom configuration transitions
- An initial mesh configuration
- An substrate configuration
- A configuration file that specifies other information about the simulation

KMC Input

Simulation Config:	step16m.dt
Database:	baza_c92
Substrate Config:	cull1r.sub
Initial Mesh:	clust9i.abk

User Interface Overview

The user interface for KMC simplifies input preparation and observing the results.



Simulation Results

Output files provide detailed records of the simulation. They allow us to:

- Observe 3D results
- Restart the simulation
- Observe database statistics
- Use the updated database in subsequent simulations

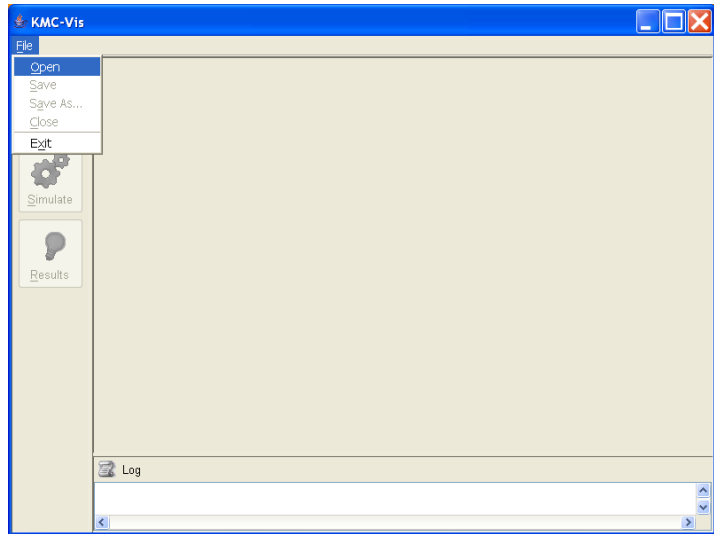
KMC Output

Updated Database:	baza_c92
Event Stack:	stackc_92
3D Movie:	clust92.m
Results Trace:	clust92.r
Final Mesh:	clust92f.abk

Initial Screen

The first step is to load a configuration file. Select the "File/Open..." option to select a .dt file. The program will automatically search for files referenced in the configuration.

Note: In the sample data, this file is "step16m.dt".

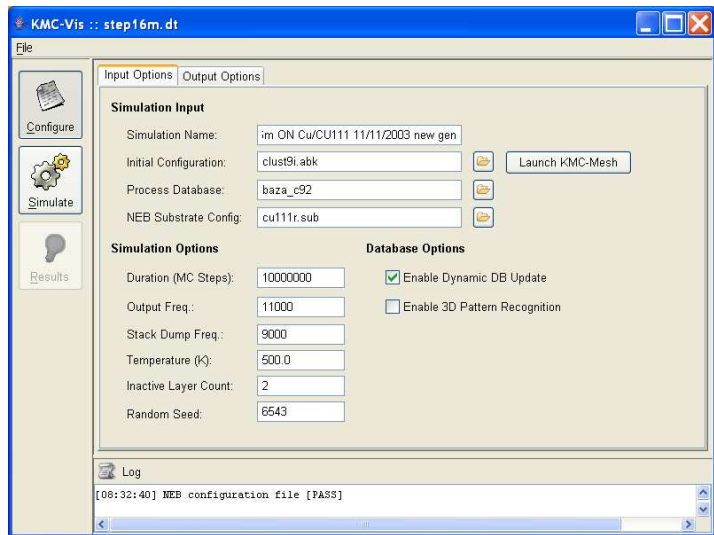


Input Options

The "Configure" view allows us to edit input and output options for the simulation. The "Input Options" tab in this view allows you to specify:

- Input files
- Parameters such as *duration* and *temperature*
- Database Options

For now, just click "Output Options".

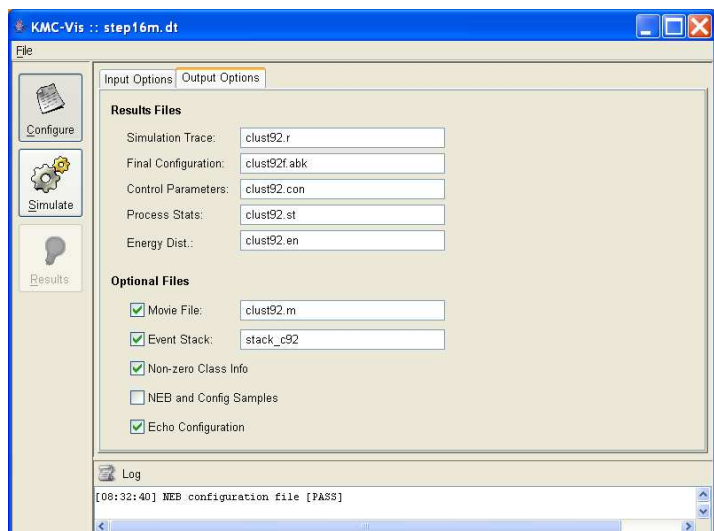


Output Options

This tab allow us to specify:

- Output files
- Optional Output

Click "Simulate" to switch to the simulation view.

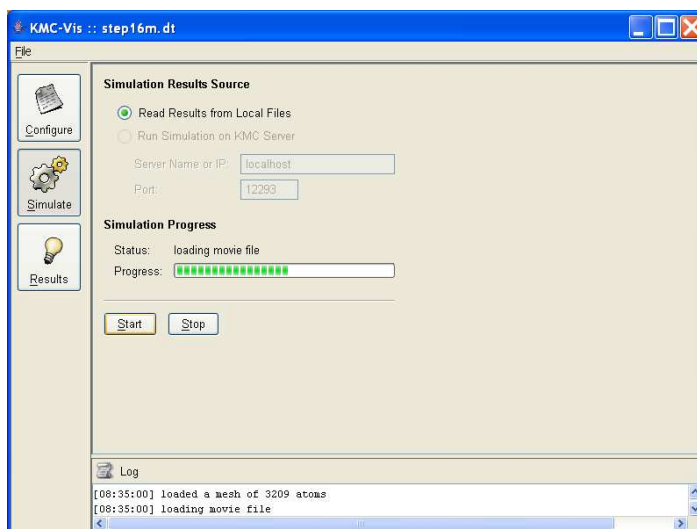


Collecting Simulation Data

Press "Start" to load results data from existing files into memory.

Notice that the "Results" button lights up immediately. This allows us to view results as they come in rather than waiting for an entire simulation to run its course.

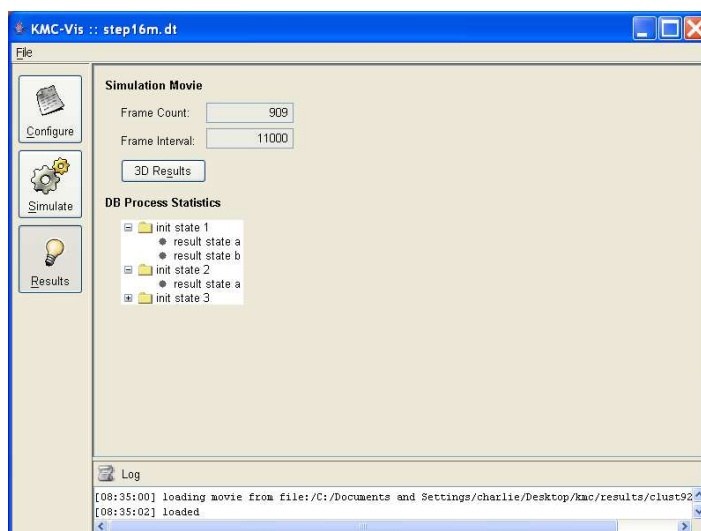
Click "Results" to view the data.



View Results

We can currently only watch the 3D simulation movie. Database statistics and transitions will soon become available in this view as well. The "Frame Count" and "Frame Interval" fields in the top of this view tell us how much movie information we have loaded. In this case we have 909 snapshots of the simulation, each of which is 11000 Monte Carlo steps apart.

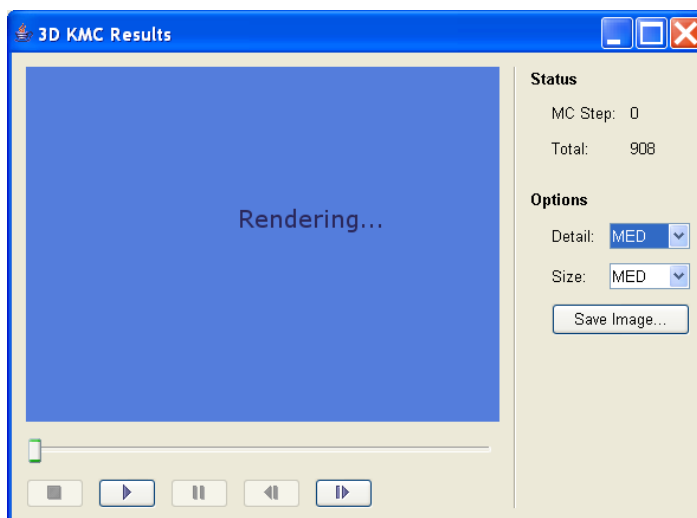
Click "3D Results" to view the 3D animation.



The 3D Movie Viewer

As the 3D subsystem renders the simulation model, a "Rendering..." message will appear. This will be replaced by the 3D animation once it is ready.

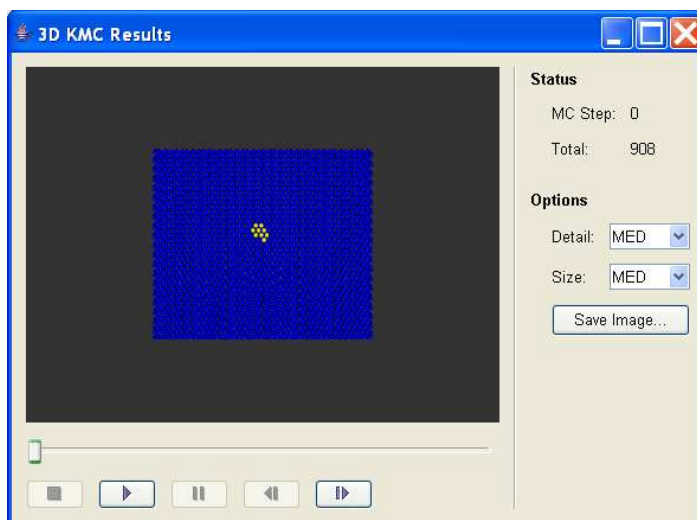
Just wait...



Movie Controls

The following playback options are available:

- STOP:** Stops the animation
- PLAY:** Starts the animation
- PAUSE:** Pauses the animation
- STEP BACK:** Steps backwards one Monte Carlo step
- STEP:** Steps forward one Monte Carlo step

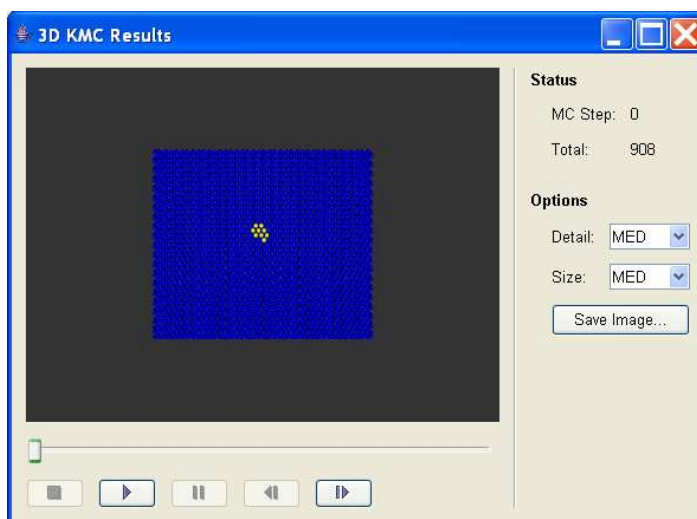


3D Rotate, Pan, and Zoom

Using the mouse and keyboard, you can manipulate the 3D view in the following ways:

- LMB + (drag):** Rotates the view
- RMB + (drag up):** Zooms out
- RMB + (drag down):** Zooms in
- RMB + SHIFT + (drag):** Shifts the view

Feel free to play with the view controls. If you ever get disoriented, you can press the 'R' button to reset the view.



Other Options

You can adjust the level of detail on the atoms using the "Detail" drop-down menu. Higher levels of detail slow down performance, but are useful for capturing graphics. The size of the atoms can also be customized. Any time the size or detail is changed the 3D subsystem must completely redraw all the atoms, which can take up to a minute.

The "Save Image..." button can be used to capture an image of just the 3D view.

