

Work flow tools

Morpheus has a number of nifty tools to optimize your work flow from model development to high performance computing.

Here, we present some use cases that use these features.

Model development and testing

Copy / paste between models

Multiscale modeling often involves the **integration of existing models**. For example, combining an existing cell-based CPM model (CPM.xml) with an ODE model (ODE.xml) regulating, say, the cell cycle of each cell.

Morpheus lets you **copy and paste** parts of a model between different documents.

This allows you to copy the `System` from ODE.xml containing the ODE equations and parameters (right-click → Copy). And then paste it inside the `CellType` element in the CPM.xml document (right-click → Copy).

You can paste elements only in appropriate places, otherwise it will be greyed out. This **ensures validity** of the model.

All copied elements are shown in the `Clipboard`.

Disable / enable

Testing models frequently involves **switch things on and off** to observe their effects. Morpheus allow you to do this without losing your contents by using Right-Click → `Disable`. The selected element and everything below it will be commented out in the XML file.

This mechanism also allows you to **compare submodels**. If you want to compare two versions of an ODE system, you can have both `System` elements in your model, with one disabled. Switching ODE systems then only involves enabling/disabling both. This provides a quick way to compare submodels within exactly the same context.

Interactive and local mode

During model construction and testing, graphical output and visual feedback is important to debugging, spot erros and guide development.

Yet, during serious simulation (production work), you do not want to be bothered by pop-up windows and graphics that slow down simulation.

Morpheus therefore distuingishes between an `interactive` and `local` simulation execution mode.

Job queue	Purpose	Behavior
Interactive	Testing mode	Start and stop simulations from toolbar buttons. Uses pop-up messages for simulation errors. Directs visual output to on-screen terminal. Overrides Gnuplotter terminal to wxt (Linux), aqua (Mac) or win (Windows).
Local	Normal simulation	Start simulations from toolbar buttons. Nonintrusive messages. Visual output to file, unless specifies otherwise.
Remote	Remote batch processing	Submit job to remote queuing system (e.g. LSF) on remote high performance computing resource. Note: Feature not available in public version

Simulation and execution

Snapshots

Checkpointing is taking snapshots of the state of an application during its execution. In computer science, this is used as a fault tolerance mechanism by using these snapshots to restart the application in case of failure.

But it is also a useful tool for modeling. It allows you to use the result of one simulation as the initial condition for the other. Ad therefore enables the construction of complex initial conditions.

You can specify the interval between snapshots in `Time / SaveInterval`. Simulation states are saved as a regular XML model description file, but compressed (`[model].xml.gz`). The current state of all cells is in `CellPopulations / Population`. You can copy this element to act as an initial population for another model.

These files can be opened within Morpheus by a double-click.

Note: PDE data is currently not stored in these files because of the amount of data. We are looking for alternative ways to store and restore these data.

Note: If you want to use checkpointing to construct a complex initial condition, you

- Image-based modeling
- In silico experiments

Parameter exploration

- Spatial parameter sweep
- Parameter sweeps
- Analysis of parameter sweeps

Analysis

- Logging and plotting raw data
- Frequency distributions / Histograms
- Colors / Labels / Arrows
- TIFF hyperstacks

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