

Standard Model of Scientific Computing

All users must do these things...

Define the Problem



Write an input file in a format reminiscent of a dead language

Run the Simulator



Manually launch jobs on impressively terrifying machines

Analyze Output

```
01100010  
01101001  
01101110  
01100001  
01110010  
01111001
```

Analyze simulation output in its most raw and unlimited form

Archive Output



Store data... somewhere!

Super-users think these are easy tasks, but most users are overwhelmed!

A cooler model of Scientific Computing

Define the Problem



Write an input file in a format reminiscent of a dead language

Run the Simulator



Manually launch jobs on impressively terrifying machines

Analyze Output

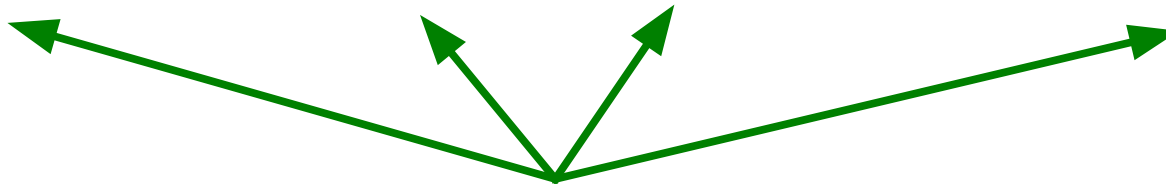
```
01100010  
01101001  
01101110  
01100001  
01110010  
01111001
```

Analyze simulation output in its most raw and unlimited form

Archive Output



Store data... somewhere!

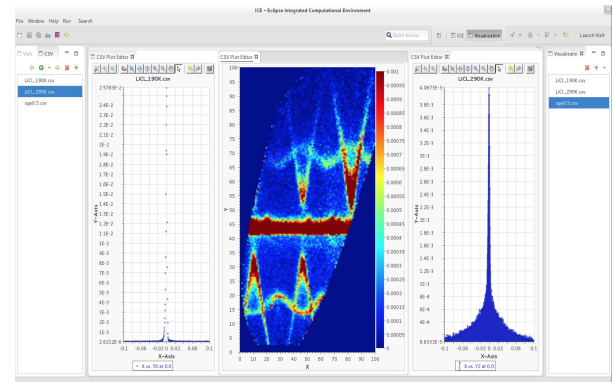
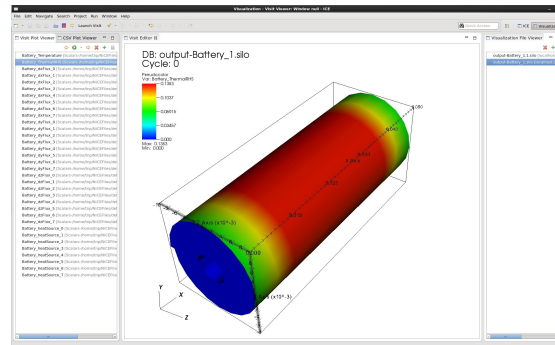
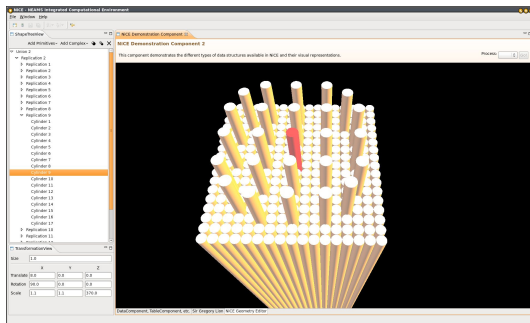
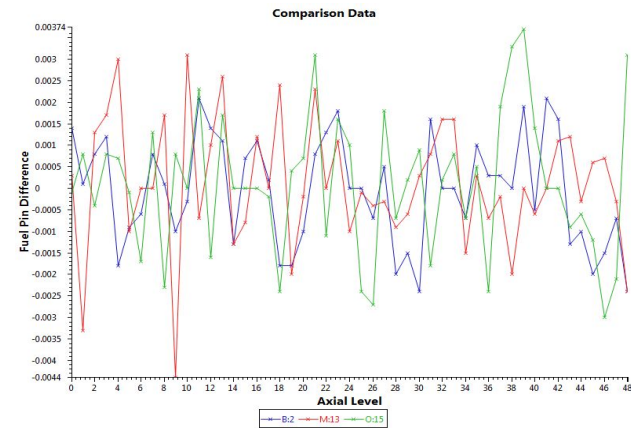
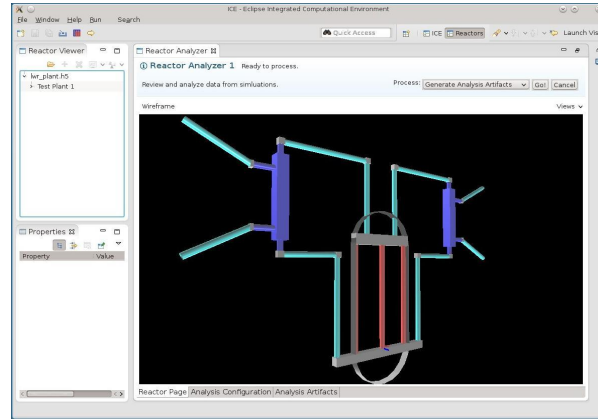
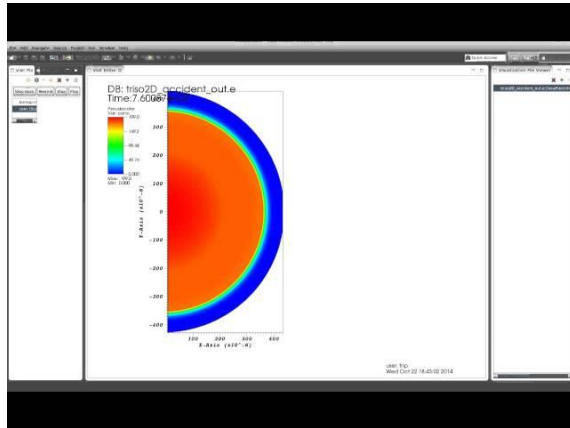
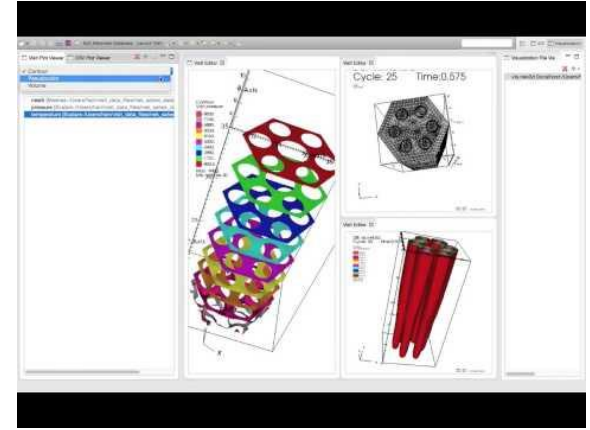
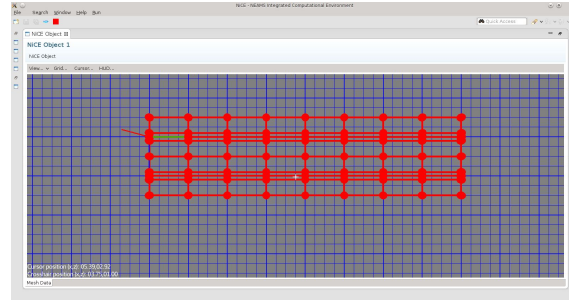
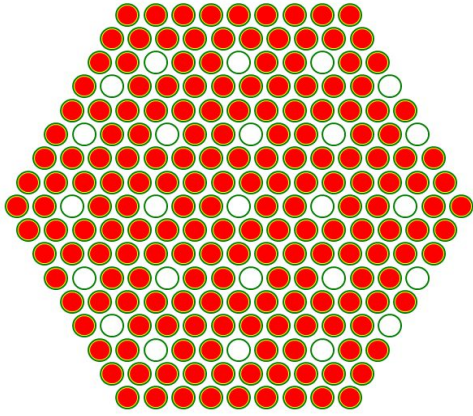


It would be better to have a computer program handle all of that...



Most of the stuff we need to do can be encapsulated for ease of use and/or automated entirely with improvements.

What can it do in 9 pictures or less?



Where does it work?

Nuclear
Energy

Data
Analysis

Advanced
Manufacturing

More 3rd Party
Tools

Coming in FY16!

Batteries



Advanced
Materials

Quantum
Computing

Astrophysics

Basic 3D Geometry
and 2D Mesh Editing

Usability in Modeling and Simulation

How I send messages around the World:



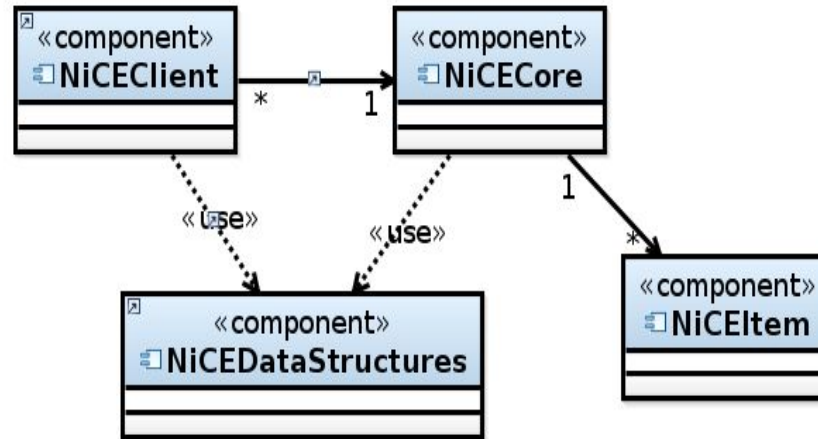
How I send messages to my code:

```
./xolotl ../benchmarks/he-W_2067.txt --  
handlers dummy --petsc -ts_final_time  
1000 -ts_final_time 1000 -  
ts_adapt_dt_max 10 -  
ts_max_snes_failures 200 -pc_type  
fieldsplit -pc_fieldsplit_detect_coupling -  
fieldsplit_0_pc_type redundant -  
fieldsplit_1_pc_type sor -ksp_monitor -  
ts_max_steps 3
```

Really?!

How does it work? Plugins!

Components of NiCE

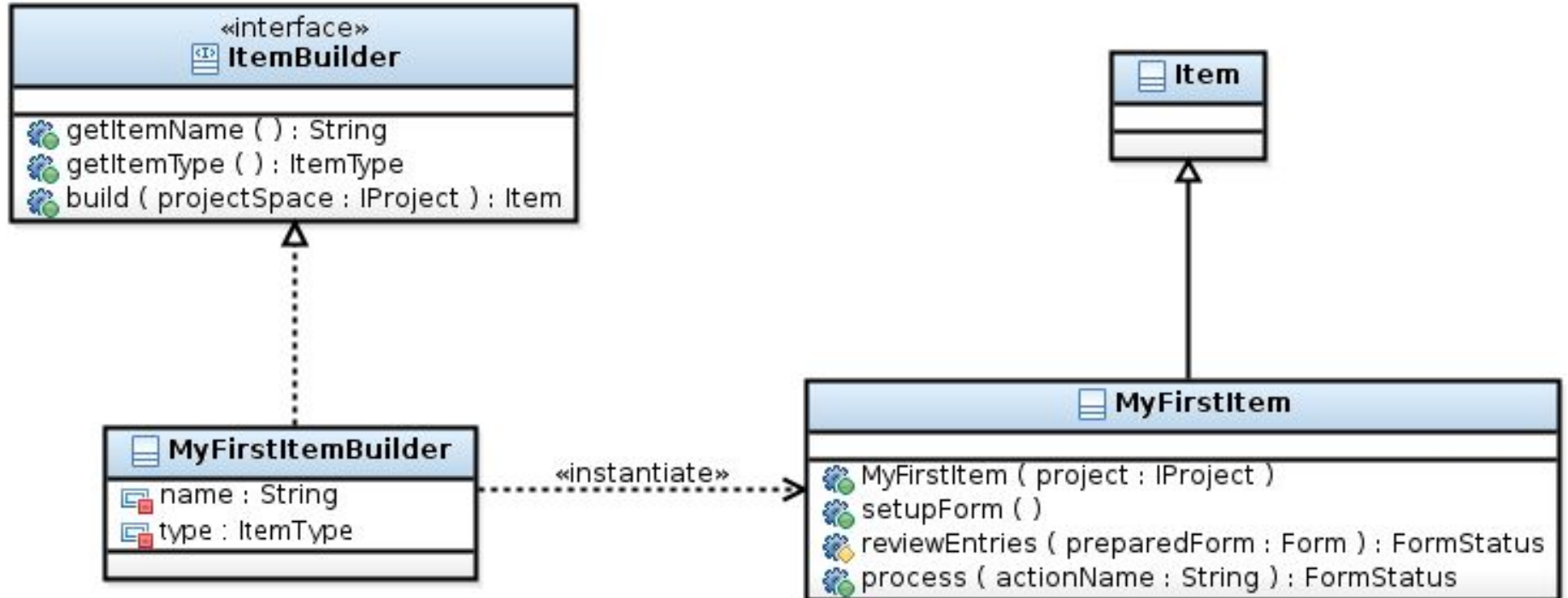


Plugins are:

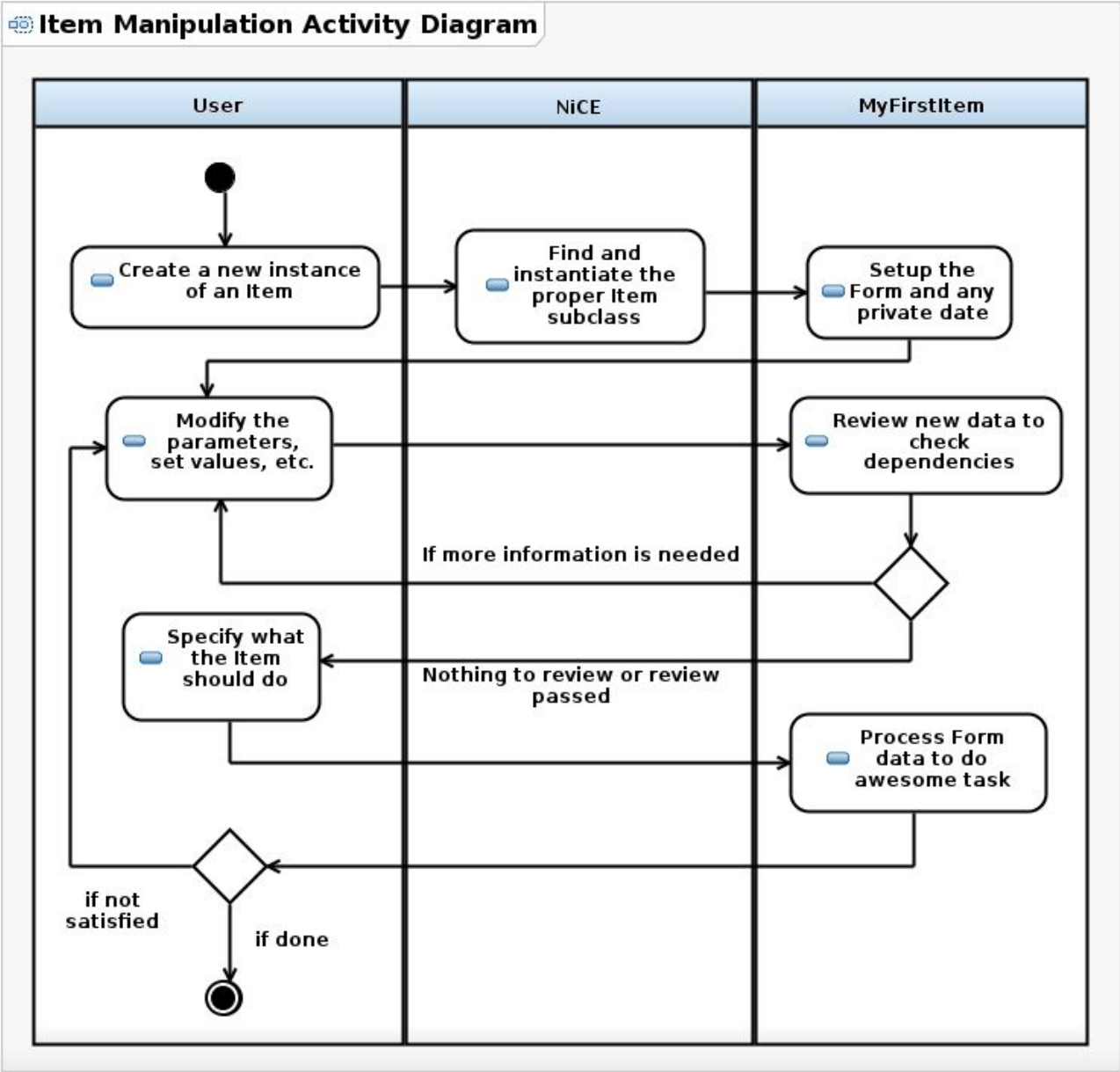
- Dynamic Services - Completely reusable components!
- “Item” Subclasses - Most of the work is already done by the platform
- Self-contained, business logic - **ONLY** your code, not UI, etc.
- Tools - Reusable components, tools, or things other

How does it work? Part 3

MyFirstItem Class Diagram



How does it work? Part 4



How does it work? Part 5

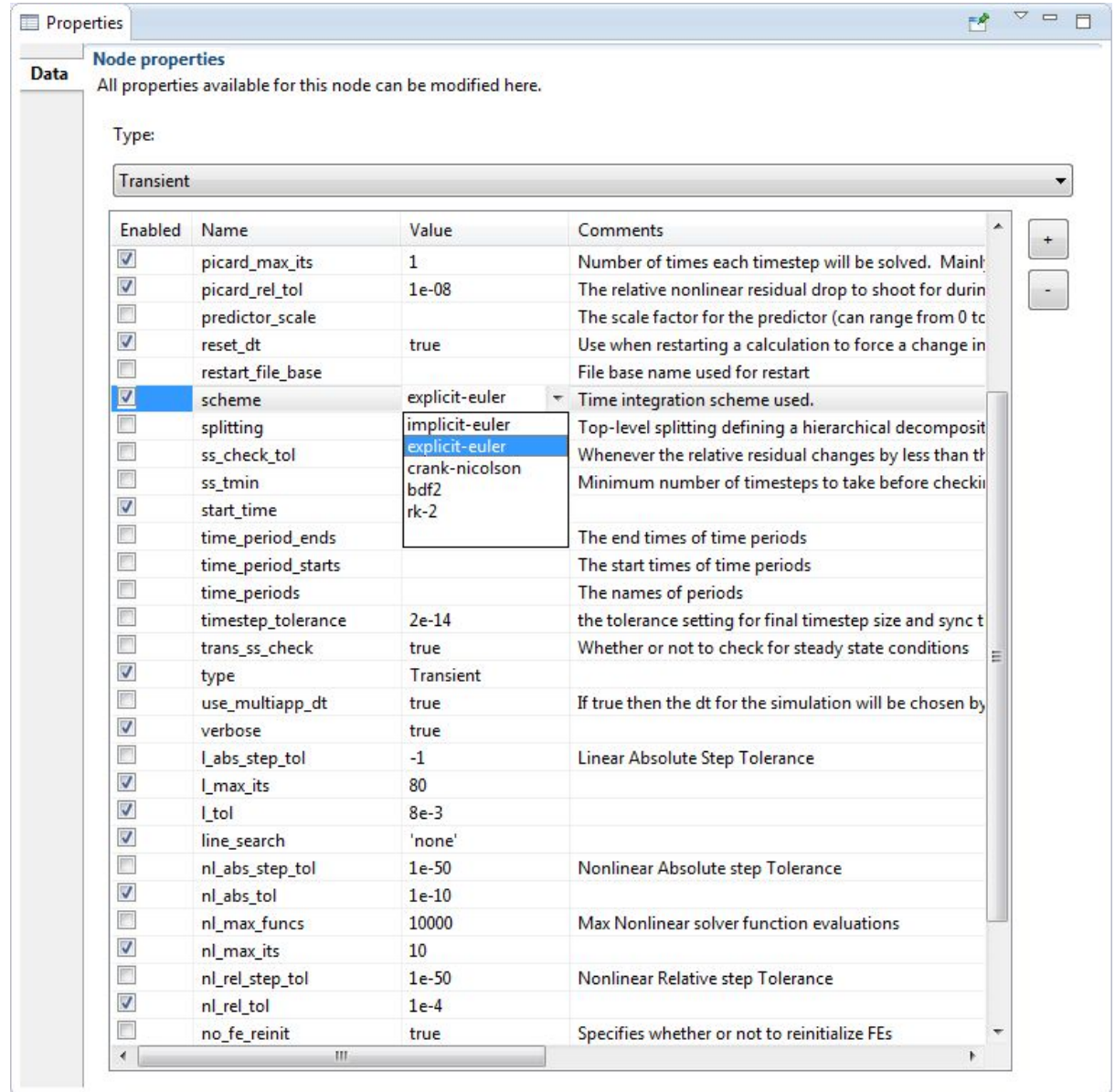
Things to keep in mind:

- You only write business code
- UI and marshalling are provided by the platform (unless you want to extend it)
- Codify only what is needed; reuse what you already have (preprocessors, etc.)

How does it work? Part 6

All of the data structures are backed by sophisticated tools so you deal with your domain.

Standardization for the win!



Different views of the same data

```
<Entry defaultValue="1.7899" ready="true" changeState="false">
  <AllowedValueType>Undefined</AllowedValueType>
</Entry>
```

```
entry1 = new Entry() {
    protected void setup() {
        allowedValues = new ArrayList<String>();
        allowedValues.add("0");
        allowedValues.add("50");
        defaultValue = "1";
        allowedValueType = AllowedValueType.Continuous;
    }
};
entry1.setName("Generic 1");
```

All of these are logically equivalent because of the standardization!

▼ Input File(s)

This section contains the name of the file(s) used by this job.

Input File:

▼ Electrical Properties

Electrical properties and settings

Current Flux:

Enabled	Name	Value	Comments
<input type="checkbox"/>	predictor_scale		The scale factor for the predictor (can range from 0 to 1)