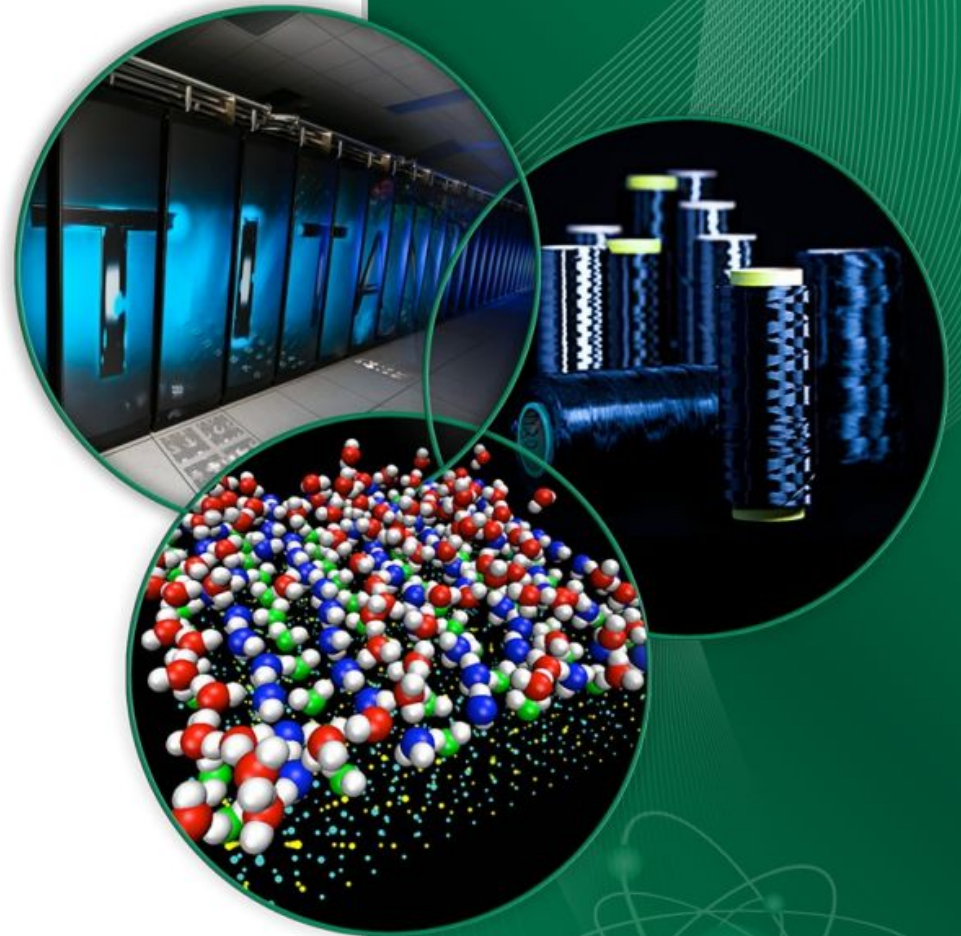


# Workflows for Dummies / Rocket Scientists

## - ORNL Part

**Jay Jay Billings**  
*Research Staff, CSMD  
Oak Ridge National Laboratory  
The Bredesen Center  
billingsjj@ornl.gov*

20160322



# Workflows We See

# Technologies and Applications

Very diverse technology landscape:

- Modeling and Simulation (M&S) tools like Eclipse ICE
- Ptolemy-based engines - Triquetrum, Kepler, Ptolemy II
- HPC engines - Pegasus, Fireworks
- Data-intensive engines - Big PanDA

Diverse Applications:

- M&S in nuclear energy, batteries, quantum computing, materials (ICE)
- High energy physics (Big PanDA)
- Visualization for advanced materials (Pegasus)
- Roughly 10-15 FTEs

# Problems, Hopes & Dreams

**This diverse technology landscape causes a diverse set of problems!**

- How do we support all of these tools?
- How do we get grant HPC resources where required?
- What about non-traditional workflows, like testing?
- What about expertise?

**Ideally we could provide uniform access through one or more end stations.**

**Streamlines user needs, centralizes service.**

# Who to talk to



Jay Jay Billings  
Modeling & Simulation, Eclipse  
billingsjj@ornl.gov



Rangan Sukumar  
NCCS Workflow GL  
sukumarsr@ornl.gov



Jeffrey Vetter  
Future Technologies GL  
vetter@ornl.gov

**Among many others!**

# Eclipse ICE & Triquetrum

# Triquetrum - Ptolemy II-based engine

The screenshot displays the Eclipse IDE interface for a Ptolemy II project. The main workspace shows a diagram with the following components and connections:

- SDF director** (orange box) is connected to the **Ramp** and **Phase** actors.
- Ramp** (blue box) has parameters: `init: 0` and `step: 440/2*PI/60`. It is connected to the **AddSubtract** actor.
- Phase** (blue box) has parameters: `value: 0.1` and `firingCountL: NONE`. It is connected to the **AddSubtract** actor.
- AddSubtract** (blue box) is connected to the **Sine** actor.
- Sine** (blue box) has parameter: `function: sin`. It is connected to the **Display** actor.
- Display** (blue box) has parameters: `rowsDisplay: 10` and `columnsDispl: 40`.

The **Console** window at the bottom shows the following output:

```
Triq Console
417 ms. Memory: 457216K Free: 377017K (82%)
0.0998334166468
-0.8117821756787
-0.9116155923255
-0.0998334166468
0.8117821756787
0.9116155923255
0.0998334166468
-0.8117821756787
-0.9116155923255
-0.0998334166468
```

**ORNL contributing, iSencia & UCB leading.**

# Spectrum of Workflows

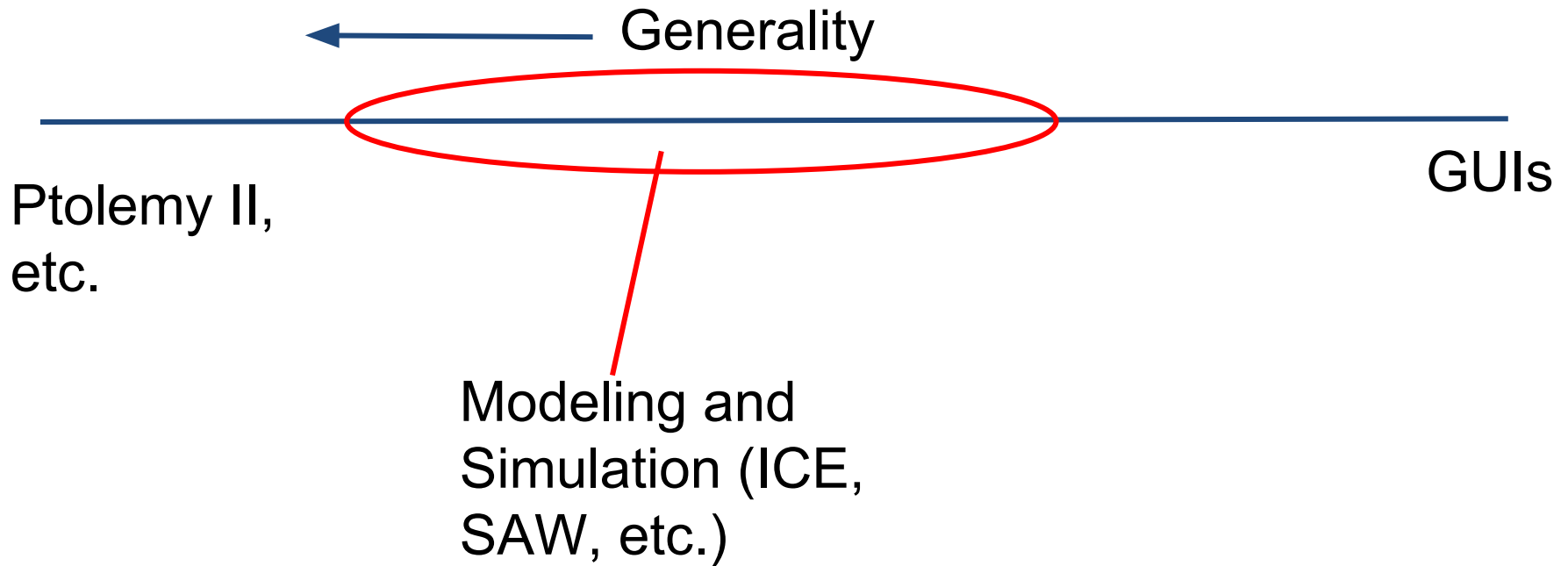
← Generality

Ptolemy II,  
etc.

GUIs



# Spectrum of Workflows



Need something in the middle that doesn't do everything,  
but enables almost that much!

# 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 and developers think these are easy tasks, but most users are overwhelmed!***

## Development

```
public Form getForm() {
    // Local Declarations
    Form actionForm = null;

    // Check the state to determine
    if (!status.equals(FormStatus.Pending))
        // Return the Item's Form
        return form;
    } else {
```

Make it do what it do...

# A cooler model of Scientific Computing

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



A. User



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

**Define the Problem**



**Run the Simulator**



**Analyze Output**

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

**Archive Output**



**Development**

```
public Form getForm() {
    // Local Declarations
    Form actionForm = null;

    // Check the state to determine
    if (!status.equals(FormState.FORM))
        // Return the Item's Form
        return form;
    } else {
```

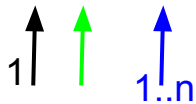
# But that doesn't cover all M&S workflows!

It more or less does...

## Define the Problem



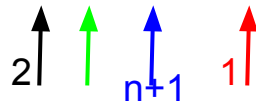
Write an input file in a format reminiscent of a dead language



## Run the Simulator



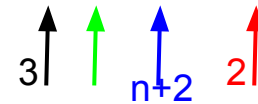
Manually launch jobs on impressively terrifying machines



## Analyze Output

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

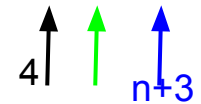
Analyze simulation output in its most raw and unlimited form



## Archive Output



Store data... somewhere!



These are activities that are mixed and matched to produce an outcome.

→ Standard    → Single Use    → Multi-Input    → "The Re-Run"

# Where does it work?



Nuclear Energy

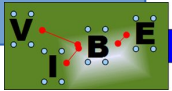
Advanced Materials

Data Analysis

Astrophysics

F

Batteries



Quantum Computing



Basic 3D Geometry and 2D Mesh Editing

Adv. Manufacturing

More 3rd Party Tools

*Coming soon!*

# Workbench Sample: Reflectivity Simulator

<ICE> - This item builds models for Reflectivity. - Eclipse Platform  
File Edit Navigate Search Project Run Window Help

Quick Access <ICE> Visualization

Reflectivity Model

Reflectivity Model 1 Done!

This item builds models for Reflectivity.

Process: Calculate Reflectivity Go! Cancel

	Name	Material ID	Thickness (Å)	Roughness (Å)	Scattering Length Density ...	mmabs/l (Å <sup>-2</sup> )	mminc (Å <sup>-1</sup> )
1	Air	1.0	200.0	0.0	0.0	0.0	0.0
2	NiOx	1.0	22.0	9.4	7.005E-6	2.27931868269305E-9	4.74626235093697E-9
3	Ni	1.0	550.0	10.105	9.31E-6	2.27931868269305E-9	4.74626235093697E-9
4	SiNiOx	1.0	42.0	16.45	5.695000000000005E-6	2.27931868269305E-9	4.74626235093697E-9
5	Si	1.0	100.0	17.5	2.07E-6	4.74981478870069E-11	1.99769988072137E-12

Rows: 2 Columns: 2 Clear

### Neutron Reflectivity

### Scattering Density Profile

Reflectivity Page

Windows Taskbar: 4:37 PM 7/22/2015

# Workbench Sample: 3D Convection

MOOSE - The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a multiphysics framework developed by Idaho National Laboratory. - Eclipse Platform

Project Explorer: AnimalApp (AnimalApp master) |> src |> include |> tests |> unit |> LICENSE |> README.md |> run\_tests |> default |> MOOSE\_Launcher\_stderr\_1.txt |> MOOSE\_Launcher\_stdout\_1.txt |> jobProfiles |> jobs |> iceLaunch\_20150721043115 |> mooseModel.i |> mug.e |> iceLaunch\_20150721043412 |> mooseModel.i |> mug.e |> iceLaunch\_20150722080545 |> mooseModel.i |> iceLaunch\_20150722081132 |> mooseModel.i |> mug.e

MOOSE Workflow 1: Ready to process. Process: Launch the Job. Rows: 2 Columns: 2 Clear

DB: result.e Cycle: 0

user: aqw Wed Jul 22 08:54:4

Plot Editor: NodalVariableValue50.csv

Time vs. NodalVariableValue50 at 0.0

Console:

Parallelization:  
Num Processors: 1  
Num Threads: 1

Mesh:  
Distribution: serial  
Mesh Dimension: 3  
Spatial Dimension: 3  
Nodes:  
Total: 3774  
Local: 3774  
Elements:  
Total: 2476  
Local: 2476  
Num Subdomains: 1  
Num Partitions: 1

Nonlinear System:  
Num DOFs: 3774  
Num Local DOFs: 3774  
Variables: "temp"  
Finite Element Types: "LAGRANGE"  
Approximation Orders: "FIRST"

Execution Information:  
Executor: Transient  
TimeStepper: ConstantDT  
Solver Mode: Preconditioned JFNK

Time Step 1, time = 1  
dt = 1  
# Nonlinear IRI = 2.231591e-01  
1 Nonlinear IRI = 1.292186e-04  
2 Nonlinear IRI = 1.282252e-09  
Solve Converged!

Postprocessor Values:  
+-----+-----+-----+-----+  
| time | NodalVariableValue10 | NodalVariableValue50 |  
+-----+-----+-----+-----+  
| 1.000000e+00 | 8.790174e-01 | 9.043408e-01 |  
+-----+-----+-----+-----+

Time Step 2, time = 2  
dt = 1  
# Nonlinear IRI = 1.659054e-01

Properties: Node properties. All properties available for this node can be modified here.

Type:	Enabled Name	Value	Comments
FileMesh	<input type="checkbox"/> centroid_partitioner_direction	x	
	<input type="checkbox"/> dim	3	
	<input type="checkbox"/> distribution	DEFAULT	
	<input checked="" type="checkbox"/> file	mug.e	
	<input checked="" type="checkbox"/> nemesis	true	
	<input type="checkbox"/> partitioner	default	
	<input type="checkbox"/> patch_update_strategy	never	
	<input checked="" type="checkbox"/> type	FileMesh	
	<input type="checkbox"/> displacements		
	<input type="checkbox"/> block_id		

Workspace Log:

Message	Plug-in	Date
invalid preference category path: org.eclipse.e...	org.eclipse.ui	7/22/15, 8:45 AM
system property http.nonProxyHosts has been...	org.eclipse.core.net	7/22/15, 8:49 AM
The workspace exited with unsaved changes l...	org.eclipse.core.resources	7/22/15, 8:49 AM
Could not bind a reference of component org.e...	org.eclipse.equinox.ds	7/22/15, 8:49 AM
Could not bind a reference of component org.e...	org.eclipse.equinox.ds	7/22/15, 8:49 AM
Could not bind a reference of component org.e...	org.eclipse.equinox.ds	7/22/15, 8:49 AM
The workspace will exit with unsaved changes...	org.eclipse.core.resources	7/22/15, 8:49 AM
Indexed 'AnimalApp' (0 sources, 0 headers) in...	org.eclipse.cdt.core	7/22/15, 8:48 AM
system property http.nonProxyHosts has been...	org.eclipse.core.net	7/22/15, 8:44 AM
The workspace exited with unsaved changes l...	org.eclipse.core.resources	7/22/15, 8:44 AM
Could not bind a reference of component org.e...	org.eclipse.equinox.ds	7/22/15, 8:44 AM
Could not bind a reference of component org.e...	org.eclipse.equinox.ds	7/22/15, 8:44 AM
Could not bind a reference of component org.e...	org.eclipse.equinox.ds	7/22/15, 8:44 AM
The workspace will exit with unsaved changes...	org.eclipse.core.resources	7/21/15, 5:08 PM
The method name 'print' from the module '...'	org.eclipse.eas	7/21/15, 5:00 PM
The Valt connection was null. Check your Valt...	org.eclipse.scs.viz.service	7/21/15, 5:00 PM

# Project Coalescence

A random surprise: ICE can aggregate other workflow engines!

The screenshot displays the Eclipse IDE interface for configuring a Triquetrum workflow. The main window is titled "ICE - An item to launch a Triquetrum workflow - Eclipse Platform". The "Triquetrum workflow Model.xml" editor shows the configuration for "TriquetrumWorkflowItemModel Item 1".

**Triquetrum Info:** Select a Triquetrum workflow from the list. Available workflows:  goodbye,  hello,  reflectivity.

**Workflow : reflectivity:** Configure the selected workflow. enableBackwardTypeInference: true. filePath: C:\data\triquetrum\ice-triquetrum\reflectivityModel\_1\_rfd.csv. smoothingFactor: 5.

The bottom left shows a "Transformation View" with a "Size" of 1.0 and a table for Translate, Rotation, and Scale. The bottom right shows a "Console" with the message "CLI Streaming output console activated."

On the right side, three data plots are shown:

- Raw data plot:** "RData raw" showing a noisy signal. Y-axis: RData (0.72 to 1.16). X-axis: X (0 to 99).
- Smoothed data plot (factor 5):** "RData smoothed ( factor 5 )" showing a smoother signal. Y-axis: RData (0.77 to 1.09). X-axis: X (0 to 99).
- Smoothed data plot (factor 10):** "RData smoothed ( factor 10 )" showing a further smoothed signal. Y-axis: RData (0.77 to 1.06). X-axis: X (0 to 99).

We're actively pursuing this



# Eclipse

# A Good Idea: Extend Eclipse for Science!



## Built on the Eclipse Platform

- Easy, extendable architecture with Rich Client Platform
- Vast amount of existing code we *\*couldn't\** reproduce (~100M lines)
- Made for Enterprise-quality software
- Cross-platform

# Science Working Group @ Eclipse

## Members

### Steering Committee



### Participating



**Workflows in 2025... or sometime later...**

## Something like this...



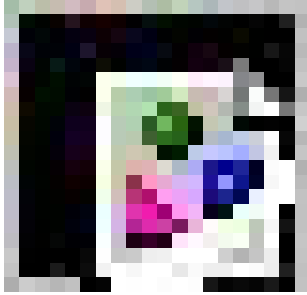
***“Hello Computer!”***

Everyone will talk to their own supercomputer. Supercomputers will talk to each other. Workflow generation will be automatic, along with data analysis and visualization.

# Any Questions?

**Catch the YouTube Videos! Thanks to our sponsors!**

Binaries @ Sourceforge.net



[niceproject.sourceforge.net](https://sourceforge.net/projects/niceproject/)

YouTube



<https://goo.gl/HpclLq>

Ohloh.net



[ohloh.net/p/eclipseice](http://ohloh.net/p/eclipseice)



**Additional Authors:** Andrew Bennett, Dasha Gorin, Hari Krishnan, Alexander J. McCaskey, Taylor Patterson, Robert Smith