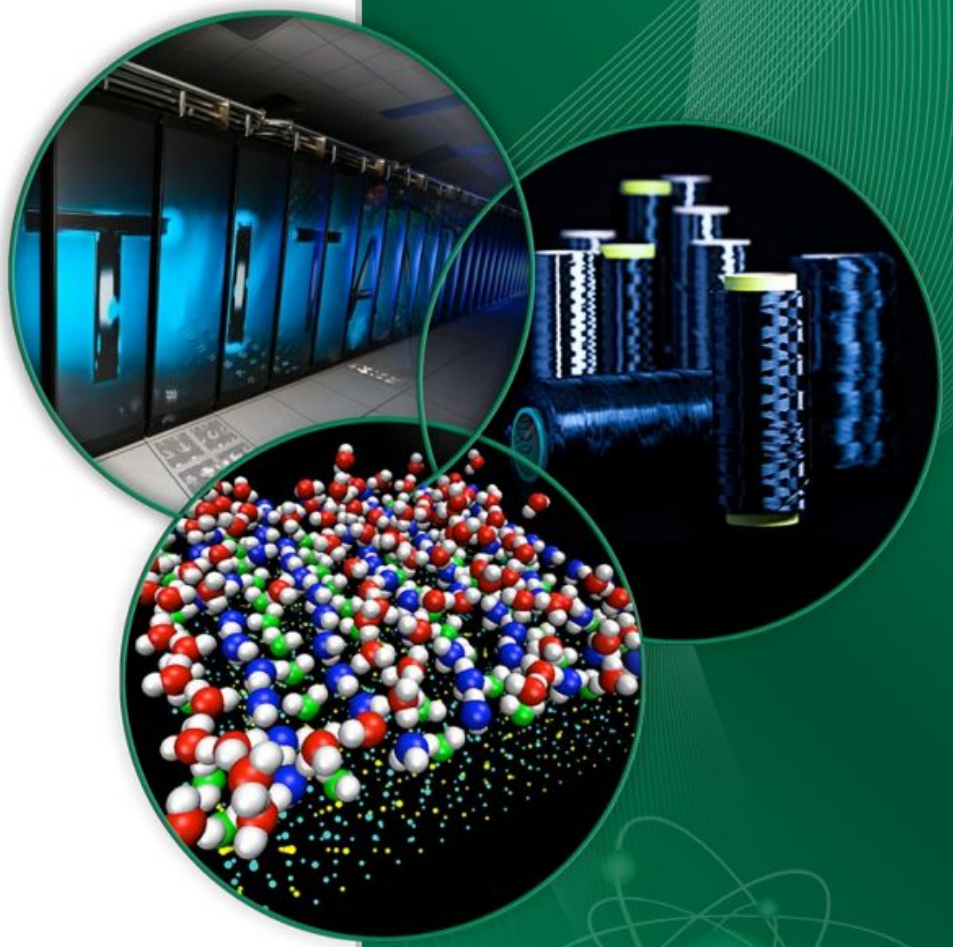
Workflows for Dummies / Rocket Scientists

- 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

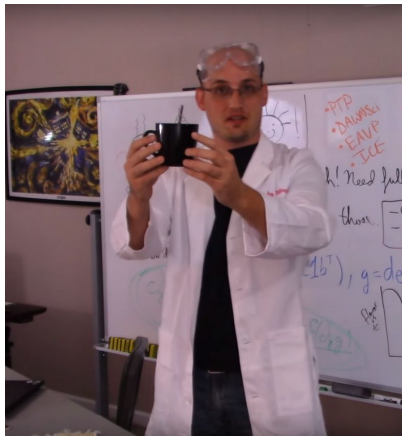
This diverse technology landscape causes a diverse set of problems!

- How do we support all of these tools?
- How do 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

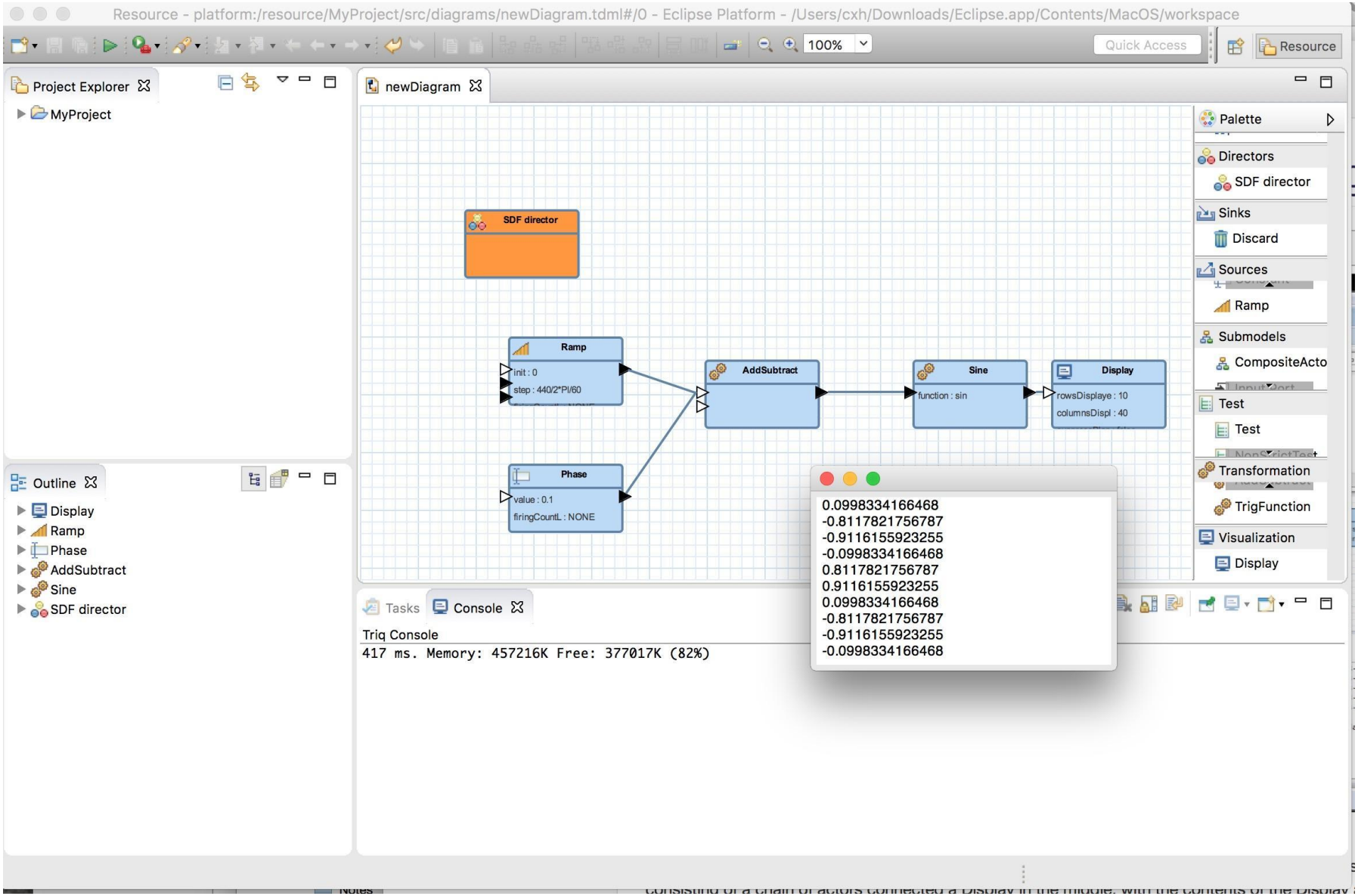
Rangan Sukumar
NCCS Workflow GL
sukumarsr@ornl.gov

Jeffrey Vetter
Future Technologies GL
vetter@ornl.gov

Among many others!

Eclipse ICE & Triquetrum

Triquetrum - Ptolemy II-based engine



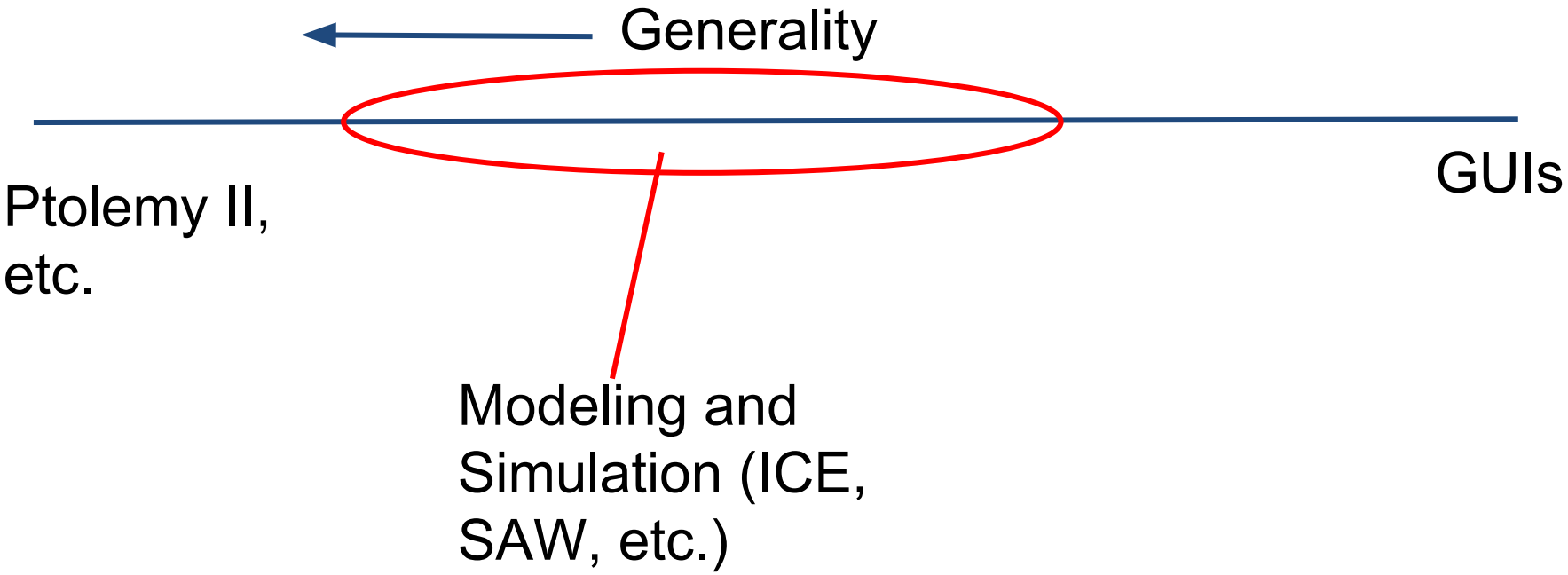
ORNL contributing, iSencia & UCB leading.

Spectrum of Workflows

GUIs

Ptolemy II,
etc.

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 dete
    if (!status.equals(FormSta
        // Return the Item's F
        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

ice

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 dete
    if (!status.equals(FormSta
        // Return the Item's F
        return form;
    } else {
```

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

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

1 ↑ ↑ 1..n ↑

Run the Simulator

Manually launch jobs on impressively terrifying machines

2 ↑ ↑ n+1 ↑ 1

Analyze Output

01100010
01101001
01101110
01100001
01110010
01111001

Analyze simulation output in its most raw and unlimited form

3 ↑ ↑ n+2 ↑ 2

Archive Output

Store data... somewhere!

4 ↑ ↑ n+3 ↑

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

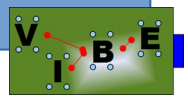
Data Analysis

Astrophysics

F

ice

Batteries



Quantum Computing

Jade
Powered by NiCE

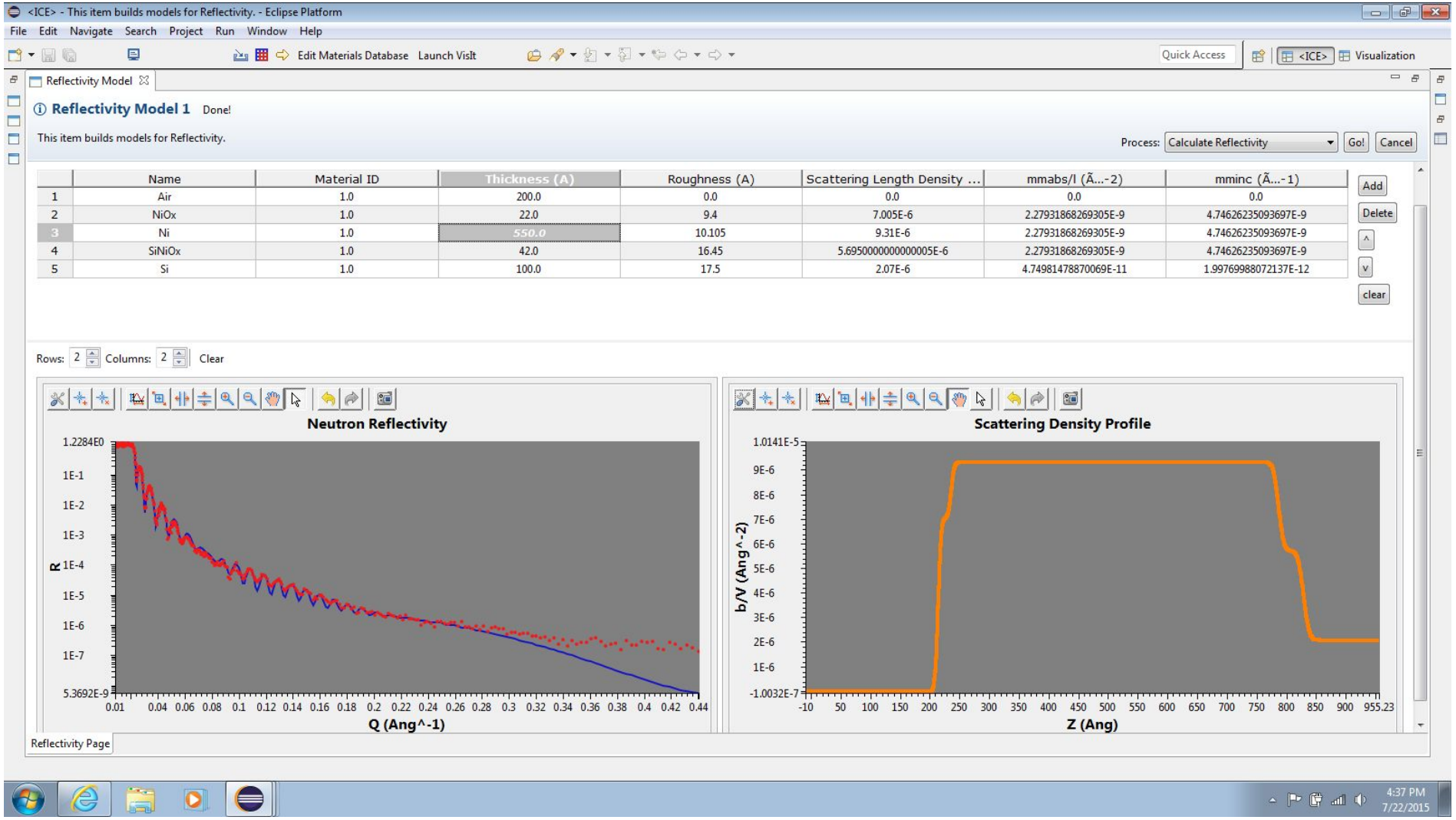
Basic 3D Geometry and 2D Mesh Editing

Adv. Manufacturing

More 3rd Party Tools

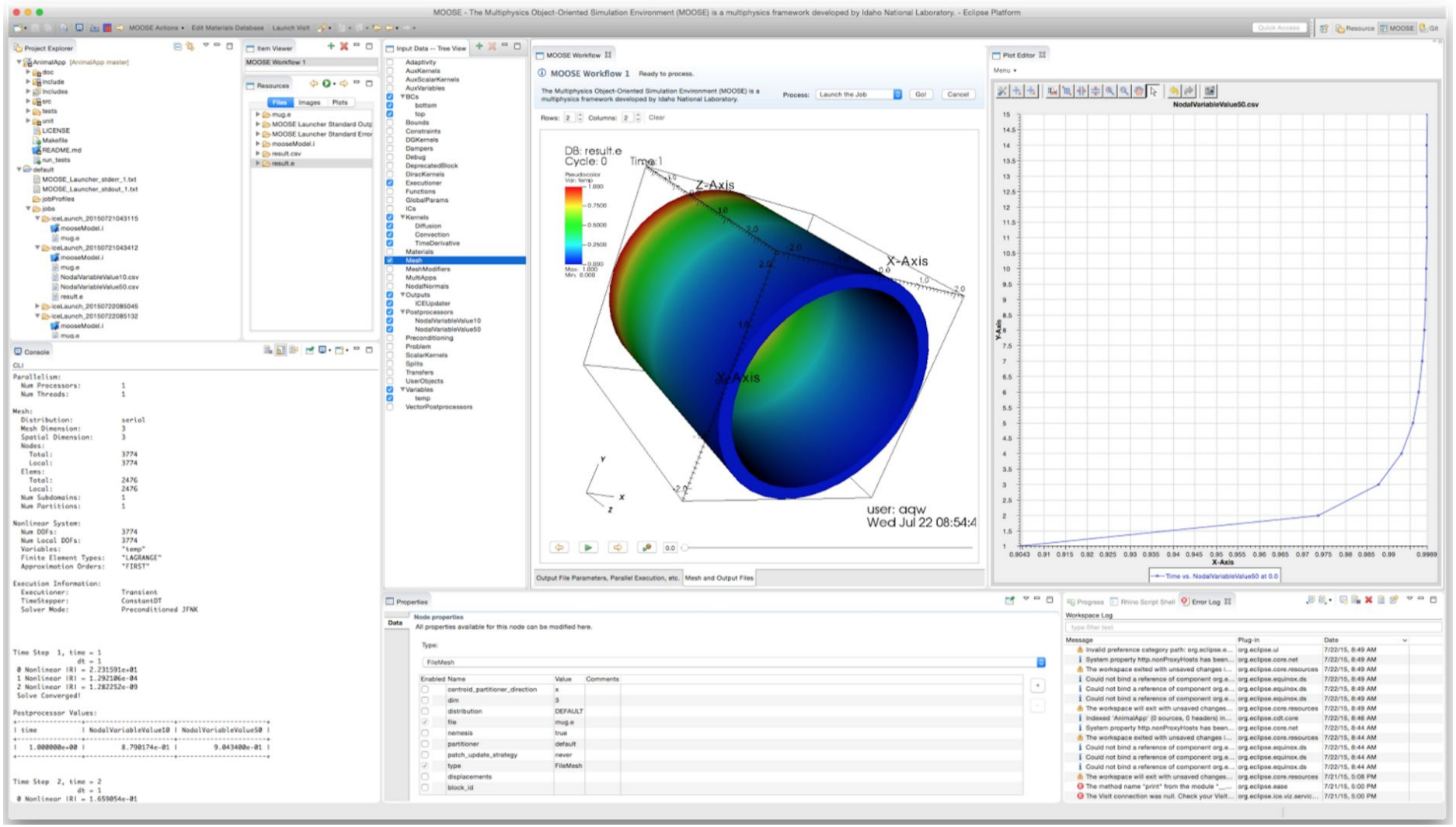
Coming soon!

Workbench Sample: Reflectivity Simulator



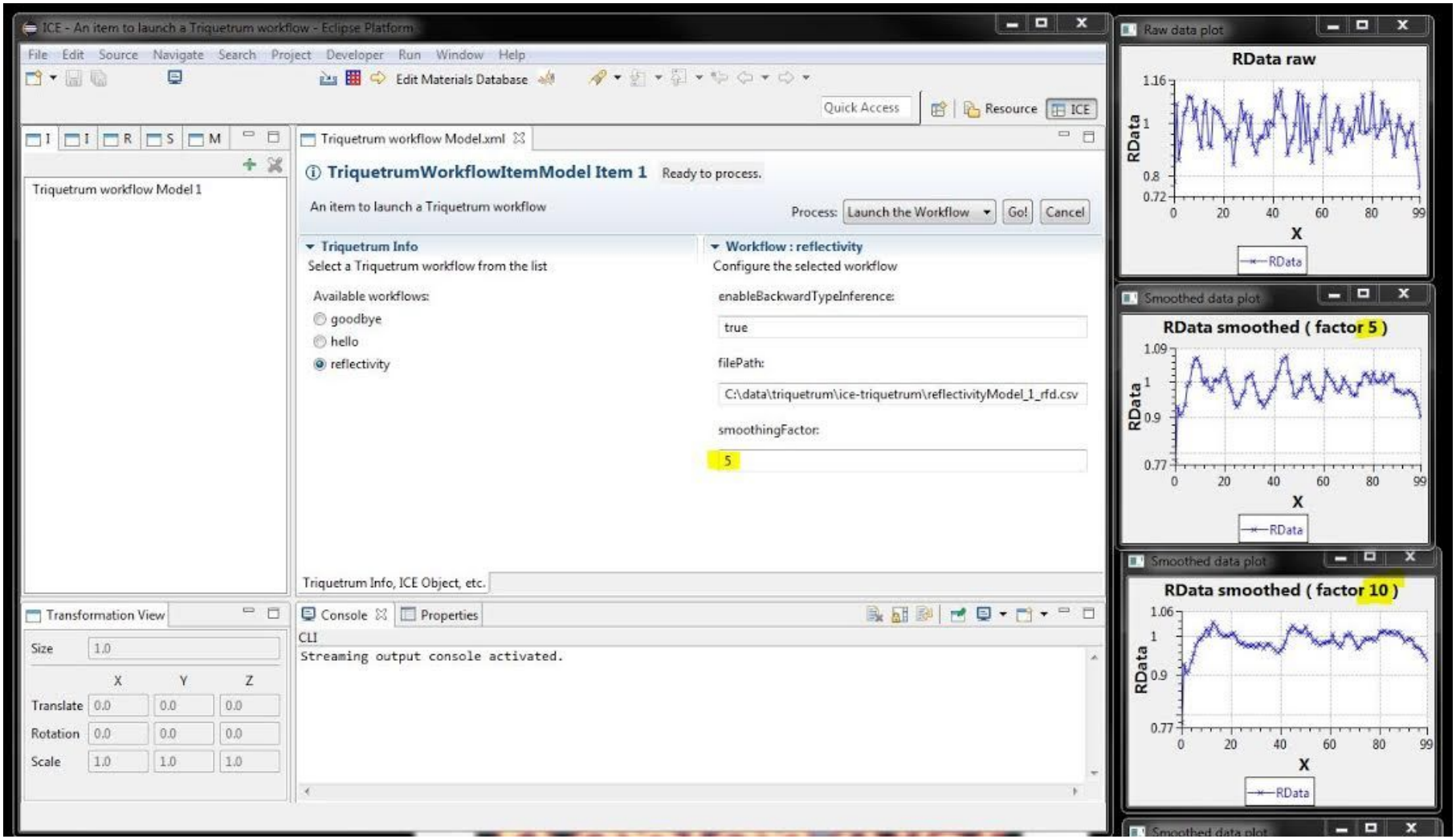
	Name	Material ID	Thickness (A)	Roughness (A)	Scattering Length Density ...	mmabs/l (Ã...-2)	mminc (Ã...-1)
1	Air	1.0	200.0	0.0	0.0	0.0	0.0
2	NiOx	1.0	22.0	9.4	7.005E-6	2.27931868269305E-9	4.74626235093697E-9
3	Ni	1.0	550.0	10.105	9.31E-6	2.27931868269305E-9	4.74626235093697E-9
4	SiNiOx	1.0	42.0	16.45	5.69500000000000005E-6	2.27931868269305E-9	4.74626235093697E-9
5	Si	1.0	100.0	17.5	2.07E-6	4.74981478870069E-11	1.99769988072137E-12

Workbench Sample: 3D Convection



Project Coalescence

A random surprise: ICE can aggregate other workflow engines!



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

diamond

IBM

itema

OAK RIDGE National Laboratory

SCIENCE
eclipse.org

Participating

AIRBUS

CLEMSON UNIVERSITY

ifp Energies nouvelles

iSencia BELGIUM

kichwa coders

Lablicate

MARINTEK

Tech advantage Groupe IFP

FACILITY FOR RARE ISOTOPE BEAMS

UPPSALA UNIVERSITET

Workflows in 2025… or sometime later...

Something like this...

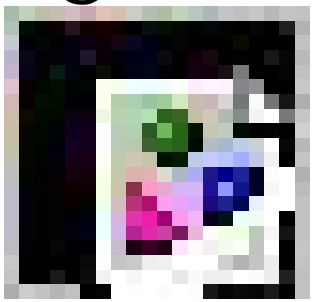
“Hello Computer!”

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

YouTube

https://goo.gl/HpclLq

Ohloh.net

ohloh.net/p/eclipseice

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