

An Update on the NEAMS Integrated Computational Environment

Jay Jay Billings, ORNL
2010 NEAMS Fall PI Meeting

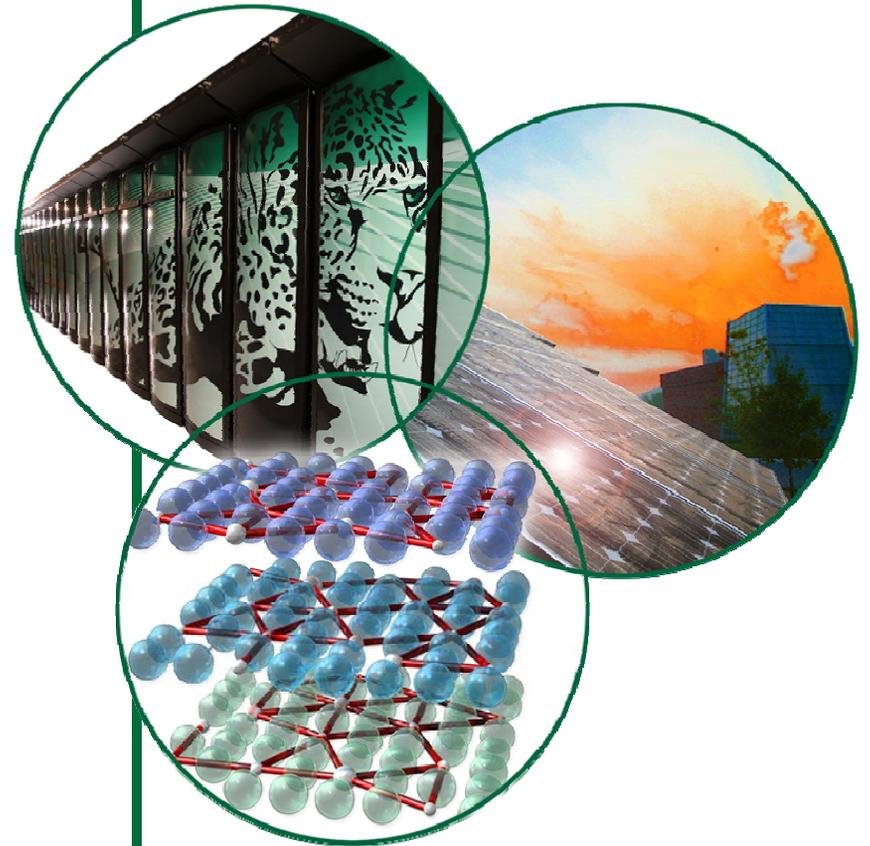
With:

David Bernholdt, ORNL

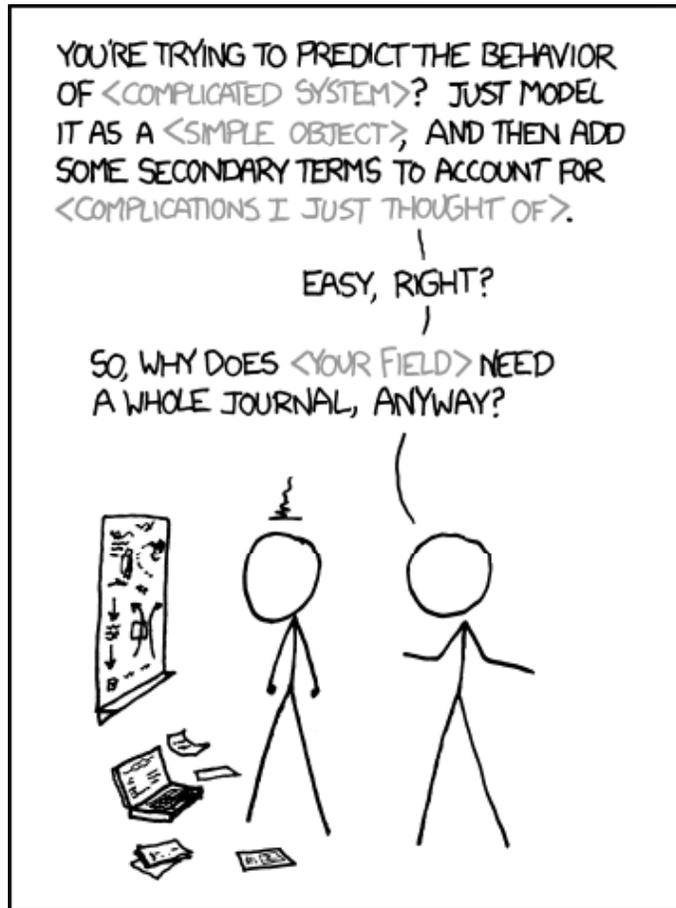
John Hetrick, IBM

Alex McCaskey, UTK

Adrian Sanchez, UTK



Talk in Brief



LIBERAL-ARTS MAJORS MAY BE ANNOYING SOMETIMES, BUT THERE'S *NOTHING* MORE OBNOXIOUS THAN A PHYSICIST FIRST ENCOUNTERING A NEW SUBJECT.

Credit: xkcd

- What is the NEAMS Integrated Computational Environment?
 - It's NiCE!
- Work in FY10
 - I forgot the User's Manual
- Future Development in FY11

What is NiCE?

We had a vision...



Vision document - March 2009 Deliverable



All of the things that ***WE*** take for granted are...

- Difficult or impossible for customers
- Are not part of software frameworks
- Common across IPSC boundaries
- NOT purely nuclear engineering issues

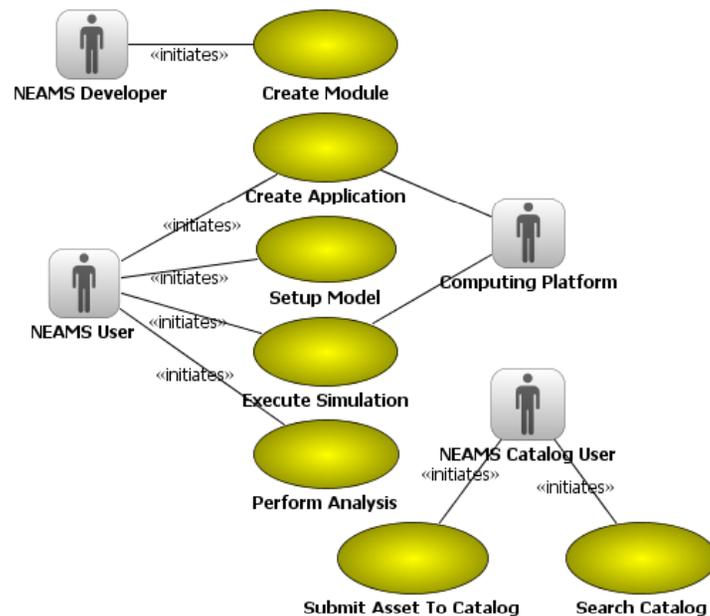
The Plot Thickens...

Relationships: - direct only	FEAT1...	FEAT2...	FEAT3...	FEAT4...	FEAT5...	FEAT6...	FEAT7...	FEAT8...	FEAT10...	FEAT14...
UC1: Execute Simulation This use case describes how a NEAMS User executes a Simulation on a Computing Platform...										
UC2: Create Application This Create Application use case allows a NEAMS User to assemble an application from a set of...										
UC3: Setup Model The Setup Model use case allows a NEAMS User to configure the input package for a simulation....										
UC4: Perform Analysis This use case describes how a NEAMS User can perform analysis on data from a Simulation.										
UC5: Create Module The Create Module use case allows a NEAMS Developer to extend the functionality of the...										
UC6: Search Catalog The Search Catalog use case allows a NEAMS Catalog User to discover existing assets available...										
UC7: Submit Asset To Catalog The Submit Asset to Catalog use case allows a NEAMS Catalog User to add new assets or update...										

Most of the requirements traced to these “other” features

NiCE

NiCE Use Case Diagram



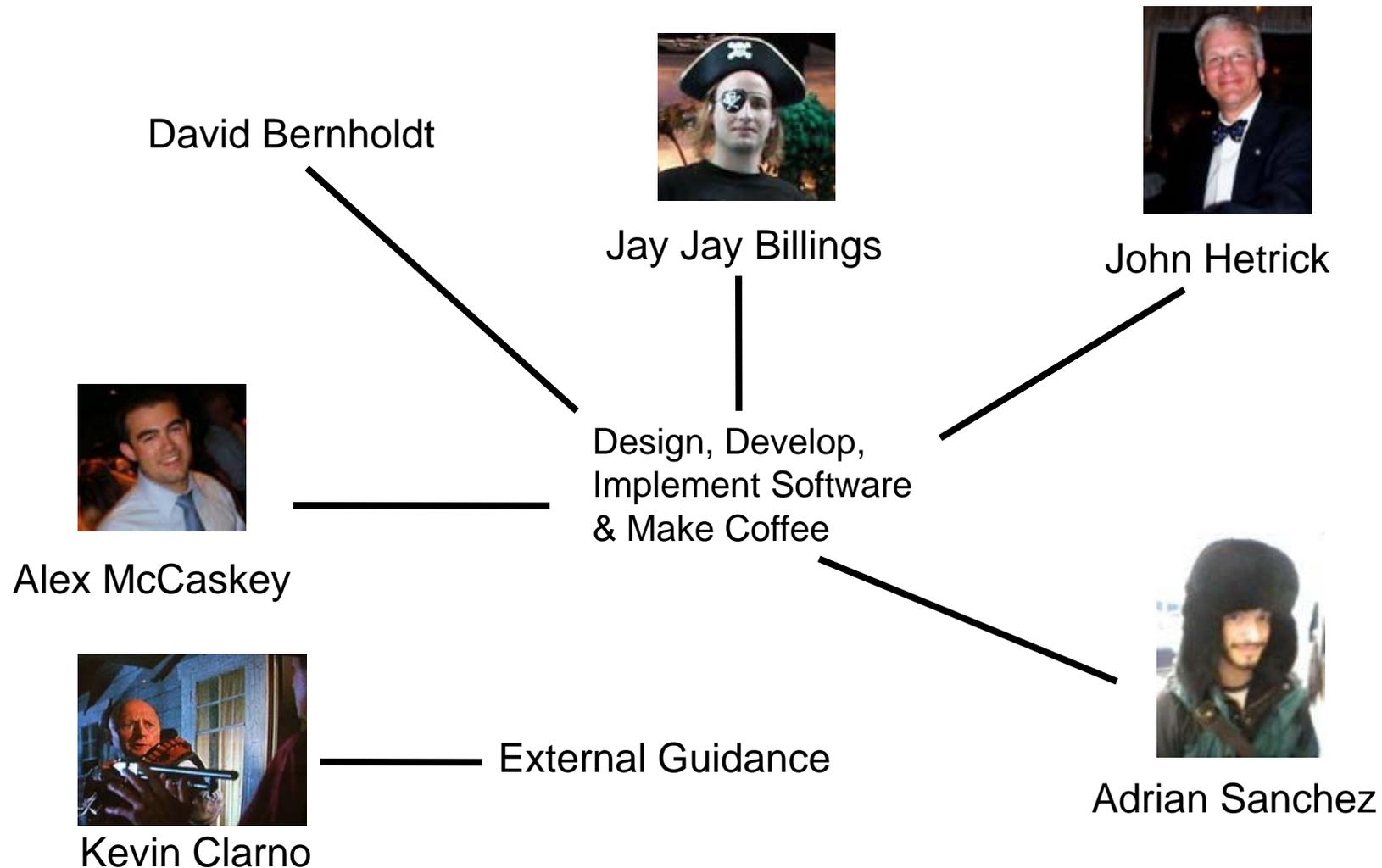
NiCE Context Diagram

Navigation: NiCE Use Cases Model

NiCE helps with all of those difficult chores...

- Getting code into new software systems
- Creating applications from new software systems
- Managing inputs, geometry, materials, and meshing
- Job launch and monitoring
- Data analysis and visualization
- “Asset” management

NiCE Dev Team



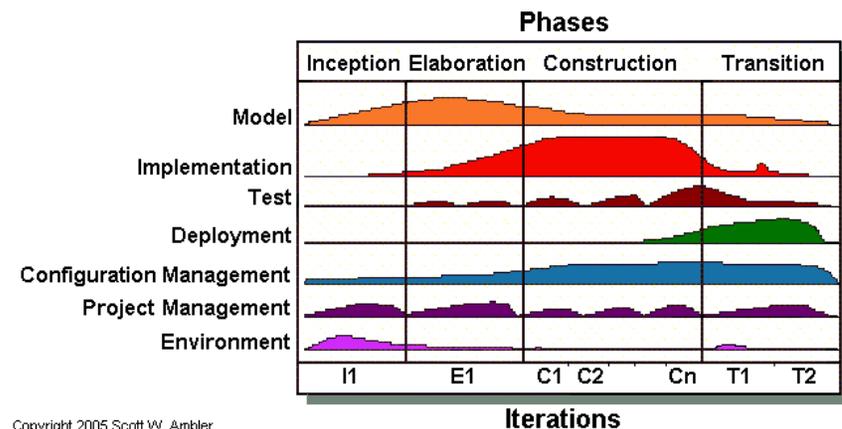
Work in FY10

FY10 Iterations and Themes

Development Iterations

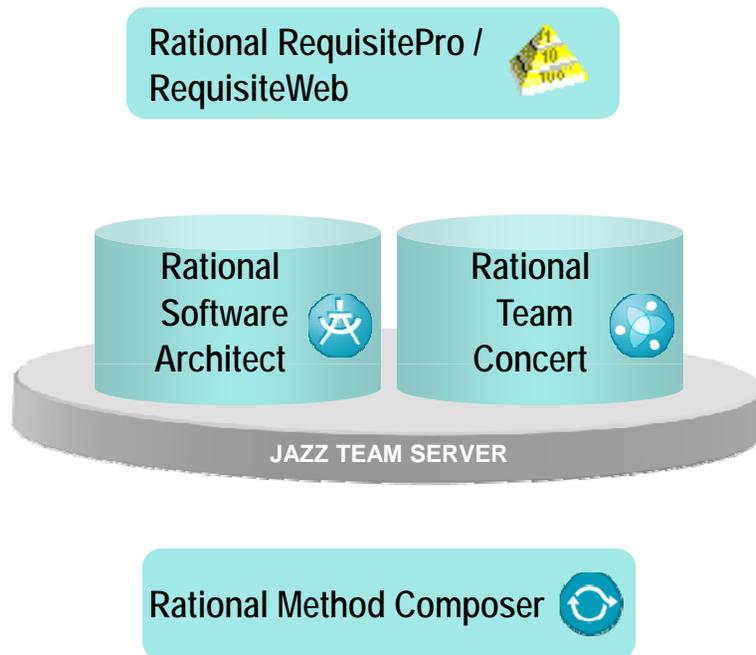
- 8 “working” iterations in total + 1 “wash out”
 - September - students gone, IBM Rational wrapping up, Jay on n projects (for $n \gg 1$).
- “Phased” iterations
- Also started requirements elicitation with Wastes, SafeSeps

Iteration(s)	Primary “Theme”
1	Dev. Environment
2-5	Design & prototyping
6-8	Active development



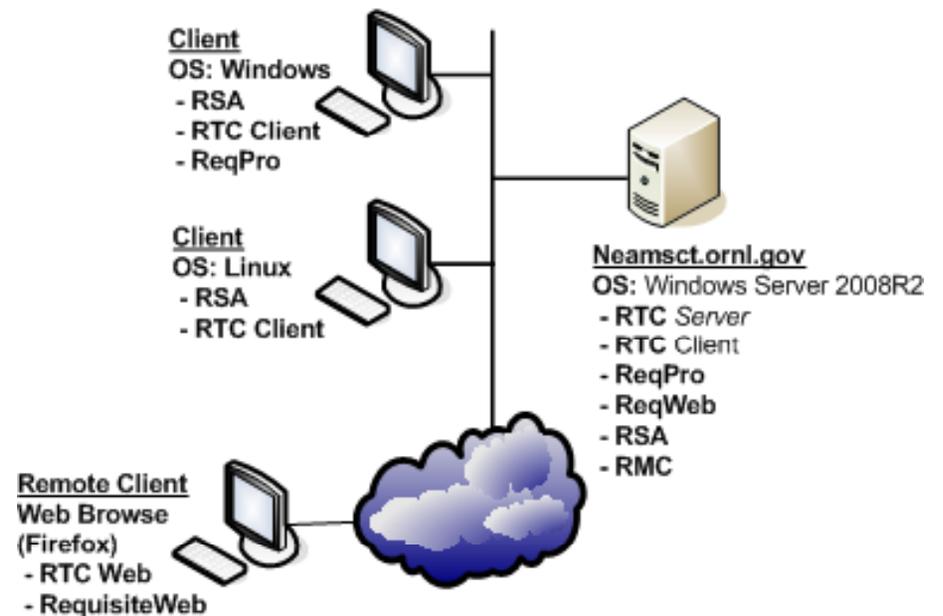
NiCE Dev Environment

Rational Tools Environment



Environment Infrastructure

ORNL NEAMS Topology

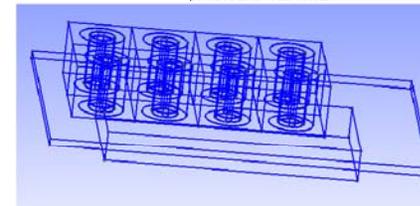
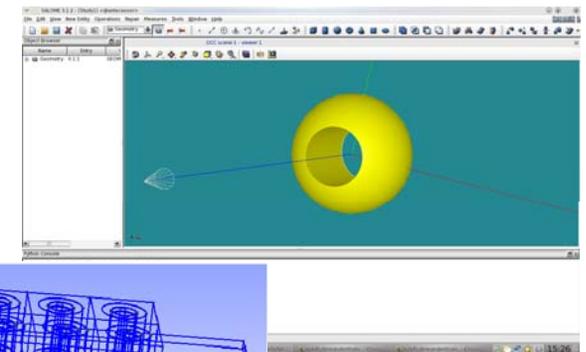
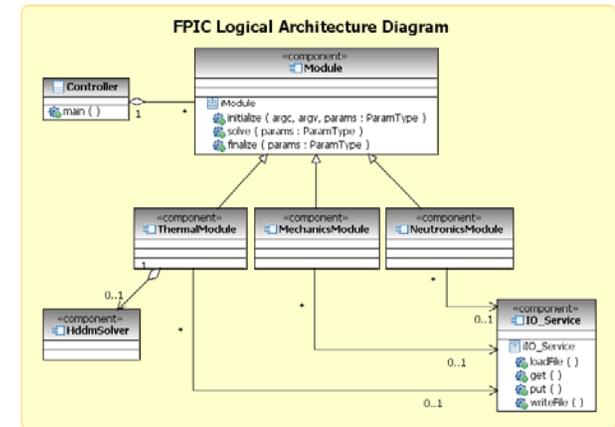


The AMP Load on NiCE

CT and Fuels work together very closely:

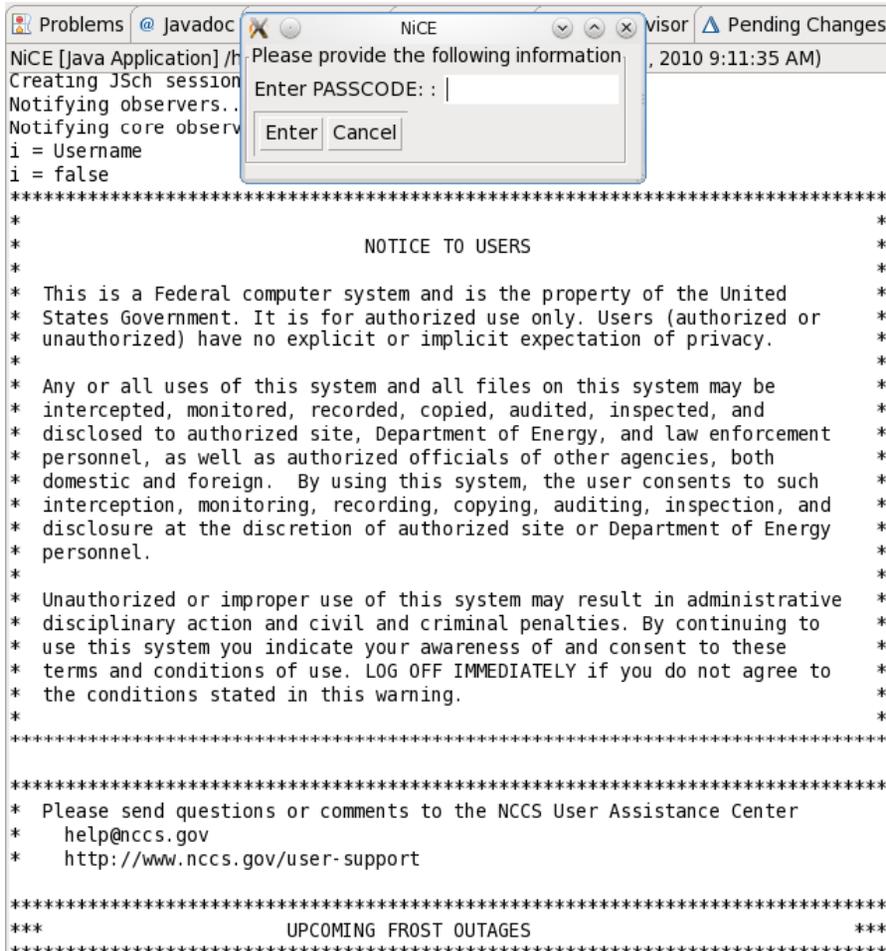
- Literally, 500ft away
- Requirements elicitation and management
- Design work on AMP
- Prototyping activities
 - Scale Geometry Converter (SCALE to ITAPS)
 - Python coupling experiments for ADVENTURE
- Process guidance

Fuels became #1 customer in 2010, Reactors not so interested...



SGC testcases

The AMP Load on NiCE – Job Launch



Job launch was #1 priority in FY10:

- Difficult for a domain scientist
- Very enabling for using “strange codes on strange computers”
- Only requires some “metadata” on the target platform, the application, and the model

Does it work?:

“When can I have it?” - Larry Ott, ORNL AMP user

Testing the Quality of a Design

Software should be easy to use, port, extend, etc.



Alex McCaskey ported NiCE to the Android Platform in less than a single workday.

We can launch AMP on Frost with our **cellphones**.

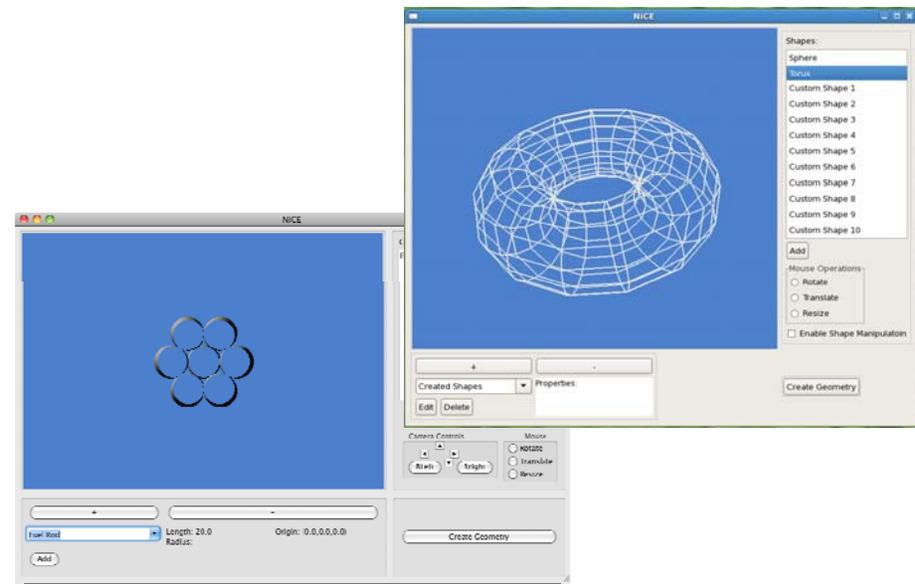
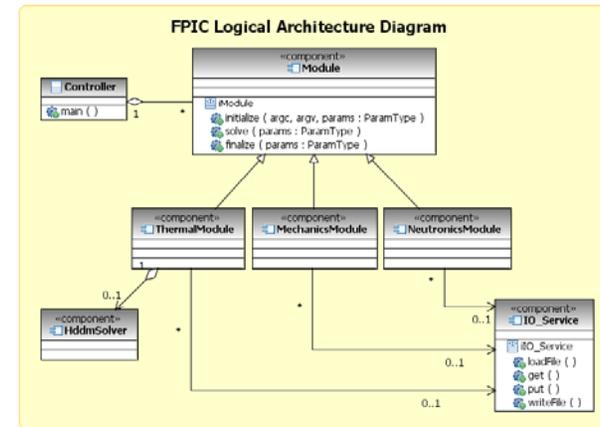
The AMP Load on NiCE – Model Setup

Several easy things:

- Setting different problem options
- Setting different module options

Several not-so-easy things:

- Geometry specification (explored & prototyped)
- Mesh generation (deferred)
- Materials definitions (deferred)



Future Development in FY11

Deliverables

This just in: NiCE is moving to ECT in FY11 and will be specifically funded!

Deliverable	Date
NiCE version 1.0	2010-12-15
NiCE version "Something Else"	2011-09-15

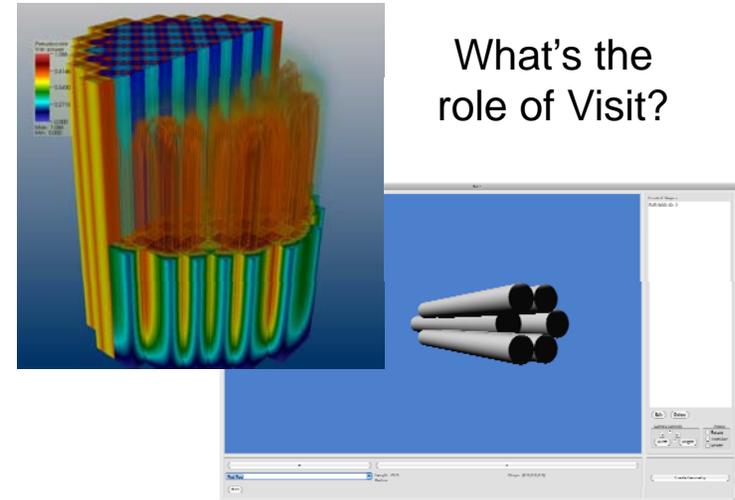
We'll be able to...

- Continuing our current dev cycle, (1 month iterations), and implement prioritized use cases
- Continue to collect, refine and "flow down" requirements to code
- Hire someone! Jay's only 50% and there's enough work to go around

Goals and things to investigate

Jay's "wish list":

- Get Keith Bradley as a user
- Implement a comprehensive analysis capability
- *Greatly* improve and deliver geometry and meshing capabilities (with Tim Tautges & CUBIT team)
- Tackle data management and workflow issues (with Carter Edwards)
- Sync up with the VU team and see what NiCE can do
- Check out possible research issues: "teaming" and real-time monitoring



What's the role of CUBIT?



Wrapping Up

Presentations & Talks



CBHPC 2009



IBM Innovate 2010

Invited talks: IADSCS&TU - Sept 27th, IBM Federal D.C. – Nov. 4th

We have a project webpage... check with Laura!

Jay's Final Thoughts

Honest thoughts about NiCE:

- There's plenty of work left. *Plenty*
- “Working software is the primary measure of progress”
- Fail and fail often – working software means downloadable, runnable, breakable and fixable!

Some thoughts about the program:

- We need to work together, programmatically, and we want to work *with* you.
- It's time to leverage collaboration tools.

Special Thanks & Questions

Questions?

Special thanks to the many subject matter experts who have taken their time to assist us:

NEAMS Reactors: Paul Fischer, Dinesh Kaushic, Andrew Siegel, Mike Smith, Tim Tautges

NEAMS Fuels: Sreekanth Allu, Kevin Clarno, Bill Cochran, Sarma Gorti, Sreekanth Pannala, Bobby Philip, Bala “Rad” Radhakrishnan, Rahul Sampath, Srdjan Simunovic, John Turner

NEAMS FMM: Doug Kothe

NEAMS SafeSeps: Valmor De Almeida

IBM: Tim Bohn, George Chiu, John Magerlein

EDF: Nicolas Geimer, Paul Rasclé, Andre Ribes

GE Hitachi: Harsh Desai, Eric Loewen, Brian Triplett

...and probably others (apologies!)

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 Rational software

