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 simulation output in its most raw and unlimited form

Analyze

Output

01100010 01101001 01101110 01100001 01110010 01110010

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



Analyze simulation output in its most raw and unlimited form



Archive

Store data... somewhere!



|CC|

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

Batteries

> ICC Advanced Manufacturing

More 3rd Party Tools

Coming in FY16!

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

MyFirstItem Class Diagram





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.)

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

Standardization for the win!

l propertie Type:	es available for this node	can be modified here.	
Transient			
Enabled	Name	Value	Comments
1	picard_max_its	1	Number of times each timestep will be solved. Main!
1	picard_rel_tol	1e-08	The relative nonlinear residual drop to shoot for durin
	predictor_scale		The scale factor for the predictor (can range from 0 tc
1	reset_dt	true	Use when restarting a calculation to force a change in
	restart_file_base		File base name used for restart
7	scheme	explicit-euler	▼ Time integration scheme used.
	splitting	implicit-euler	Top-level splitting defining a hierarchical decomposit
F	ss_check_tol	explicit-euler	Whenever the relative residual changes by less than th
	ss_tmin	crank-nicolson	Minimum number of timesteps to take before checkin
V	start_time	rk-2	
	time_period_ends		The end times of time periods
	time_period_starts		The start times of time periods
	time_periods		The names of periods
(T)	timestep_tolerance	2e-14	the tolerance setting for final timestep size and sync t
[m]	trans_ss_check	true	Whether or not to check for steady state conditions
1	type	Transient	
	use_multiapp_dt	true	If true then the dt for the simulation will be chosen by
V	verbose	true	
	l_abs_step_tol	-1	Linear Absolute Step Tolerance
V	I_max_its	80	
V	l_tol	8e-3	
1	line_search	'none'	
	nl_abs_step_tol	1e-50	Nonlinear Absolute step Tolerance
1	nl_abs_tol	1e-10	
	nl_max_funcs	10000	Max Nonlinear solver function evaluations
V	nl_max_its	10	
	nl_rel_step_tol	1e-50	Nonlinear Relative step Tolerance
1	nl_rel_tol	1e-4	
	no fe reinit	true	Specifies whether or not to reinitialize FFs

Different views of the same data

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 Jo	b

Input File: Caebat_Model_1.conf

 Electrica 	Properties	
Electrical pro	perties and setttings	
Current Flux	÷	
3602431		

Enabled	Name	Value	Comments	^
	predictor scale		The scale factor for the predictor (can range from 0 to 1)	

The Eclipse ICE Item Project Generator

This tutorial will teach you how to create new ICE Item Projects

You will need:

- Experience writing simple Java code
- Docker Image with Fern science code

You will learn:

- How to create an Item project
- How to create Model and JobLauncher Items
- How to use those Items in ICE.



The Eclipse ICE Item Project Generator

Wizards: I construction of the second sec	Select a wizard		Enable users	s to go from working ICE
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Visualization Components

Resource Components, Geometry Editor Components, and Mesh Editor Components



Resource Component

 Add a component to your item which will display output using CSV graphs or VisIt 3D visualization.



Editing 3D Structures

- Add a Geometry Component to your Item to edit 3D shapes.
- Add a Mesh Component to your Item to create polygonal meshes.





Scripting ICE with EASE







Outline

- Install and Configure EASE
- Creating and Running Scripts
- Using the Sample Scripts

Installing and Configuring EASE

- EASE Jython Installation
- PyDev Installation
- EASE Configuration





Creating and Running Scripts

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XX

- Creating a Python Script
- Writing a Python Script
- Running a Python Script

🖹 Problems Target Platform State 📃 Console 🔀

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result was: InfoError

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Using the Sample Scripts

- createAndEditPython.py
- createAndProcessPython.py
- iterateChangeParameterPython.py
- listFromScratchPython.py

ICE Dynamic UI Tutorial

This tutorial will teach you how to change the ICE UI with only some small amounts of text.

You will need:

- Experience creating Eclipse plugins
- Experience writing UI code with SWT
- Experience creating an ICE Item

You will learn:

- How to create news pages in ICE's FormEditor
- How to create new EntryComposites in ICE's Form editor
- How to publish UI updates to the Eclipse 4 Context



Change this...

▼ Data		
Some Data		
Data Entry:		

... into this...



... without changing the way ICE draws the UI.

The Eclipse ICE Developer Menu

This tutorial will teach you how extend the ICE Developer Menu

You will need:

- Experience creating Eclipse plugins
- Experience adding Extensions

You will learn:

• How extend the Developer Menu with custom actions





Eclipse for Science

How the Parallel Tools Platform can enhance the development of scientific applications



Parallel Tools Platform

Enabling Parallel Application Development





PTP Application Development Cycle



CAK RIDGE

Dynamic & Performance Analysis

3 Eclipse for Science

Coding & Static Analysis

- Eclipse provides a wide variety of coding assistance tools
 - Project management, Editing and formatting, Navigation, Advanced searching, Refactoring, Version control
- C/C++ Development Tools (CDT)
 - Standard (Makefile) and managed builders, Support for arbitrary toolchains, Visual debugging using GDB, High level views (outline view, call hierarchy, type hierarchy, include browser), Refactorings
- Parallel Tools Platform (PTP)
 - Fortran, New project wizards (MPI, OpenMP) Content Assist, Hover help, Built-in API descriptions (MPI, OpenMP, LAPI, UPC), Location of parallel "artifacts" in code (MPI, OpenMP, PAMI, and UPC), Barrier analysis, Deadlock detection
 - Python Development (PyDev)
 - Code completion, type hinting, refactoring, debugging, interactive console, unittest, code coverage, Django integration



Coding & Static Analysis

- Assistance tools to increase productivity of parallel programmers
 - New project wizards (MPI, OpenMP)
 - Content Assist (command/API completion), hover help, built-in API help descriptions in an html help "view" (MPI, OpenMP, LAPI, UPC)
 - Location of parallel "artifacts" in code: MPI, OpenMP, and UPC

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MPI_Comm_size	MyMPIproject.c
MPI_Send	MyMPIproject.c
MPI_Recv	MyMPIproject.c
	MyMPIproject.c
	MyMPIproject.c





Fortran Development Tools

- Photran features:
 - Supports Fortran 77-2008
 - Syntax-highlighting editor
 - GUI interface to gdb
 - Makefile-based compilation
 - Compiler error extraction
 - Outline view
 - Open declaration
 - Fortran refactorings
 - C preprocessor support





Python Development

🖶 PyDev - Robots/src/robots/tests/test_robo	r.py - Eclipse SDK
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- PyDev is a Python IDE for Eclipse
- Create/manage Python modules
- Full array of Eclipse editing features for Python
- Python debugger
- Interactive console with Python
 interpreter
- Integration with Python unittest and code coverage modules



PTP Application Development Cycle



CAK RIDGE

Dynamic & Performance Analysis

8 Eclipse for Science

Application Execution

Launching & Monitoring

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- Improves visibility into target system
- Single point of interface for launching and control
- Manages interaction with different runtime systems and job schedulers

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Application Execution

- Target Configuration Framework
 - Extensible framework for launching & monitoring
 - System and node status information
 - Job status (e.g. position in queue) & application status
 - Job submission & control
 - Debugger launch
 - Configuration files to support different resource managers
 - Job schedulers (LoadLeveler, PBS, Torque, SLURM, GridEngine)
 - Interactive runtimes (e.g. PE, Open MPI, MPICH2, MVAPICH)
 - Systems (AIX, Linux, Power, x86, BG/Q, Cray)
 - Local or remote system support
 - Command-line tools executed locally or via ssh connection



PTP Application Development Cycle



11 Eclipse for Science

Application Debugging

PTP Parallel Debugger

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<pre>{ fint my_rank; /* rank of process */ int num_procs; /* number of processes */ int source; /* rank of sender */ int dest = 0; /* rank of receiver */ int tag = 0; /* tag for messages */ char message[100]; /* storage for message */ MPI_Status status; /* return status for receive */ /* start up MPI */ MPI_Init(&argc, &argv); /* find out process rank */ MPI_Comm_rank(MPI_COMM_WORLD, &my_rank); c </pre>		142 № № ∞ # mpi.h # stdio.h # string.h • calc_pi(int, int) : void • main(int, char4]) : int
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- Mid-scale integrated debugger
- Tightly integrated with Eclipse
- Supports debugging multiple jobs simultaneously
- Utilizes backend debugger (e.g. gdb) for low level operations
- Targeted at SPMD programming models
- Supports mixed MPI & thread debugging
- Single process and group operations
- Platform for building new debugging paradigms



Application Debugging

- Scalable debugger using multicast reduction network
- Integrated with PTP and launched using target configurations
- Supports basic debug commands



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PTP Application Development Cycle=





Application Execution

Dynamic & Performance Analysis

Dynamic Analysis Tools

- Perform analysis on the running application using external tools
- Generate results that must be brought back into Eclipse as part of the development workflow

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 May require external tool for visualization or other purposes





Dynamic & Performance Analysis

- Tuning and Analysis Utilities (TAU)
 - Instrumentation and transparent re-build of application executable
 - Execution of profiled application and collect performance data
 - Performance data visible in UI
 - Launches paraprof visualization client from Eclipse
- Graphical Explorer of MPI Programs (GEM)
 - Formal Dynamic Verification of MPI Applications
 - Detects all deadlocks, assert violations, MPI object leaks, and default safety properties
 - Matches sends and receives
 - Allows post-verification review of highlighted bugs
 - Works with a variety of MPI implementations





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Online Information

Information about PTP

- Main web site for downloads, documentation, etc.
 - http://eclipse.org/ptp
- Developers' wiki for designs, planning, meetings, etc.
 - http://wiki.eclipse.org/PTP
- Articles and other documents
 - <u>http://wiki.eclipse.org/PTP/articles</u>



Community

PTP Mailing lists

- Major announcements (new releases, etc.) low volume
 - <u>http://dev.eclipse.org/mailman/listinfo/ptp-announce</u>
- User discussion and queries medium volume
 - http://dev.eclipse.org/mailman/listinfo/ptp-user
- Developer discussions higher volume
 - <u>http://dev.eclipse.org/mailman/listinfo/ptp-dev</u>

