



Exceptional service in the

national

interest

The Sandia Analysis Workbench Leveraging a COTS Framework To Provide Integrated Engineering Analysis Workflows On HPC Systems

Ernest J. Friedman-Hill Edward L. Hoffman Robert L. Clay



Ø

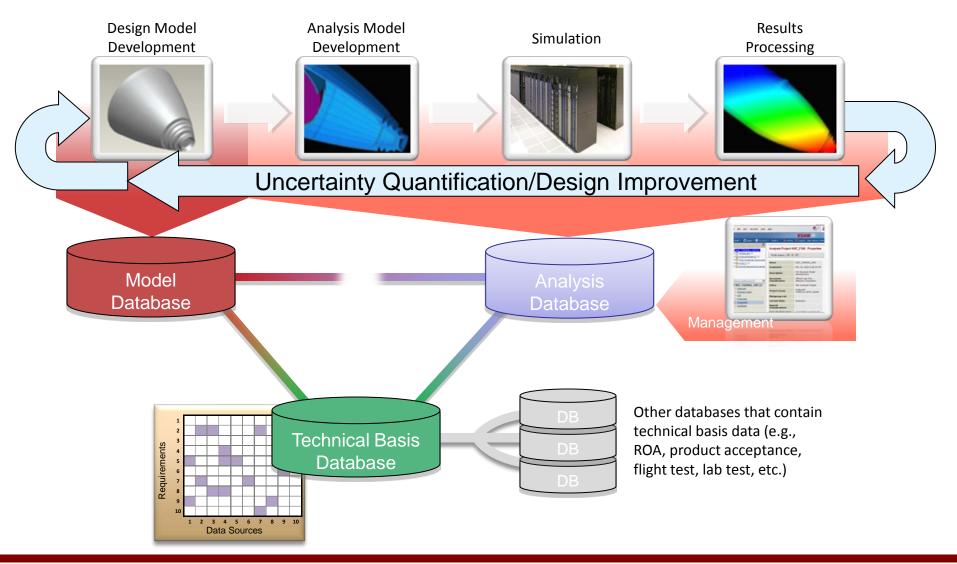
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Outline



- Problem Space
- The Eclipse Framework
- Tool Case Studies

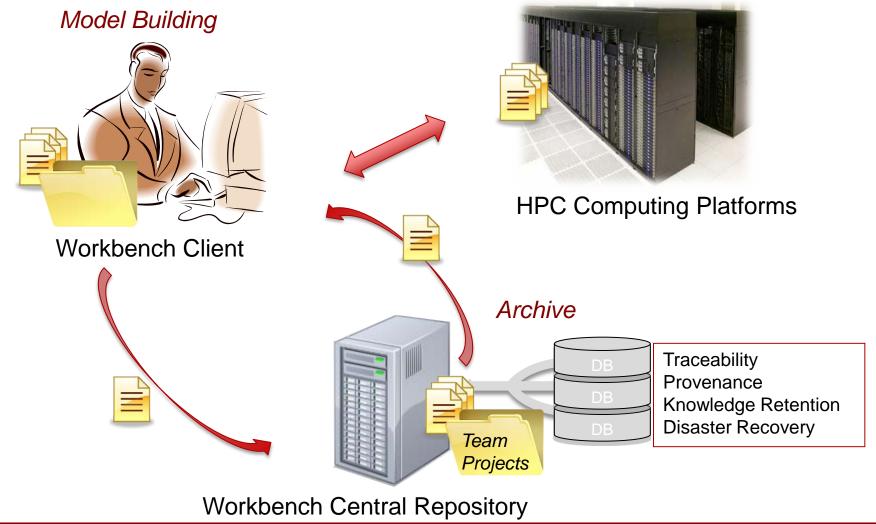
Support the Design-To-Analysis process, capturing data in context





Integrating Analysis Systems

Job Submission & Remote Viz



Sandia Laboratories



- Scientists
- Engineers
- Developers

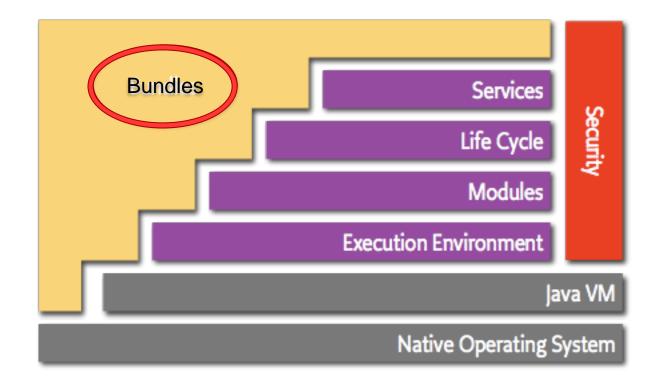
All working together

- Wide variety of software in use
 - Commercial
 - In-house
- Corporate services available
- Change is a given
- How to make everything work together?



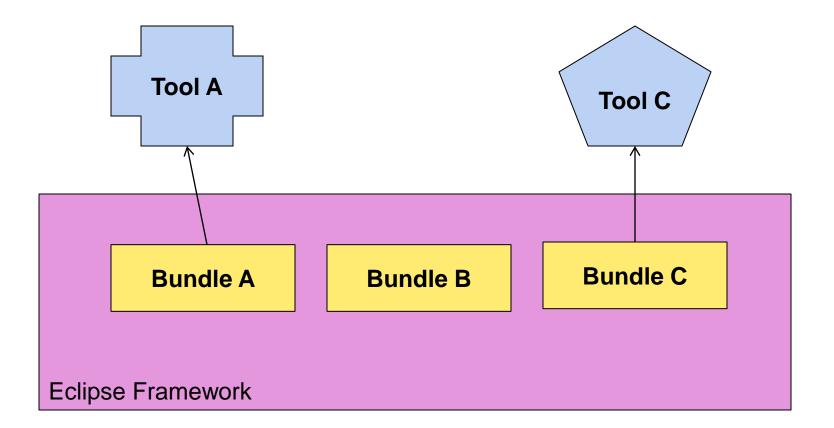


OSGi Architecture



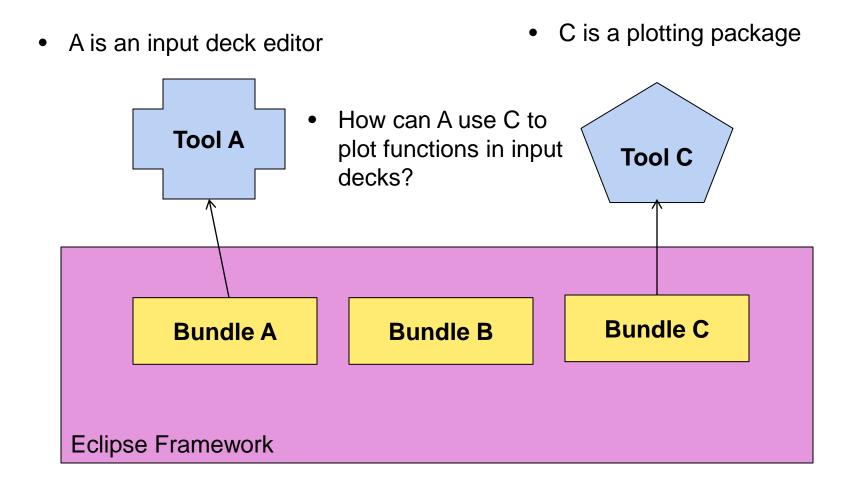






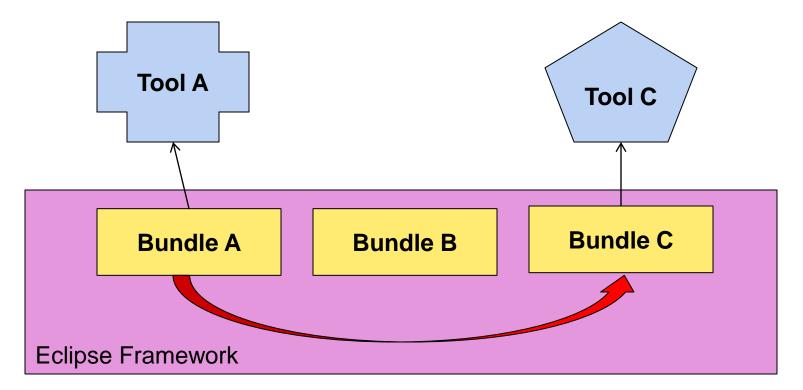
Tool Interactions





Direct Dependencies





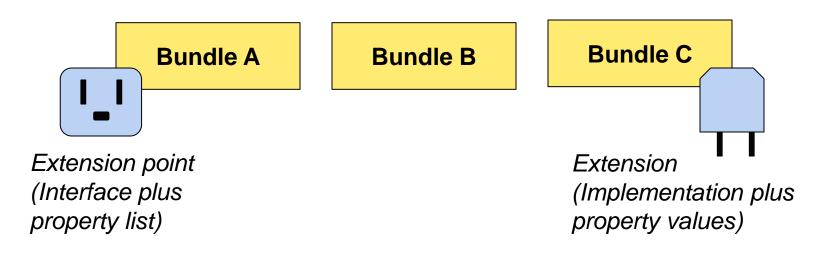
- Hard-wired dependency
- No user choice

Extension Points



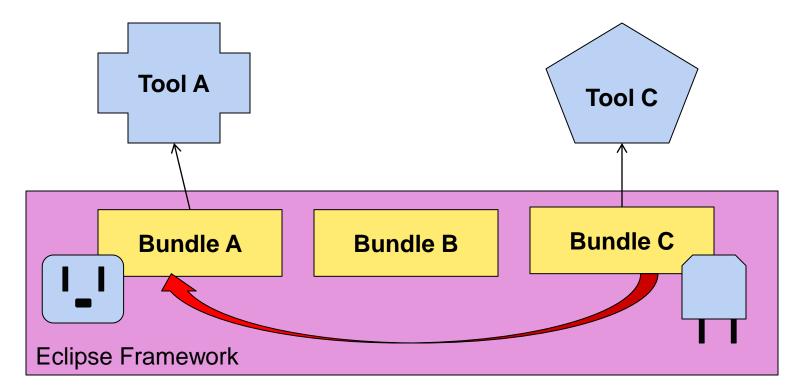
• "Inversion of Control"

• Framework gives A a list of extensions at runtime



Extension Points

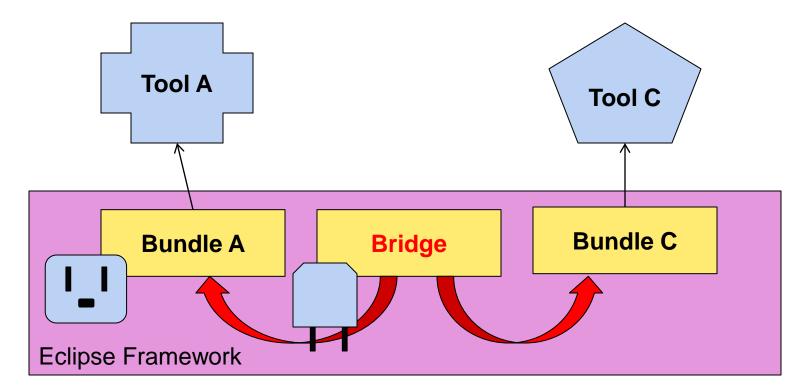




- Compile-time dependencies
- User choice enabled

Bridge Plugins





- Tools are independent
- User choice enabled

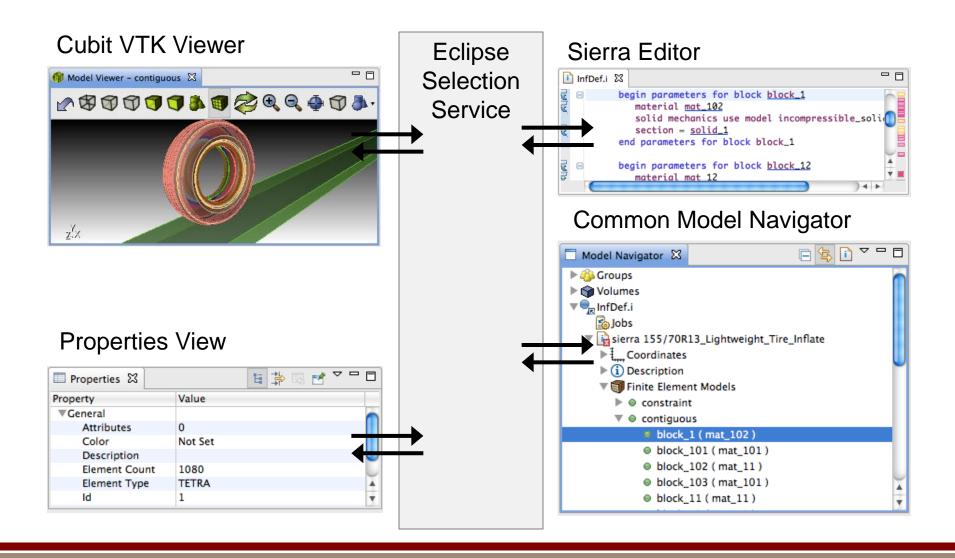
Object Adapters



- Adapt one object type to another
- IAdaptable interface
- AdapterManager
 - Any bundle can provide adapters
- No need to use common interfaces!

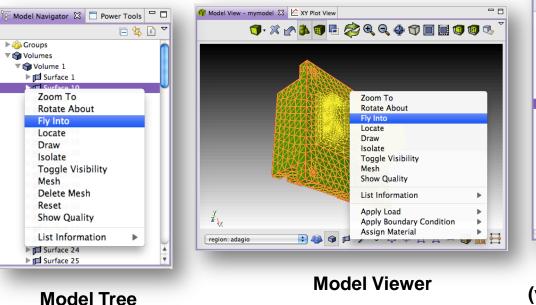


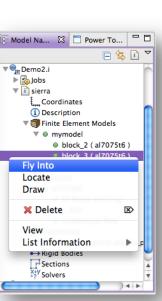
Eclipse platform selection service



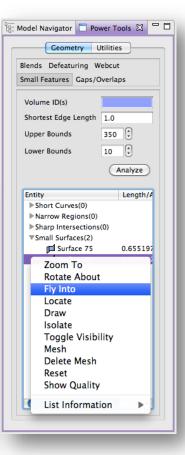
Object Action Contributions

- Eclipse Command/Handler/Menu framework
- Action enablement based on selected object type
- Implemented once, available in many places





Sierra Editor Tree (via Object Adapter)



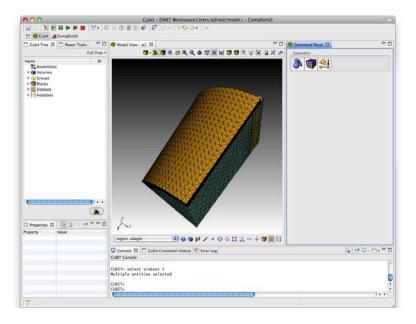
Cubit Model Tree

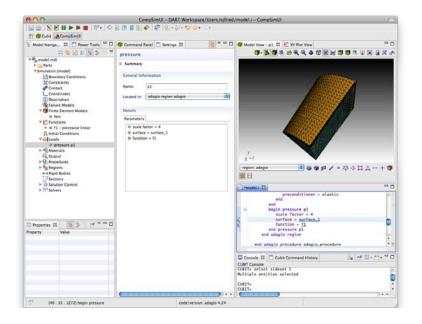


Eclipse "Perspectives"



- An arrangement of views, buttons, menus
- One button push separates these two screens





Sierra Analysis Codes



- Single framework
- Many different physics codes (Thermal, Structural)
- Used separately or coupled
- Available commands described in XML



Sierra Editor



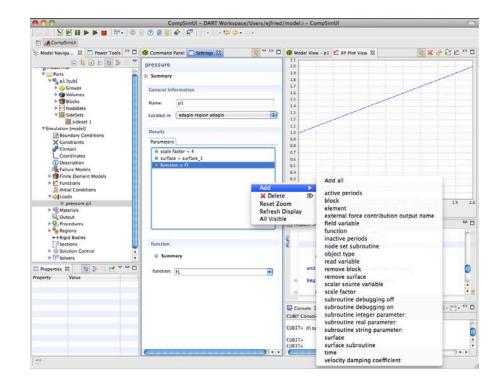
- Reads XML and provides
 - Syntax highlighting
 - Validation
 - Completion
 - Content assist
 - Hyperlinking
- Supporting other codes
 - Same XML format for commands
 - Syntax implemented with code module

Begin Finite Element Model AFF-tet-fine Dotbose Name =	- 0
<pre>2 d Database Name =AFF-tet-fine.g 5 5 6 End Finite Element Model AFF-tet-fine 7 8 Begin presto Procedure prestoProcedure 9 10 begin presto region prestoRegion 11 use finite element model <u>afF-tet-fine 12 begin prestope</u> pp 13 block = block.g 14 end pore pressure pp 15 begin fixed displacement fd1 19 begin prescribed displacement fd1 19 begin prescribed displacement fd1 19 begin prescribed displacement pd 20 components = x Y 18 end prescribed displacement pd 20 components = y 21 function = horizontal 22 block = block.g 23 end prescribed displacement pd 24 end prestoregion prestoRegion 25 26 End presto Procedure prestoProcedure 27 </pre>	C .
Q A Database Nome =/AFF-tet-fine.g 5 End Finite Element Model AFF-tet-fine 7 Begin presto Procedure prestoProcedure 9 begin presto region prestoRegion 11 use finite element model <u>afF-tet-fine</u> 12 begin presto region prestoRegion 13 block - block_8 14 end pore pressure pp 15 begin prescribed displacement fd1 16 block - block_9 17 components = x Y 18 end prescribed displacement pd 20 component = y 21 function = horizontal 22 block - block_8 23 end prestribed displacement pd 24 end prestribed displacement pd 25 End presto region prestoRegion 25 End presto Procedure prestoRegion	
6 End Finite Element Model AFF-tet-fine 7 Begin presto Procedure prestoProcedure 9 begin presto region prestoRegion 11 use finite element model <u>aff-tet-fine</u> 12 begin presto region prestoRegion 13 block - block_8 14 end pore pressure pp 15 begin fixed displacement fd1 16 block - block_9 17 components = x Y 18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block_8 23 end prestor region prestoRegion 25 End presto Procedure prestoProcedure	
7 8 9 Begin presto Procedure prestoProcedure 9 begin presto region prestoRegion 11 use finite element model <u>off-tet-fine</u> 12 begin pres pressure pp 13 block - block_8 14 end pore pressure pp 15 begin fixed displacement fd1 16 block - block_9 17 components - x Y 18 end fixed displacement pd 20 component - y 21 function - horizontal 22 block - block_8 23 end prescribed displacement pd 24 end prescribed displacement pd 25 block - block_8 24 end prescribed displacement pd 25 block - block_8 26 End presto region prestoRgion 25 End presto Procedure prestoProcedure	
Begin presto Procedure prestoProcedure 9 100 begin presto region prestoRegion 11 use finite element model <u>aff-tet-fine</u> 120 begin presto region prestoRegion 121 begin prestore pressure pp 13 block - block_8 14 end pore pressure pp 15 begin fixed displacement fd1 16 block - block_9 17 components - x Y 18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component - y 21 function - horizontal 22 block - block_8 23 end prestorbed displacement pd 24 end prestorbed displacement pd 25 End presto region prestoRegion 25 End presto Procedure prestoProcedure	
9 begin presto region prestoRegion 10 use finite element model <u>aff-tet-fine</u> 12 begin pore pressure pp 13 block - block 8 14 end pore pressure pp 15 begin fixed displacement fd1 16 block - block 9 17 components - x Y 18 end fixed displacement pd 20 component - y 21 function - horizontal 22 block - block.8 23 end prescribed displacement pd 24 end presto region prestoRegion 25 End presto Procedure prestoProcedure	
10- begin presto region prestoRegion 11 use finite element model <u>off-tet-fine</u> 12- begin pore pressure pp 13 block - block_8 14 end pore pressure pp 15= begin fixed displacement fd1 16 block - block_9 17 components - x Y 18 end fixed displacement fd1 19- begin prescribed displacement pd 20 component - y 21 function - horizontal 22 block - block_2 23 end prestoregion prestoRegion 25 End presto Procedure prestoProcedure 27 End presto Procedure prestoProcedure	
12 use finite element model aff-tet-fine 12 block = block_8 14 end pore pressure pp 15 begin fixed displacement fd1 16 block = block_9 17 components = x Y 18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block_8 23 end prescribed displacement pd 24 end prestoregion prestoRegion 25 End presto Procedure prestoProcedure	
12e begin pore pressure pp 213 block = block.8 15e begin fixed displacement fd1 15e block = block.9 17 components = x Y 18 end fixed displacement fd1 19e begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block.8 23 end prescribed displacement pd 24 end presto region prestoRgion 25 End presto Procedure prestoProcedure 27 End presto Procedure	
13 block - block.8 14 end pore pressure pp 15 begin fixed displacement fd1 16 block - block 9 17 components = x Y 18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block - block.8 23 end prescribed displacement pd 24 end prescribed displacement pd 25 End presto region prestoRegion 26 End presto Procedure prestoProcedure	
14 end pore pressure pp 15= begin fixed displacement fd1 16 block = block_9 17 components = x Y 18 end fixed displacement fd1 19= begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block - block_8 23 end prescribed displacement pd 24 end presto region prestoRgion 25 End presto Procedure prestoProcedure 27 End presto Procedure	
15 begin fixed displacement fd1 216 block - block 9 17 components - x Y 18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component - y 21 function - horizontal 22 block - block 8 23 end prestorribed displacement pd 24 end prestorribed displacement pd 25 end prestorribed displacement pd 26 End presto Procedure prestoProcedure 27 Prosto Procedure prestoProcedure	
2 16 block = block.9 17 components = x Y 18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block.8 23 end prescribed displacement pd 24 end prestoregion prestoRegion 25 26 26 End presto Procedure prestoProcedure	
17 components = x Y 18 end fixed displacement fd1 19= begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block & block & block 23 end prescribed displacement pd 24 end prescribed displacement pd 25 end prestorregion prestoRegion 25 End presto Procedure prestoProcedure 27 Presto Procedure	
18 end fixed displacement fd1 19 begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block = 23 end prescribed displacement pd 24 end presto region prestoRegion 25 End presto Procedure prestoProcedure 27 For presto Procedure	
19- begin prescribed displacement pd 20 component = y 21 function = horizontal 22 block = block_8 23 end prescribed displacement pd 24 end prescribed displacement pd 25 26 26 End presto Procedure prestoProcedure 27 27	
20 component = y 21 function = horizontal 22 block = block & 23 end prescribed displacement pd 24 end presto region prestoRegion 25 End presto Procedure prestoProcedure 27 27	
21 function = horizontal 22 block = block.8 23 end prescribed displacement pd 24 end presto region prestoRegion 25 26 26 End presto Procedure prestoProcedure 27 27	
23 end prescribed displacement pd 24 end presto region prestoRegion 25 End presto Procedure prestoProcedure 27 27	
23 end prescribed displacement pd 24 end presto region prestoRegion 25 End presto Procedure prestoProcedure 27 27	
24 end presto region prestoRegion 25 End presto Procedure prestoProcedure 27 27	
25 26 End presto Procedure prestoProcedure 27	
27	
27	
20	
28	
290 BEGIN DEFINITION FOR FUNCTION horizontal	
30e BEGIN VALUES	
31 12	
32 3 4	Ŧ
**	

Sierra Builder



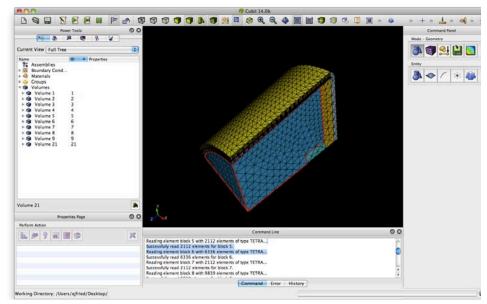
- Builds on editor to provide
 - Fully-graphical model building
 - Generated dialogs
 - Custom dialogs (via extension point)
 - Tree-based navigation



CUBIT Mesh Generator



- C++ library
- Interactive application
- Existing Qt GUI
 - Imperative command panels
 - Properties view
 - VTK-based viewer
 - Console
- Our approach: keep mesh viewer, recreate the rest of the GUI





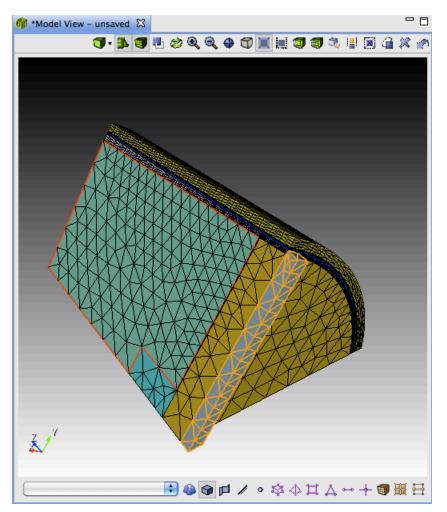
CUBIT: Command Panel Builder

- Novel XML format
- Describe command, not GUI
 - "Hints" for GUI implementation
- Testing for panel generator

👘 Command Panel 🛛 🗧 🗖
Geometry
Volume
Modify
Auto Clean
Volume ID(s) all
Select Auto Clean Method
Small Curves
O Small Surfaces
O Split Narrow Regions
O Force Sweepability
Small Feature Threshold Size 0.1
Update Threshold
Preview Apply
×
Ŧ

CUBIT: Native Code Integration

- Generate glue code with SWIG
- Less than 500 lines of handwritten C++
- Platform-specific fragments





Data Management

Teaming

NTK



Simulation Data Management Job Management 0 0 SDM JoeDemo2/Files/3_point_bend_test1.i - DART Workbench - /Users/elhoffm/Desktop/workspace_nov_training । 🔛 🗁 💋 🐠 🍘 🌄 🌄 🔍 । 🏇 • 🔘 • - | 🖉 - | © 📄 🕐 🞒 🚰 - 🍋 💥 - 👉 | 😓 - 🏹 - 🏷 - 🔶 -📑 🖀 SDM 🖀 Model Building 🖀 JobSubmissio 🗞 🗙 🔄 🗸 🗖 😢 Project Navigator 🚺 *3_point_bend_test1.i 🛛 🗄 Outline 🖏 Job Status 🖾 Teams 1⊖# Generated by: 🄁 🚰 🔊 🔥 🖂 🕏 Name Aachine Stage Oueue Status 2 # SIMBA version 67 Build number 3201(Ad-hoc). loint model SALINA shasta Finished Completed Tue Nov 24 15:56:2 DAKOTA-Milestone 3 # Built on ejfried-dell at 4/23/2009 12:03:47 loint model SALINAS Tue Nov 24 16:01:1 shasta Finished Ed_March_Training Completed 4 # Exported on Fri Mar 19 10:23:14 MDT 2010 Joint_model_SALINAS shasta Finished Completed Tue Nov 24 16:20:1 🔻 🔓 >JoeDemo2 5 1 6@begin sierra 3_point_bend_test1 dt1b_blivet_060515 Tue Nov 24 16:37:1 thunderbird Finished Completed 🚹 .DS_Store [1/1] Joint_model_SALINAS thunderbird Finished Completed Wed Nov 25 12:09:2 AnalysisFolder Metagroups {include("gpm_functions.txt")} 8 # Wed Nov 25 12:25:4 Tail_assy thunderbird Finished Completed Deleted Items {include("gpm_functions.txt")} Wod Nov 25 12.20.2 Tail acc underhird Einicher 🔻 旑 Files 10 {include("gpm.txt")} 3_point_bend_test1.i [2/2] 🔗 🗍 • 🗍 • XY • 💋 🏥 🔠 🏢 🎐 🌵 🏇 🖉 🖓 🖯 💁 Model View 🖾 🛐 3_point_bend_test1a.g [1/1] begin property specification for material Default beam.g 14 density = 1000. 🔒 cmcc.i [1/1] begin parameters for model ELASTIC Web services Ę displacement y.txt [1/1] 16 poissons ratio = 0.3333 17 youngs modulus = 3E7 🔒 fetidp.txt [1/1] 18 end parameters for model ELASTIC gpm_functions.txt [1/1] 19 end property specification for material Default gpm.txt [1/1] 20 results_output.txt [1/1] begin property specification for material mat_1 solver.txt [1/1] density = 8000 test.inp [1/1] 230 begin parameters for model elastic 24 poissons ratio = 0.245 清 y_reaction.bdf [1/1] 25 youngs modulus = 195.0e+09 y_reaction.h [1/1] 26 end parameters for model elastic ▶ 🚰 > Materials end property specification for material mat_1 SIMBAWS 28 WorkProductsDocumentFolder 29 # Functions for conditions 🚰 *>LPC_Demo Proble... | 🕸 Engine... 🙋 Progress 🔗 Search 🖆 XY Plot ... 🔀 📮 Console 🧮 🗖 🔂 glory 🕱 (> <> 🗛 🔻 🗖 🗖 🔒 🗳 🗎 🚔 🟠 0.0000 - 0 🖀 Team Members 🛛 🔲 Properties /gscratch1/elhoffm/JoeDemo2/Files -0.0001🐴 🕂 🗶 🎬 Size Modified 3_point_bend_test1.i 7.9 KB Nov 3, 2010 1:00:07 P Role Email Name -0.0002 3_point_bend_test1a.cfg 284 bytes Nov 3, 2010 1:00:16 P Team Member mjgibso@sandia.gov Gibson, Marcus J -0.0003 1 MB Nov 3, 2010 1:00:09 P 3_point_bend_test1a.g Project Manager elhoffm@sandia.gov Hoffman, Edward Team Member jagreen@sandia.gov Greenfield, John 3_point_bend_test1a.g.4.0 322 KB Nov 3, 2010 1:00:16 P -0.0004 3_point_bend_test1a.g.4.1 355.9 KB Nov 3, 2010 1:00:16 P 385.2 KB, Nov 3, 2010 1:00:17 P 3 point bend test1a.g.4.2 -0.0005 _bend_test1a.g.4.3 345.9 KB Nov 3, 2010 1:00:17 P point bend test1a.lbd.er 0 bytes Nov 3, 2010 1:00:16 P -0.0006 3_point_bend_test1a.lbd.out 2.1 KB Nov 3, 2010 1:00:16 P -0.0007 3_point_bend_test1a.nem 204.7 KB Nov 3, 2010 1:00:16 P 3_point_bend_test1a.pex 588 bytes Nov 3, 2010 1:00:16 P 🔻 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2) 4 + | 🕈 🗐 111M of 508M

Distributed File Management

Job Submission

Sandia National Laboratories

- Modular architecture
 - Machine templates
 - Code templates
 - Defaults
 - Custom templates
- Remote access
 - Heterogeneous machines
- Local access

	e O O Edit Configuration
	Edit configuration and launch.
	Select the code and machine for the job submission, then select an execution template. Set the parameters of the job submission (input files, oueve, number of nodes, job time, etc) under the Resources. Machine, and Execution Instructions tabs
	Name: far_field_pressure
	🕅 Main 🗉 Common 🦣 APC Repository
	Code: Presto Execution Template: presto-glory Execution Template: presto-glory
	Resources Machine Execution Instructions
	Input Deck: //Users/elhoffm/Documents/runtime-DART-Workbench-feature.product/DryRunTestProjec Browse
	Input files:
	Output files: *.e Add
) 🔘	Edit Configuration Edit
ne: far_field_p Main Comr de: Presto cchine: glory Queue: Remote Directo	Revert Revert Resources Machine Execution Instructions Run
Under Of Proc Job Time: Account:	
	Apply Revert

Multiple Configurations









- Workbench
 - Everything
- CompSimUI
 - Model Building
 - Meshing
 - Job Submission
- Sierra Editor
 - Model Building
 - Job Submission

Eclipse allows us to build multiple application distributions by choosing from among our set of components

Conclusions



- Eclipse and the OSGi architecture let us
 - ... reduce dependencies between integrated software projects
 - ... integrate diverse components smoothly and robustly
 - ... create and deploy customized solutions easily

Acknowledgements



The DART Team

Douglas Clay, Marcus Gibson, John Greenfield, Stephen Mueller, Kevin Olson, Edward Walsh

The CUBIT Team

Randy Morris, Matt Staten

The SIERRA Team

• Mike Glass, Martin Heinstein, Garth Reese, Brett Robertson



This work is supported by the Advanced Strategic Computing program of the NNSA.

Questions



Technical contact: Ernest Friedman-Hill 925-294-2154 <u>ejfried@sandia.gov</u>

Programmatic contact: Robert Clay 925-294-3114 <u>rlclay@sandia.gov</u>