

ENGINEERING SCIENCES WORKFLOWS FOR V&V APPLICATIONS

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The Sandia Analysis Workbench

An integrated environment for engineering analysis

The screenshot displays the Sandia Analysis Workbench interface with the following components:

- Project Navigator:** A tree view showing the project structure, including folders like 'DAKOTA-Milestone', 'Ed_March_Training', and 'JoeDemo2'. The 'Files' folder is expanded to show various input files such as '3_point_bend_test1.i', 'beam.g', 'cmcc1', and 'displacement_y.txt'.
- Code Editor:** Displays the input file '3_point_bend_test1.i' with a pre-processor script. The script includes material and model definitions, such as:

```
begin property specification for material Default
density = 1000.
begin parameters for model ELASTIC
poissons ratio = 0.3333
youngs modulus = 3E7
end parameters for model ELASTIC
end property specification for material Default

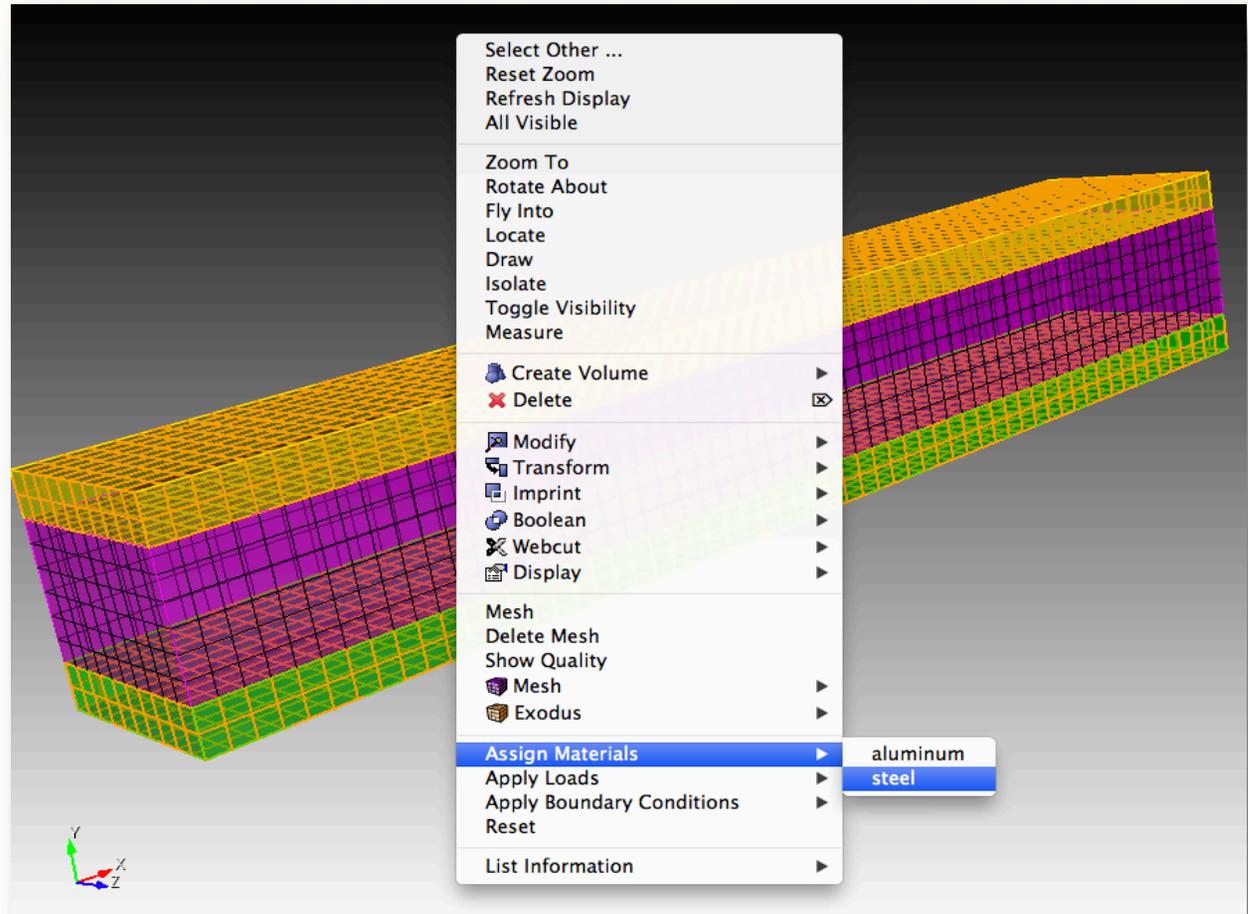
begin property specification for material mat_1
density = 8000
begin parameters for model elastic
poissons ratio = 0.245
youngs modulus = 195.0e+09
end parameters for model elastic
end property specification for material mat_1

# Functions for conditions
```
- Job Status Table:** A table listing the execution status of various jobs. The table has columns for Name, Machine, Stage, Queue Status, and Submit Date.

Name	Machine	Stage	Queue Status	Submit Date
Joint_model_SALINAS	shasta	Finished	Completed	Tue Nov 24 15:56:2
Joint_model_SALINAS	shasta	Finished	Completed	Tue Nov 24 16:01:1
Joint_model_SALINAS	shasta	Finished	Completed	Tue Nov 24 16:20:1
dt1b_blivet_060515	thunderbird	Finished	Completed	Tue Nov 24 16:37:1
Joint_model_SALINAS	thunderbird	Finished	Completed	Wed Nov 25 12:09:2
Tail Assy	thunderbird	Finished	Completed	Wed Nov 25 12:25:4
Tail Assy	thunderbird	Finished	Completed	Wed Nov 25 13:03:9
- Model View:** A 3D visualization of a mechanical assembly, showing a cylindrical component with a mesh overlay.
- Console:** A plot showing a linear relationship between two variables, with the x-axis ranging from 0.0 to 1.3 and the y-axis from -0.0007 to 0.0000.
- File Explorer:** A file browser showing the contents of the '/gscratch1/elhoffm/JoeDemo2/Files' directory, listing files like '3_point_bend_test1.i', '3_point_bend_test1a.cfg', and '3_point_bend_test1a.g'.

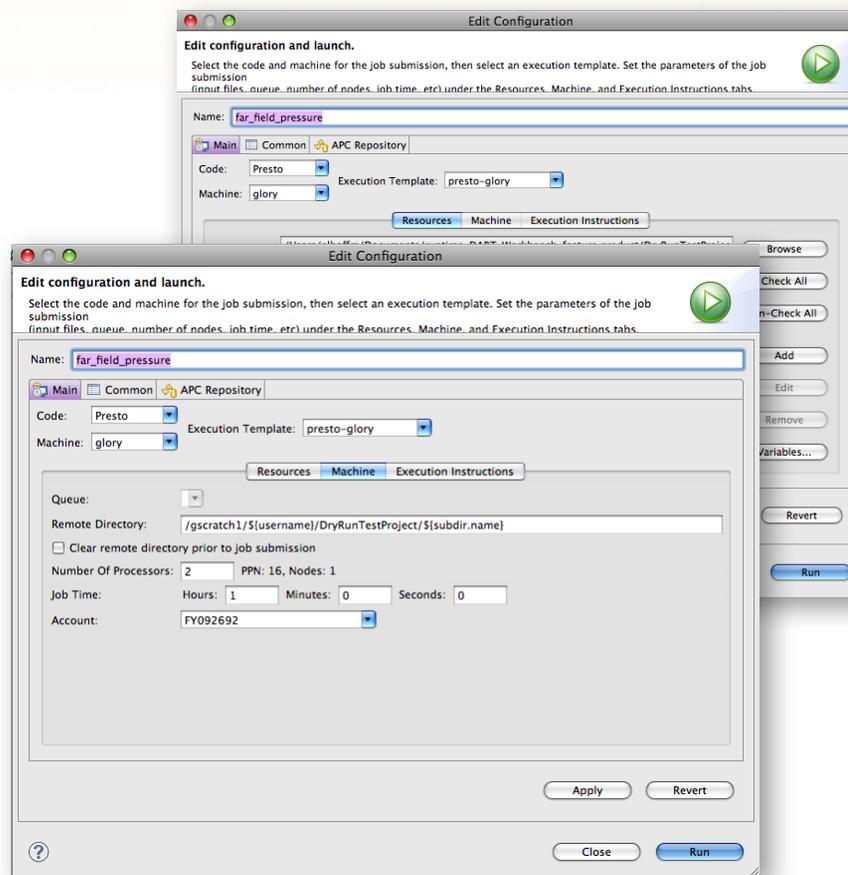
Model Building

Graphical model building for many in-house codes including the Sierra suite and CTH



Job Submission

Template driven,
easily user
customized,
makes access to
heterogeneous
resources
uniform



Job Monitoring and Distributed File Management

Debug, track, and access jobs

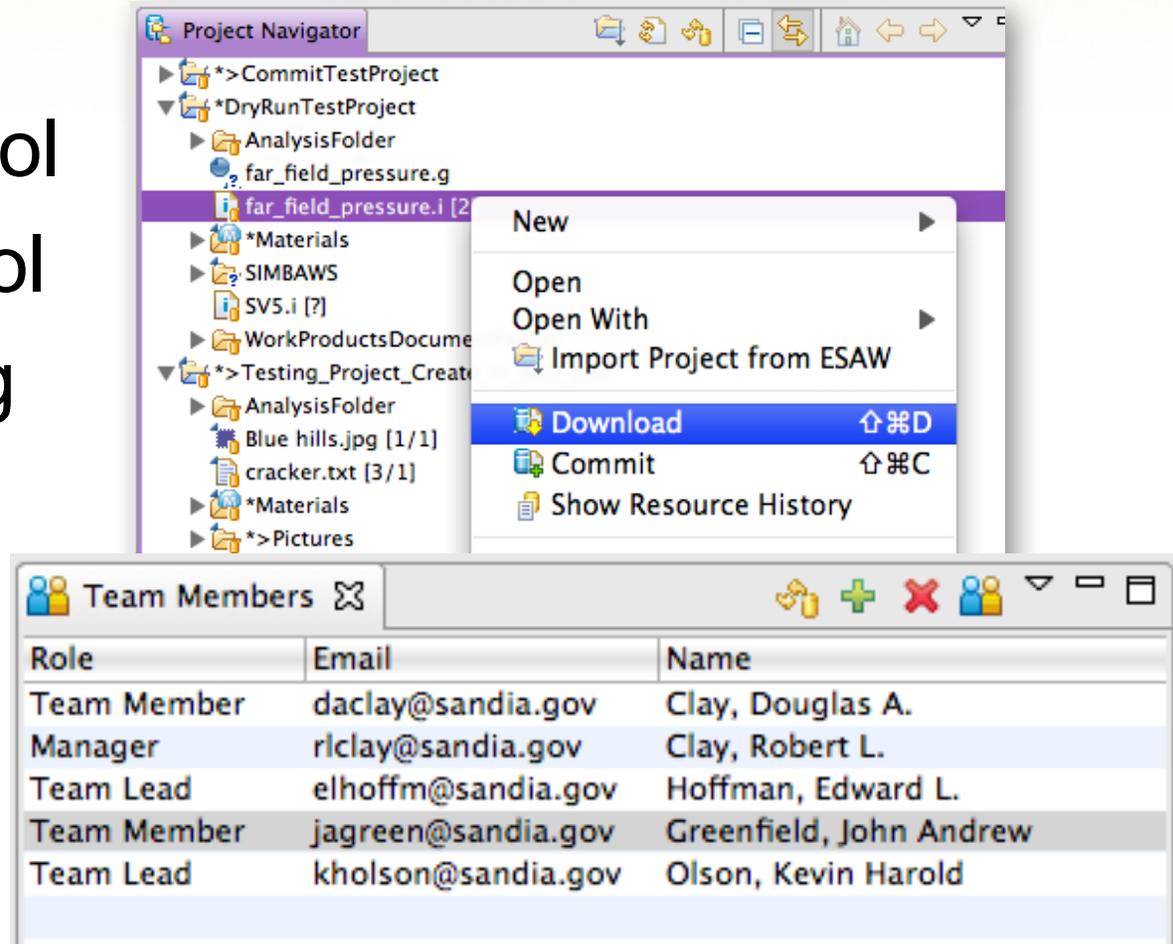
The screenshot displays a job monitoring application with two main panels. The left panel shows a list of machines with their utilization percentages and estimated job start times. The right panel shows a table of job status.

Name	URL	% Utilized	Estimated Job Start for: 16 procs @ 01:~
skybridge	ssh://skybridge.sandia.gov/fscratc...	96%	Immediately (2017-02-22 09:28:...
chama	ssh://chama.sandia.gov/fscratch/ej...	97%	Immediately (2017-02-22 09:51:...
uno	ssh://uno.sandia.gov/fscratch/ejfried	93%	
serrano	ssh://serrano.sandia.gov/gscratch/...	92%	
redsky	ssh://redsky.sandia.gov/fscratch/ej...	90%	
local	file://localhost/		

Job Name	Stage	Queue Status	Submit Dat
test	Finished		2017-02-
test	Finished		2017-02-
Crush_e...	Finished	Completed	2017-02-
Crush_e...	Finished	Completed	2017-02-
Crush_e...	Finished	Completed	2017-02-
Crush_e...	Killed	Removed	2017-02-
Crush_e...	Finished	Completed	2017-02-

Scientific Data Management

- Version control
- Access control
- Team sharing
- Repository search

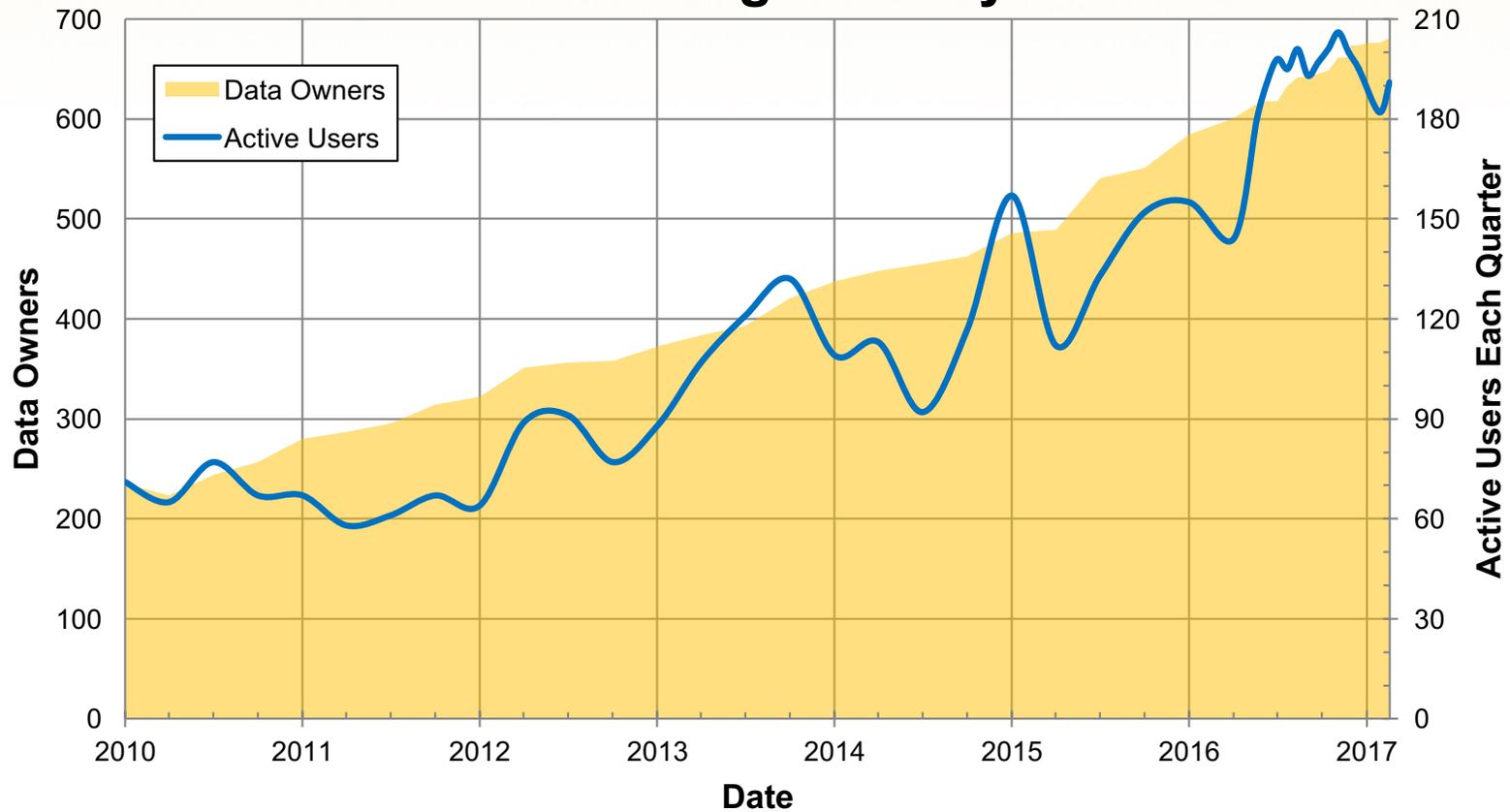


The screenshot displays two windows from a software application. The top window, titled 'Project Navigator', shows a hierarchical tree of project folders and files. A context menu is open over a file named 'far_field_pressure.i', with options including 'New', 'Open', 'Open With', 'Import Project from ESAW', 'Download', 'Commit', and 'Show Resource History'. The bottom window, titled 'Team Members', contains a table with the following data:

Role	Email	Name
Team Member	daclay@sandia.gov	Clay, Douglas A.
Manager	rlclay@sandia.gov	Clay, Robert L.
Team Lead	elhoffm@sandia.gov	Hoffman, Edward L.
Team Member	jagreen@sandia.gov	Greenfield, John Andrew
Team Lead	kholson@sandia.gov	Olson, Kevin Harold

Metrics show widespread adoption of SAW

SAW Usage History



Data are for internal Sandia users only

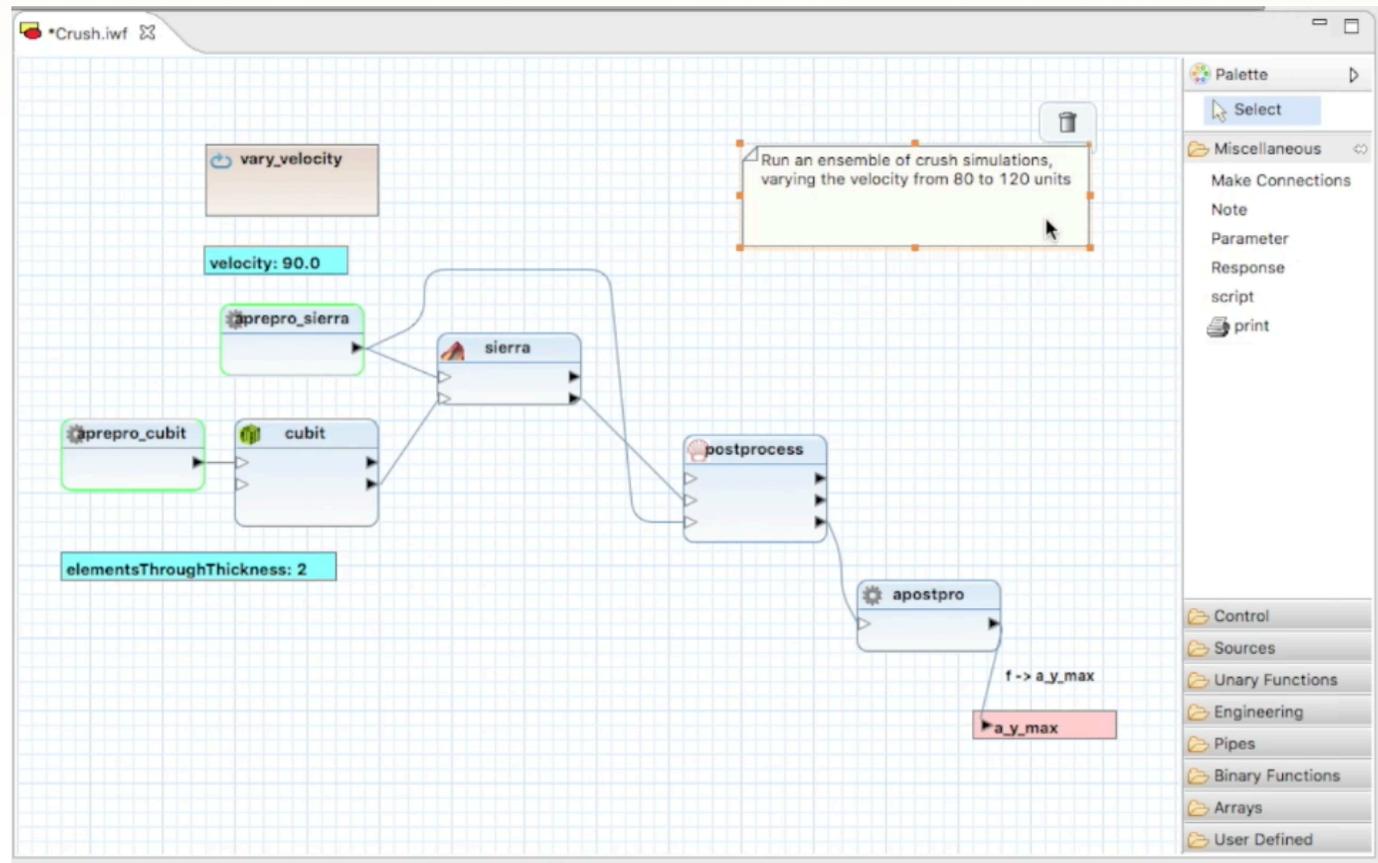
New Challenges

Ensembles

- ...of multi-step processes
- ...with constant variations
- ...often needing manual intervention
- ...running on unreliable machines
- ...providing high-consequence evidence

The Solution

Automated workflow...
integrated with everything else in SAW



Workflow System Requirements

- Workflow engine independence
- Minimal server installation
- Flexible system architecture
 - “Everything executes anywhere”
- Low cognitive load
- Transparent and escapable

SAW Workflow Architecture

- Graphical Workflow Editor
 - Leverages some tech from Triquetrum/ESWG
 - Data-driven
- Workflow Runtime
 - “Abstract dataflow” (exoscale)
 - Integration layer for workflow engine independence
 - Highly portable

Model Building

Edit model components naturally using familiar tools

The screenshot displays a multi-paneled software interface for model building. The top-left pane shows a workflow diagram with components like 'vary_velocity', 'aprepro_Sierra', 'cubit', 'sierra', 'bashScript', and 'apostpro'. The top-right pane is a code editor showing a piecewise linear function definition for 'pmdi20_modulus'. The bottom-left pane is a settings window for the 'pmdi20_modulus' function, showing its type and a table of data points. The bottom-right pane is a plot view showing a linear decrease in temperature over time.

```
92  ordinate is temperature
93  abscissa is time
94  begin values
95    -500.00 1.0
96    0.00 1.0
97    500.00 1.0
98  end values
99  end definition for function pmdi20_constant
100
101  begin definition for function pmdi20_modulus
102  type is piecewise linear
103  ordinate is temperature
104  abscissa is time
105  begin values
106    -53.90 1.23
107    21.10 1.0
108    73.90 0.80
109    82.20 0.75
110  end values
111  end definition for function pmdi20_modulus
112
113  begin definition for function pmdi20_rate
114  type is piecewise linear
115  ordinate is temperature
116  abscissa is time
```

definition for function

General Function Info

pmdi20_modulus Plot

Type piecewise linear

Function Definition

Value Properties

Use Data File

x value	y value
-53.90	1.23
21.10	1.0
73.90	0.80
82.20	0.75

Plot View

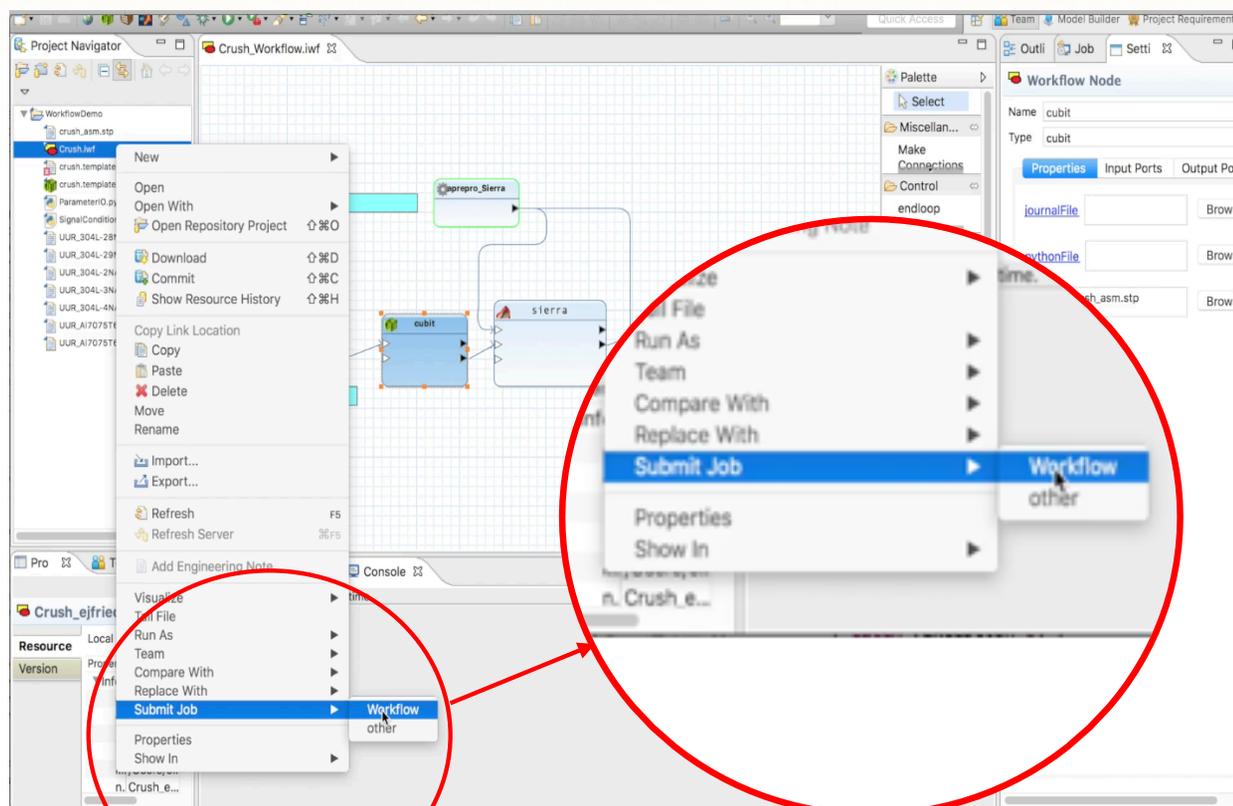
Temperature

time

pmdi20_modulus

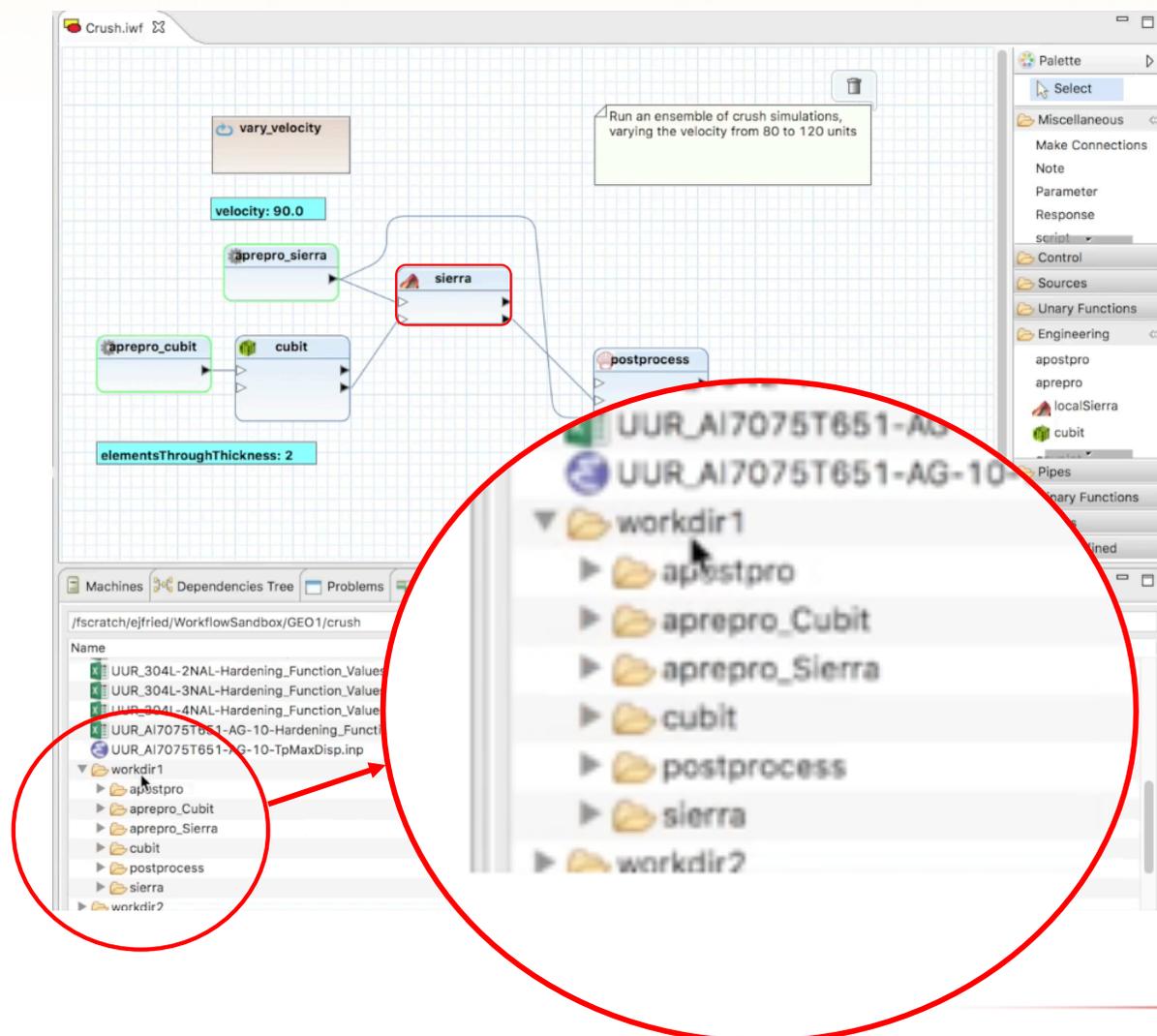
Job Submission

Workflow
executed locally
or remotely
using SAW job
submission



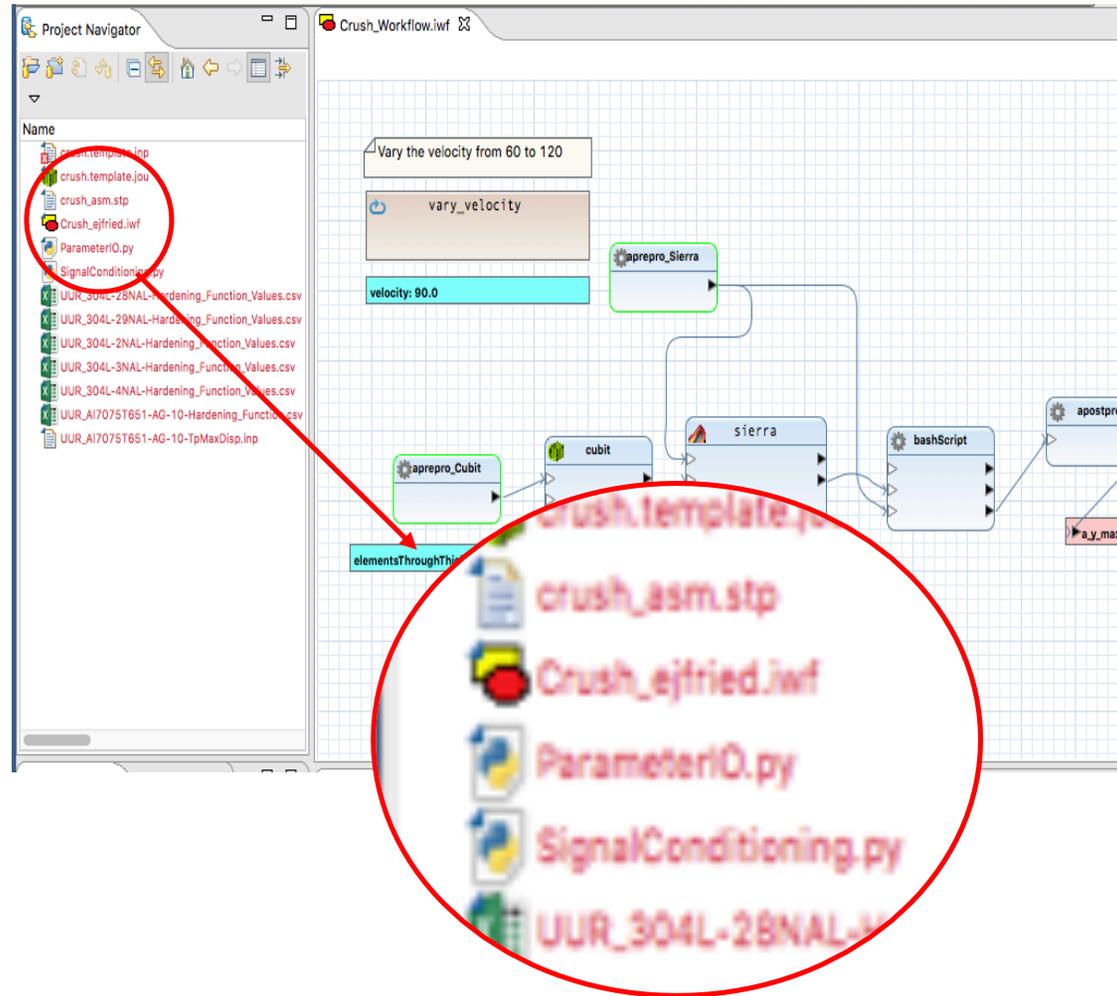
Job Monitoring and Distributed File Management

Workflow status reported graphically using standard views; clicking a workflow node opens its runtime data directory



Scientific Data Management

A workflow is just a file, and it can be stored along with all the data it uses



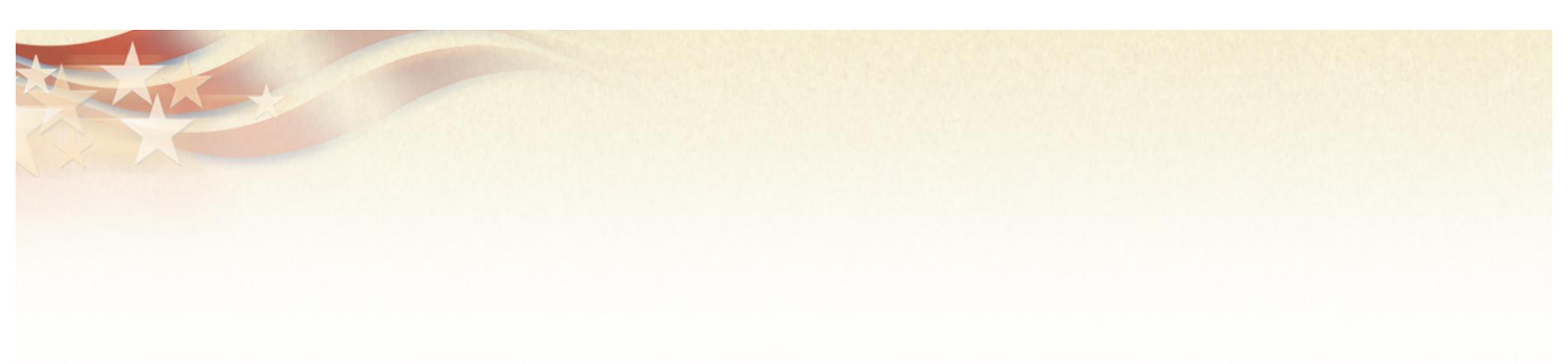
Benefits

- Reproducibility
 - It's easy to make sure you're performing the same steps
- Reliability
 - Errors handled robustly
- Reusability
 - No reinventing the wheel
- Team communication
 - Intrinsically documented processes

Acknowledgements

- Marcus Gibson
- Matt Glickman
- Andrew Rothfuss
- Kevin Olson
- George Orient (V&V apps)

www.sandia.gov/saw



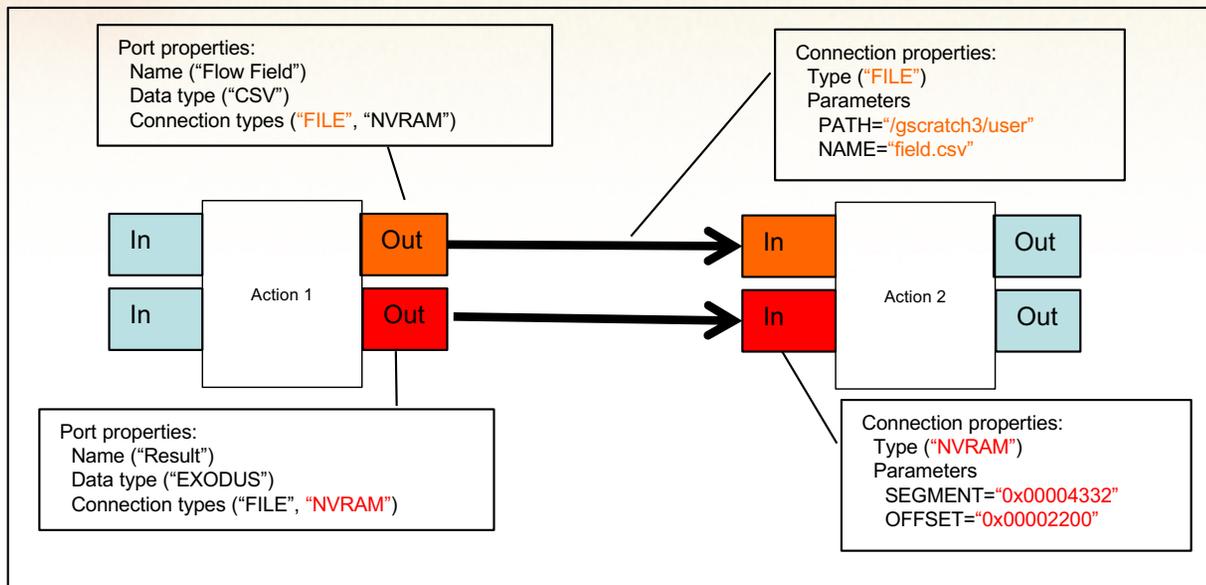
Extra slides



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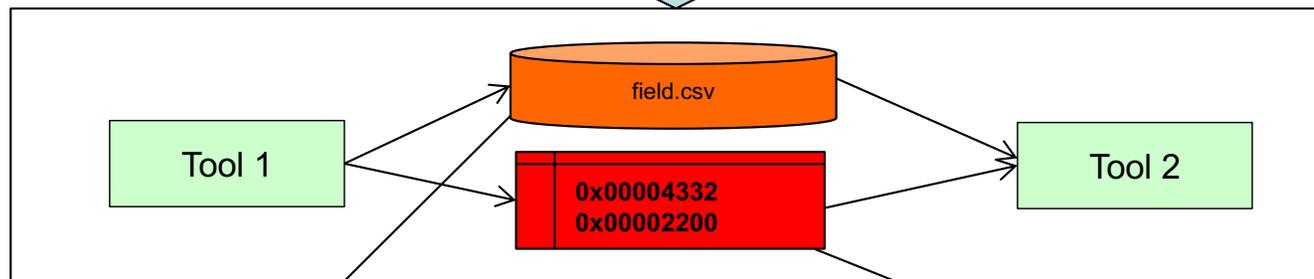


Final Scalable Workflow Architecture Directly Connects Actions Using Any Available Comms



Descriptions of all inputs and outputs of workflow actions include available connection types. At runtime, in-situ connections are used as available. Result is distributed-area workflow containing embedded in-situ workflows.

Execute using COTS Workflow Engine



"Distributed-Area" Link

"In-Situ" Link