

# ENGINEERING SCIENCES WORKFLOWS FOR V&V APPLICATIONS

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SAND2016-7247 PE



# The Sandia Analysis Workbench

An integrated environment for engineering analysis

The screenshot displays the Sandia Analysis Workbench interface. The main window is titled "SDM - JoeDemo2/Files/3\_point\_bend\_test1.i - DART Workbench". The interface is divided into several panes:

- Project Navigator:** Shows a tree view of the project structure, including folders like "DAKOTA-Milestone", "Ed\_March\_Training", "JoeDemo2", "DS\_Store", "AnalysisFolder", "Deleted Items", "Files", "Materials", "SIMBAWS", and "WorkProductsDocumentFolder".
- Code Editor:** Displays the input file "3\_point\_bend\_test1.i" with the following content:

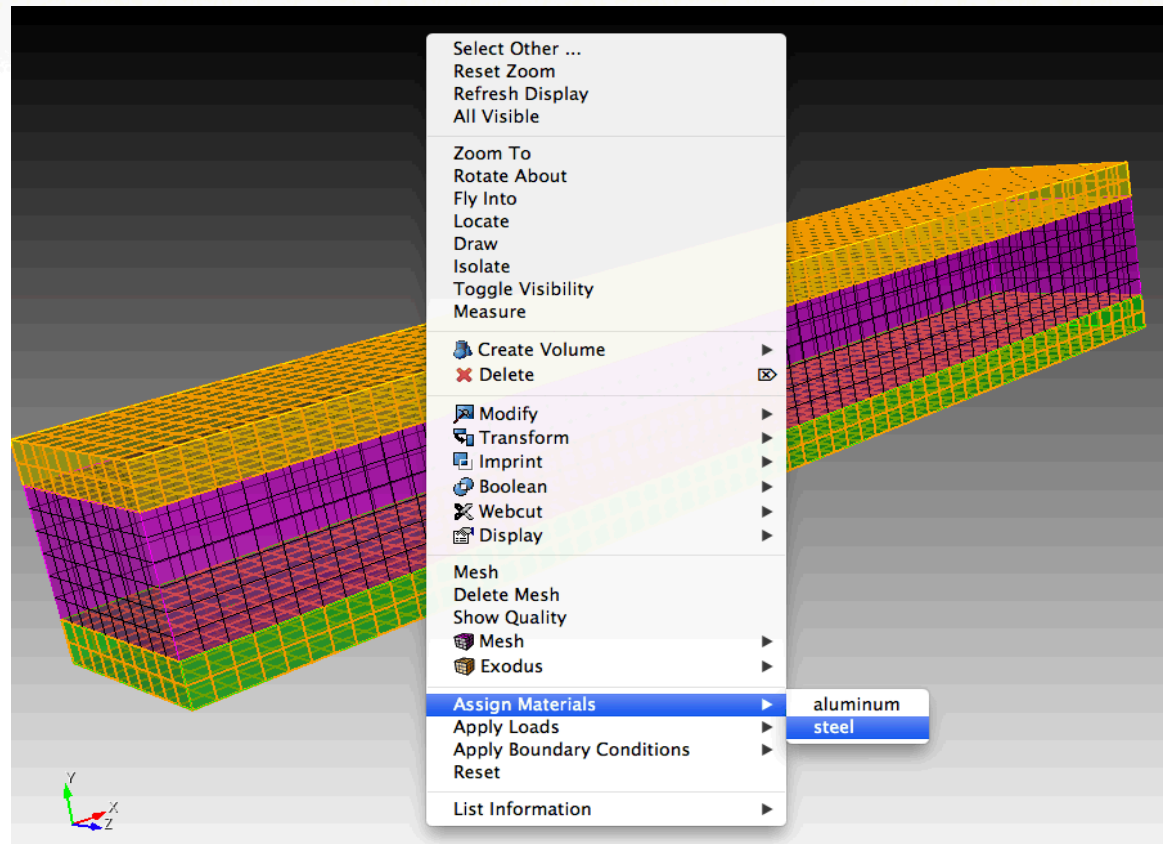
```
1: Generated by:
2: # SIMBA version 67 Build number 3201(Ad-hoc).
3: # Built on ejfried-dell at 4/23/2009 12:03:47
4: # Exported on Fri Mar 19 10:23:14 MDT 2010
5:
6: begin sierra 3_point_bend_test1
7:
8:   {include("gpm_functions.txt")}
9:   {include("gpm_functions.txt")}
10:
11:   {include("gpm.txt")}
12:
13: begin property specification for material Default
14:   density = 1900.
15: begin parameters for model ELASTIC
16:   poissons ratio = 0.3333
17:   youngs modulus = 3E7
18: end parameters for model ELASTIC
19: end property specification for material Default
20:
21: begin property specification for material mat.1
22:   density = 8000
23: begin parameters for model elastic
24:   poissons ratio = 0.245
25:   youngs modulus = 195.0e+09
26: end parameters for model elastic
27: end property specification for material mat.1
28:
29: # Functions for conditions
```
- Job Status:** A table showing the status of various jobs:

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
dtlb_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
- Model View:** A 3D visualization of a mechanical assembly, showing a cylindrical component with a central hole and a flange, rendered in a mesh format.
- Plot:** A line graph showing a linear relationship between two variables. The x-axis ranges from 0.0 to 1.3, and the y-axis ranges from 0.0000 to -0.0007. The plot shows a straight line starting at (0,0) and ending at approximately (1.2, -0.0007).
- Team Members:** A table listing team members:

Role	Email	Name
Team Member	mjigbso@sandia.gov	Gibson, Marcus J
Project Manager	elhoffm@sandia.gov	Hoffman, Edward
Team Member	jagreen@sandia.gov	Greenfield, John
- 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", "3\_point\_bend\_test1a.g", etc.

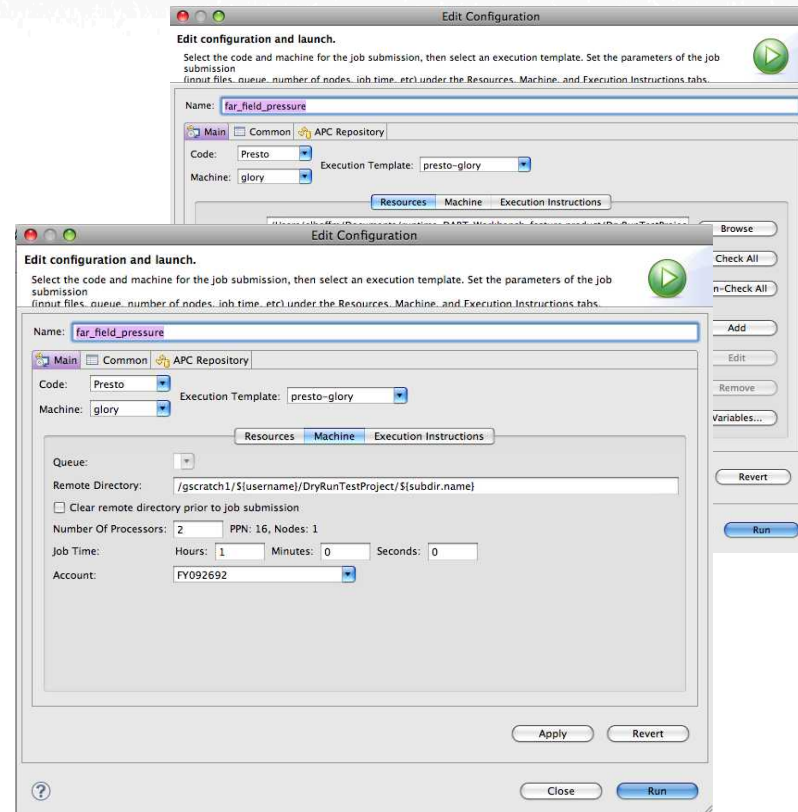
# Model Building

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 windows. The left window, titled 'Machines', shows a list of machines and their utilization. The right window, titled 'Job Status', shows a list of jobs and their status.

**Machines Window:**

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 Status Window:**

Showing 7 jobs (limited to 500). 2 filters are active.

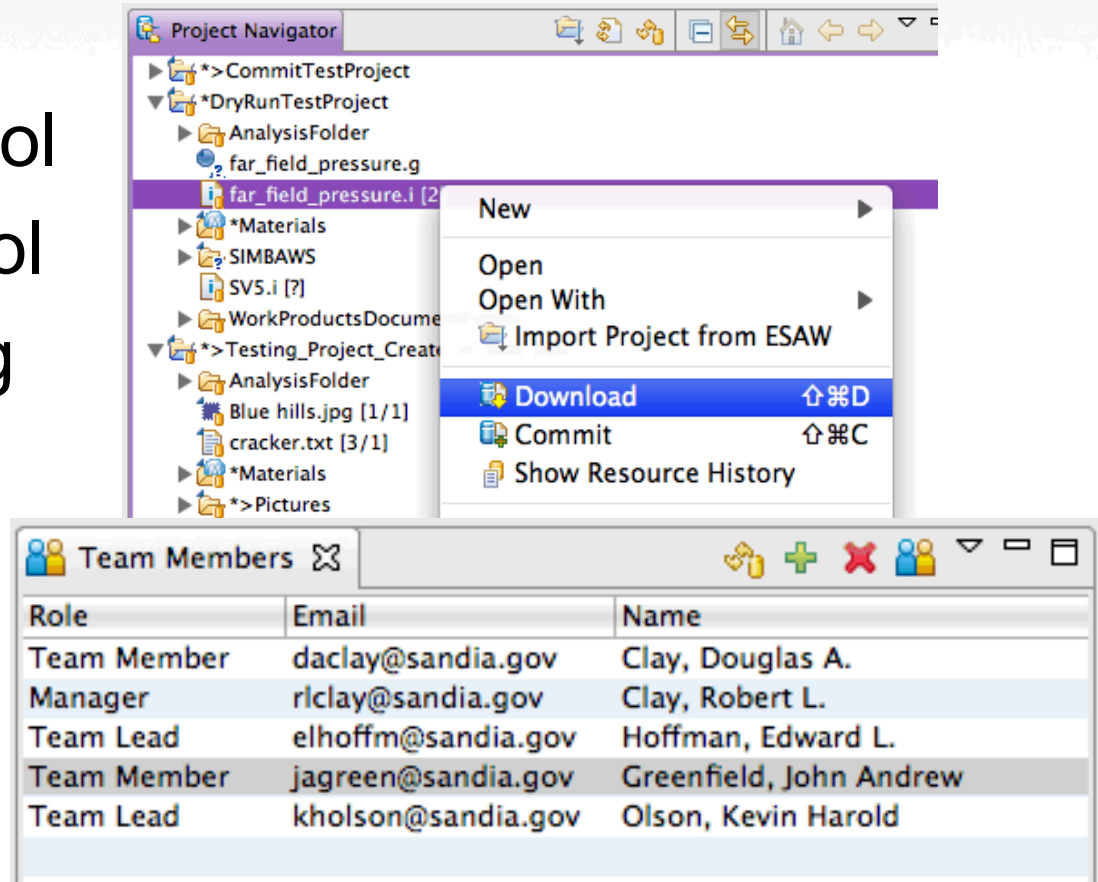
Job Name	Stage	Queue Status	Submit Dat
test	Finished		2017-02-
test	Finished		2017-02-
Crush_e...	Finished	Completed	2017-02-
Crush_e...	Finished	Completed	2017-02-
Crush_e...	Finished	Completed	2017-02-
Crush_e...	Killed	Removed	2017-02-
Crush_e...	Finished	Completed	2017-02-

**Context Menu for 'redsky':**

- Browse File System
- Refresh Utilization Information
- Stop utilization refresh jobs on redsky
- Reset Connection on redsky
- Disable Connections
- Edit properties for redsky
- Queue Info
- Open Terminal

# Scientific Data Management

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

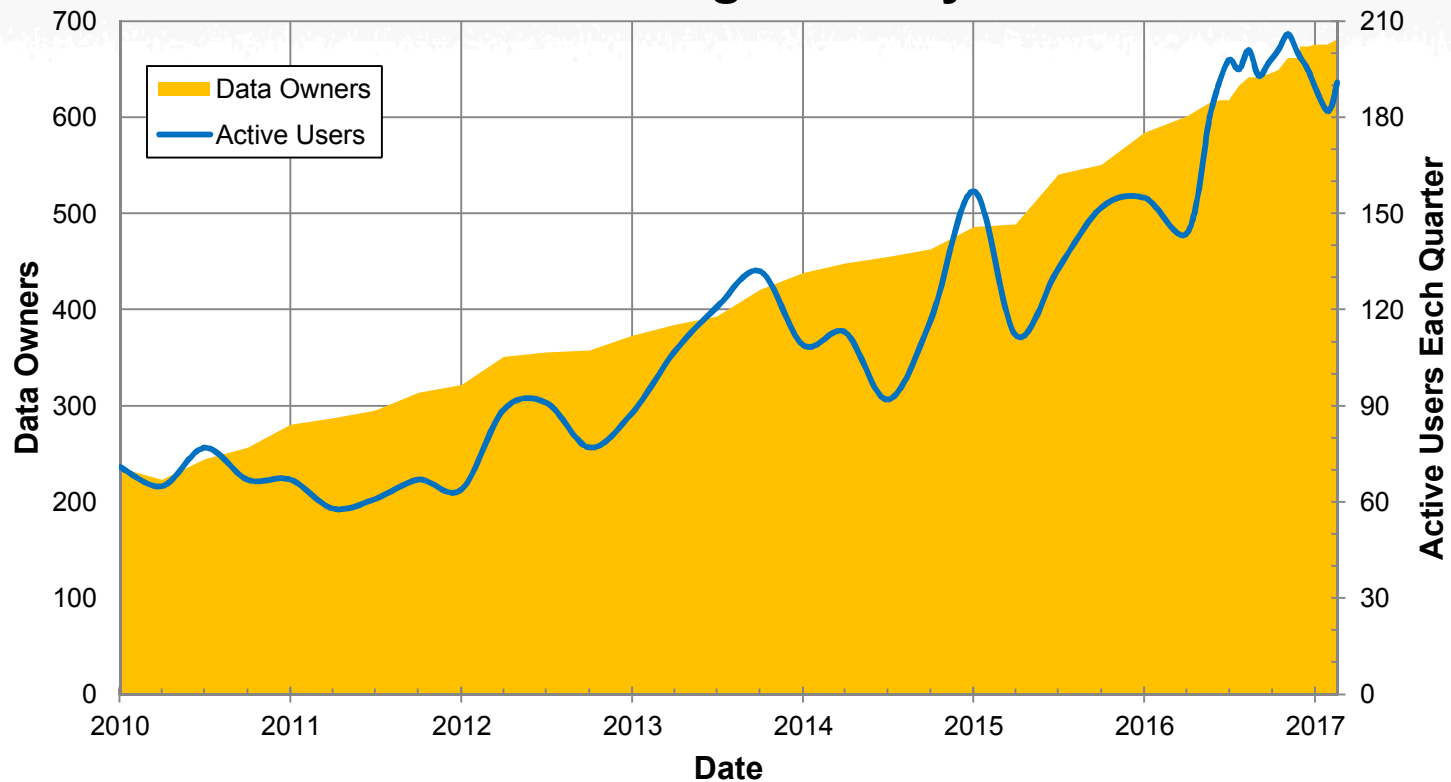


The screenshot displays a software interface with two main components. The top component is a 'Project Navigator' window showing a hierarchical tree of project folders and files. A context menu is open over a file named 'far\_field\_pressure.i [2]', listing actions such as 'New', 'Open', 'Open With', 'Import Project from ESAW', 'Download', 'Commit', and 'Show Resource History'. The bottom component is a 'Team Members' window containing a table with columns for Role, Email, and Name.

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*

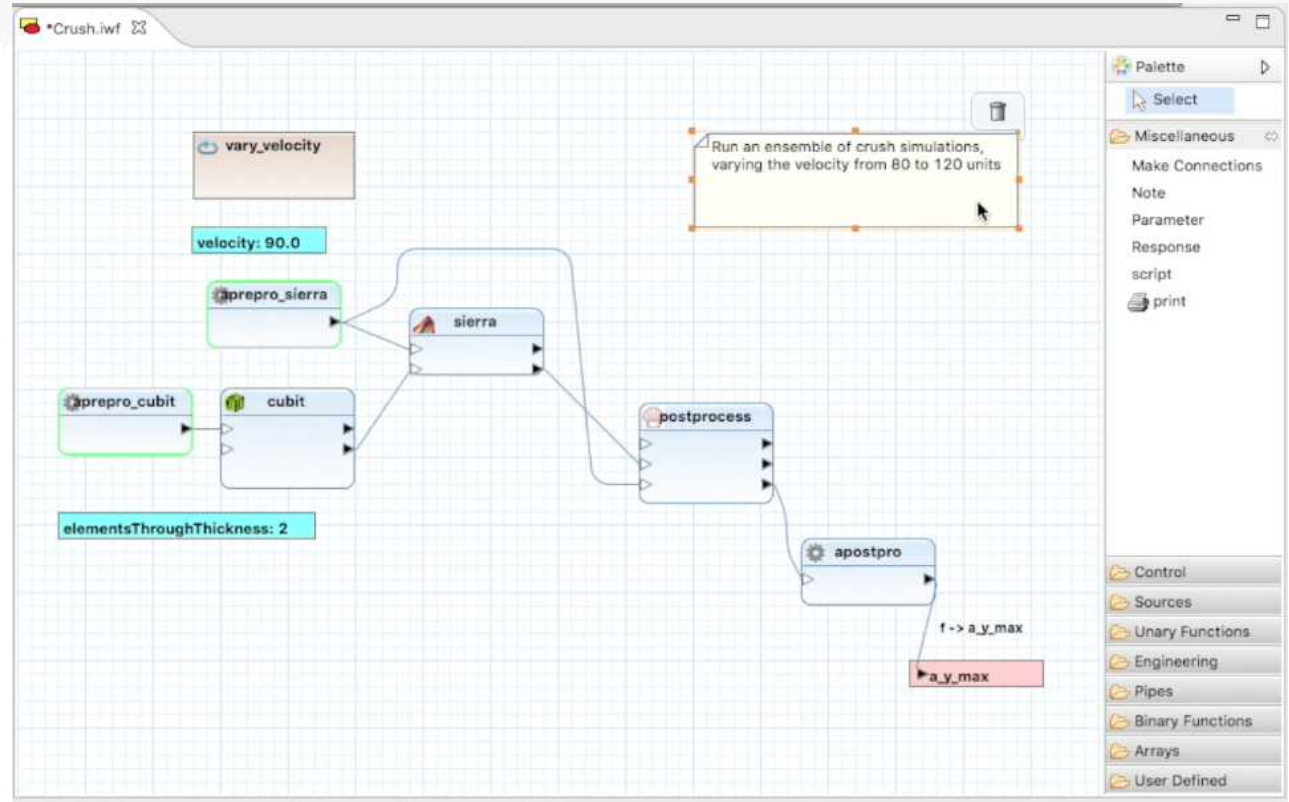
# New Challenges

## *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

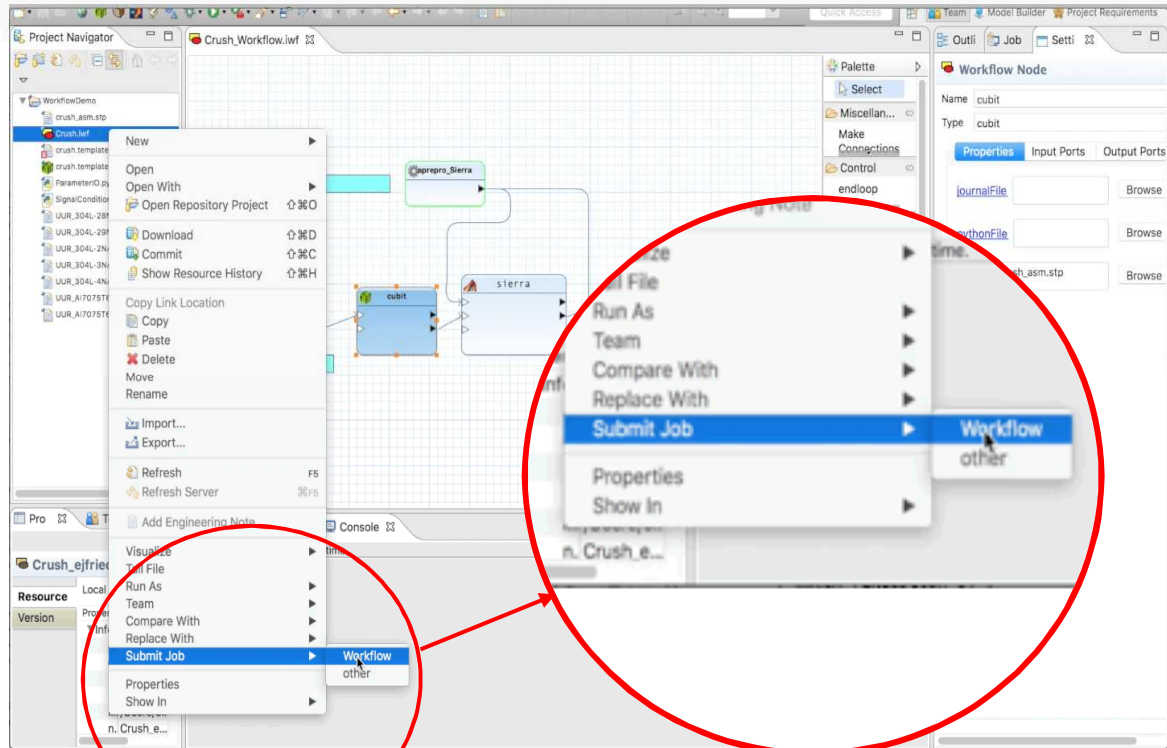
The screenshot displays a multi-paneled software interface for model building. The top-left pane shows a workflow diagram with components: 'Vary the velocity from 60 to 120', 'vary\_velocity', 'velocity: 90.0', 'aprepro\_Sierra', 'aprepro\_Cubit', 'cubit', 'sierra', 'bashScript', 'apostpro', and 'a\_y\_max'. The top-right pane shows a code editor with a Fortran-like script defining functions for temperature and time. The bottom-left pane shows a 'definition for function' dialog for 'pmdi20\_modulus', with a 'Type' of 'piecewise linear' and a table of data points. The bottom-right pane shows a 'Plot View' of a line graph with 'temperature' on the y-axis and 'time' on the x-axis.

```
92 ordiante 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   ordiante 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   ordiante is temperature
116   abscissa is time
```

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

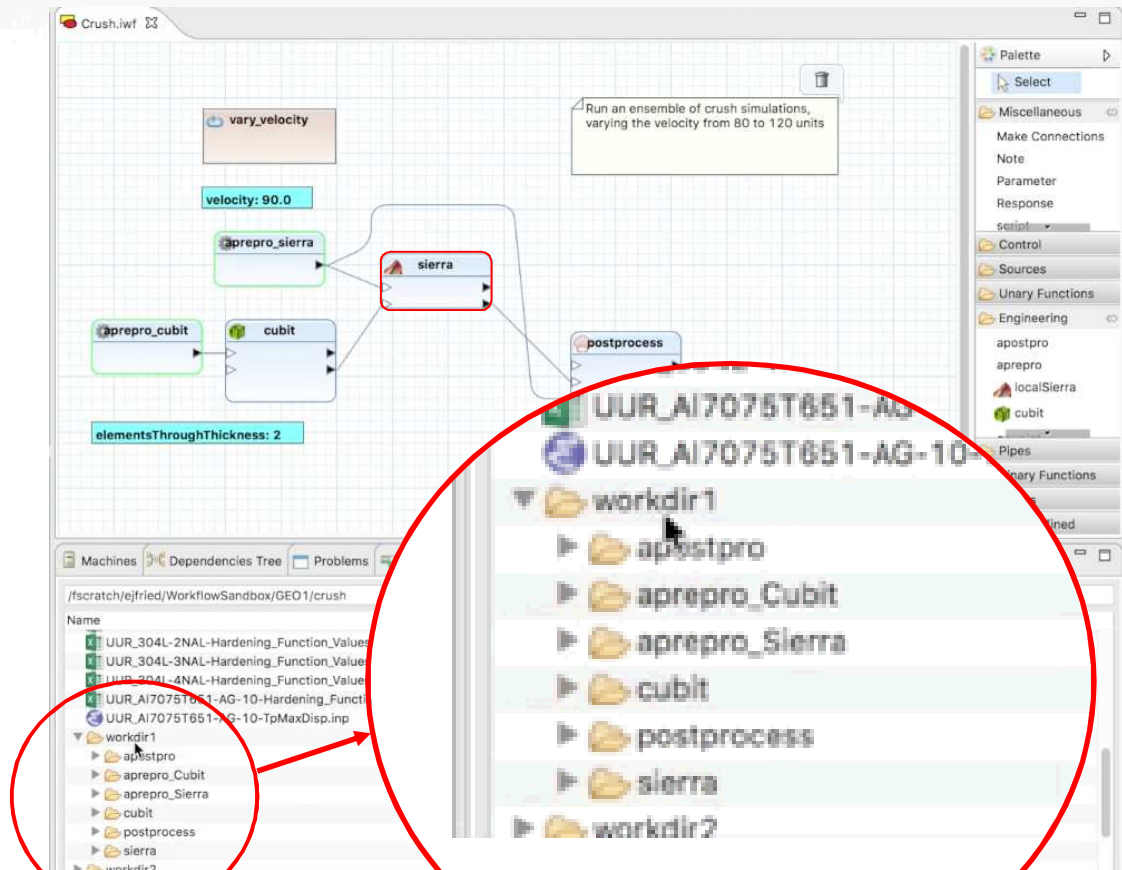
# Job Submission

Workflow  
executed locally  
or remotely  
using SAW job  
submission



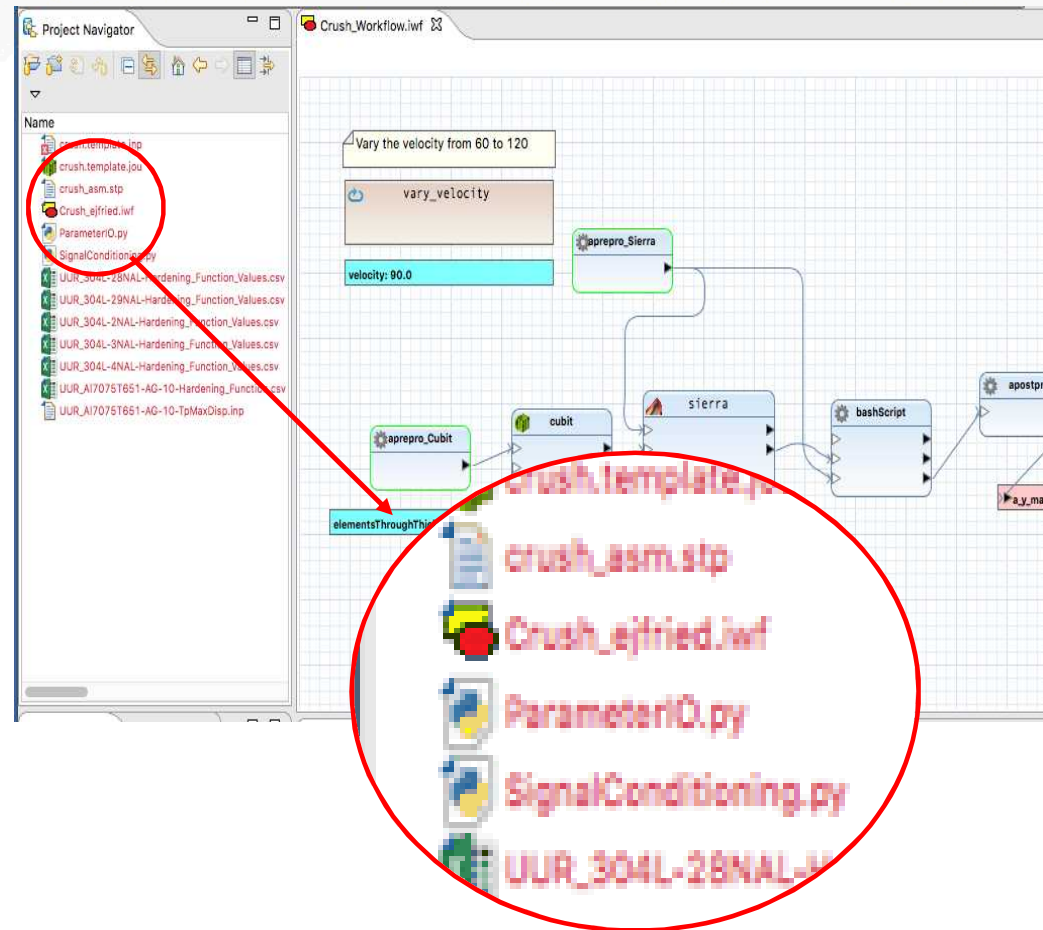
# Job Monitoring and Distributed File Management

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)



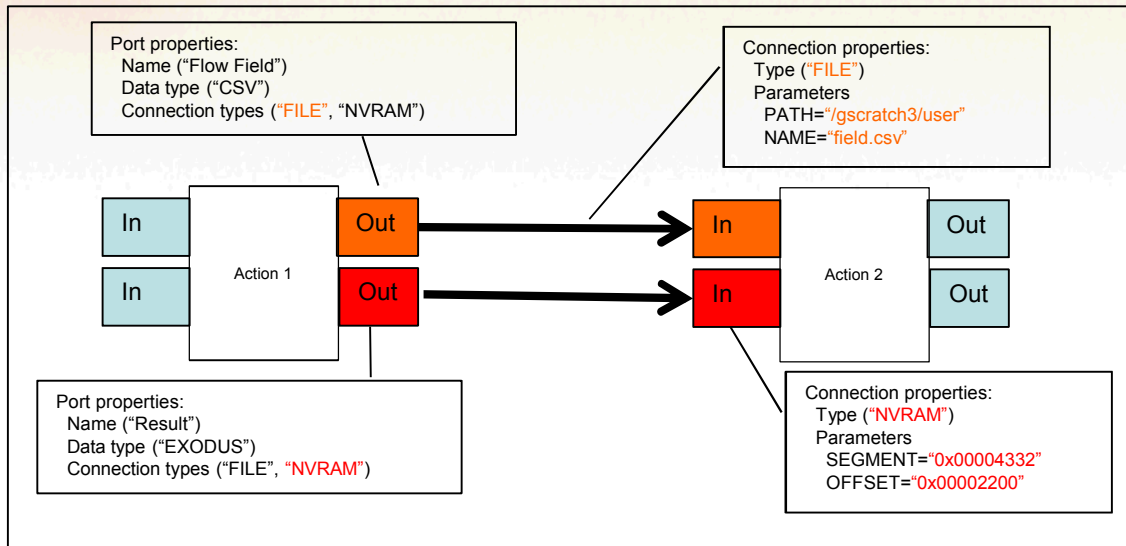
# Extra slides



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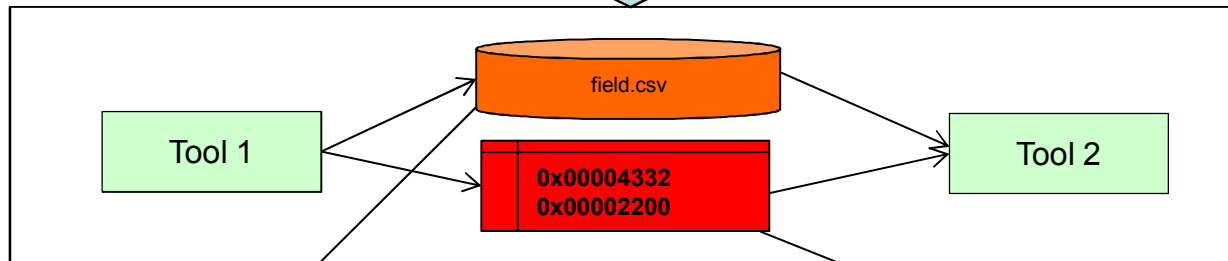


# Final Scalable Workflow Architecture Directly Connects Actions Using Any Available Comms



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