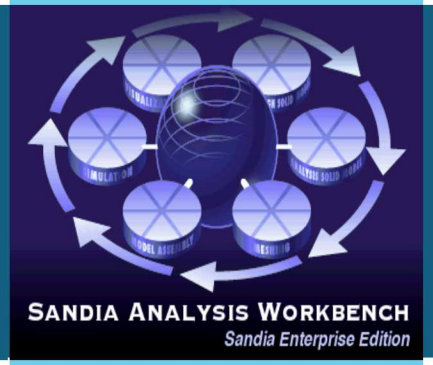
SAND2019-2986C

The SAW Next Generation Workflow System



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Motivation

Our Users

- Engineers and scientists
- Computer-literate
- Know scripting or programming
  - Not "programmers"
- Run lots of complex, in-house research codes
  - Experts with some, novices with others
- Need to follow best practices
  - Verification and validation

Motivation

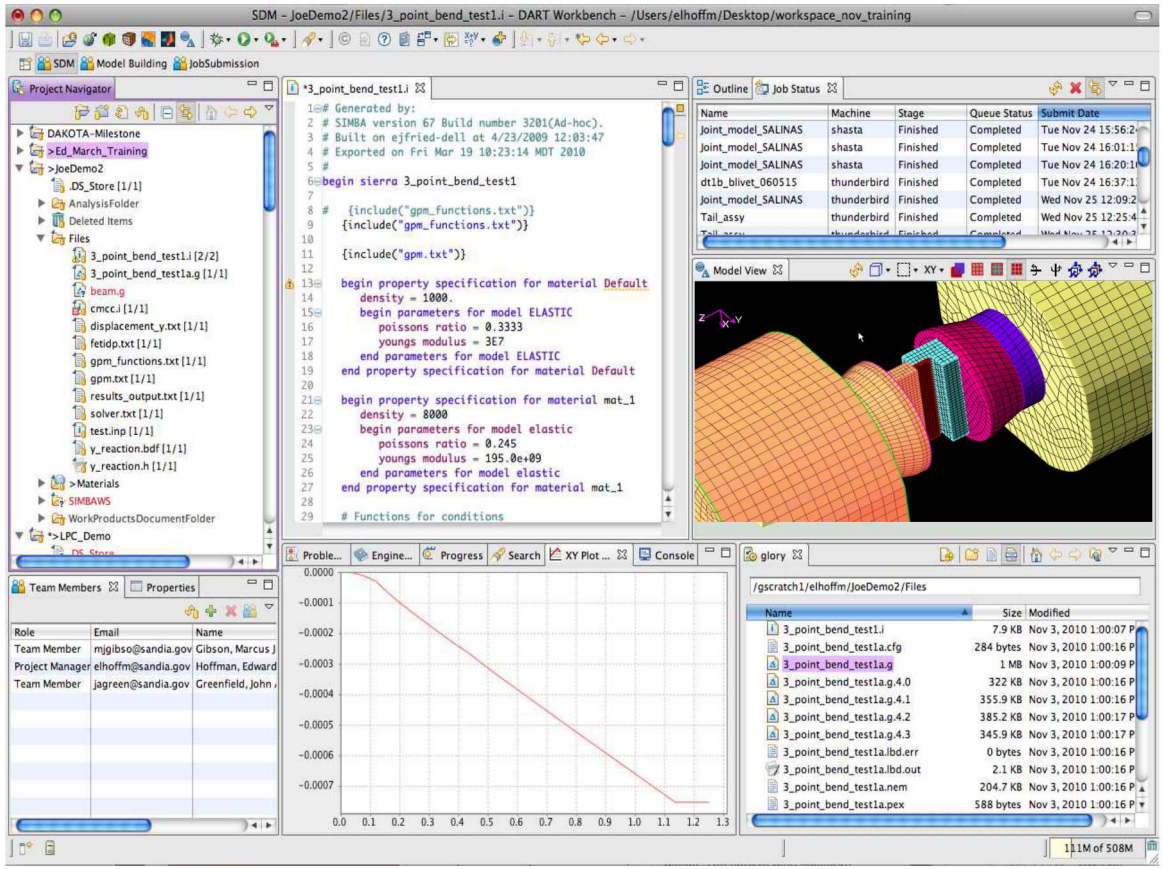
Environment

- Heterogeneous hardware
- Multiple, secure networks
- Need-to-know
- *Decentralized*
- Compartmentalized

The Sandia Analysis Workbench

An integrated environment for engineering analysis

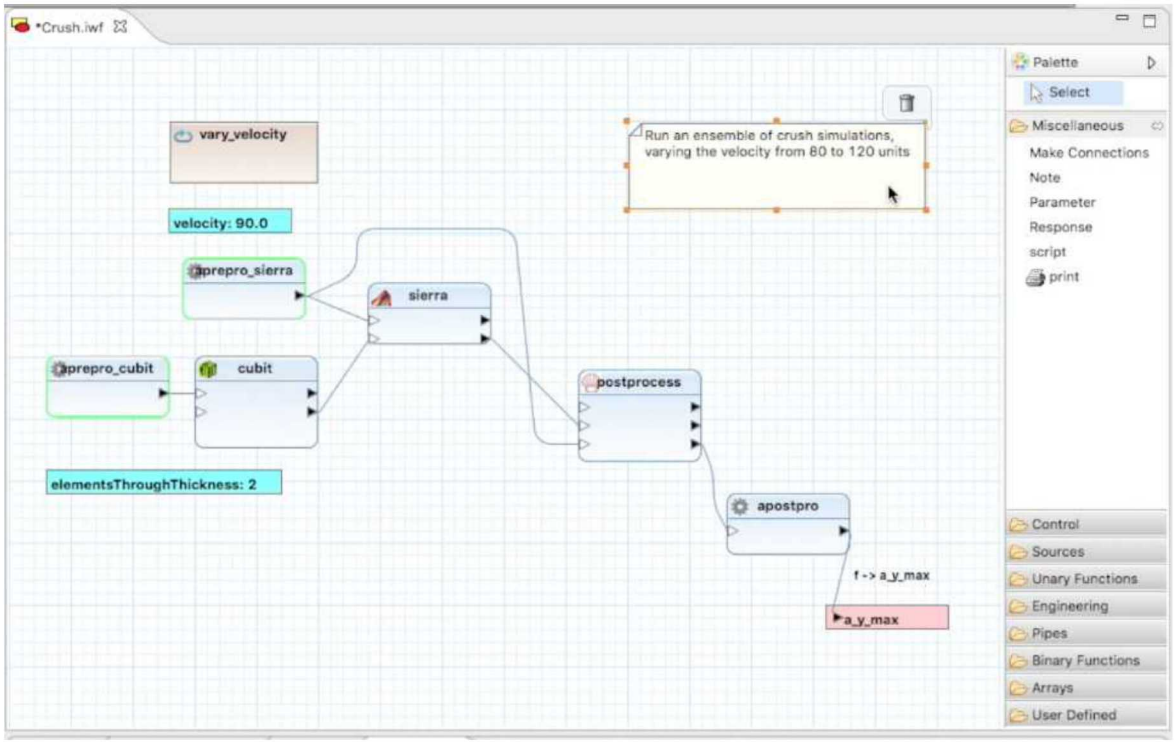
- Graphical model building
- Job submission
- Distributed file management
- Scientific data management
- Requirements management



SAW Next Gen Workflow (NGW)

Automated workflow that

- is integrated with everything else in SAW
- works with with external codes
- runs inside or outside SAW
- is intuitive



NGW System Requirements

Low cognitive load

- Users can think in the domain, not about the workflow system
- You don't *program* workflow, you *build* it

Transparent and "escapable"

- It's always obvious what the system is doing
- It's always possible for user to customize behavior

Flexible system architecture

- Everything can execute anywhere

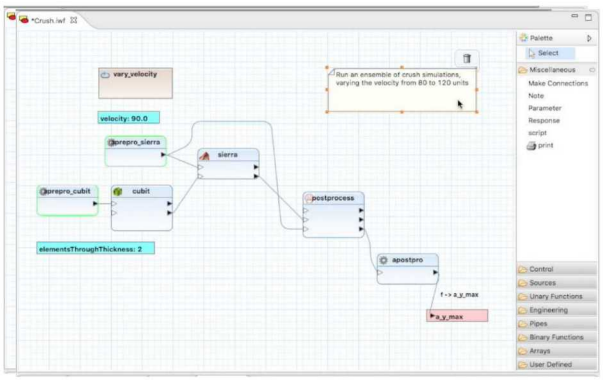
Zero-install

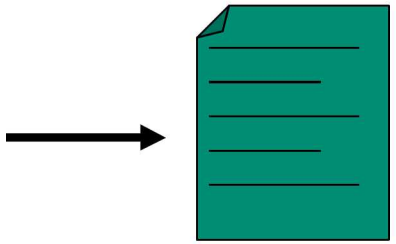
- *Can't assume root access on runtime system*
- *Can't install a persistent server*

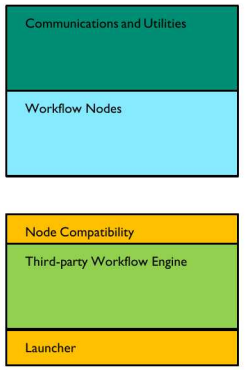
Workflow engine independence

- Can be implemented on multiple products

Next-Gen Workflow Architecture







1. Graphical Editor

2. Workflow File

3. Layered Runtime

Graphical editor and runtime are independent and can be used separately in time and space. Editor runs on desktop, while runtime can execute anywhere from desktop to HPC clusters

NGW Definitions

A workflow is an executable graph of connected components

A component or "node" represents an activity

- Executing an external code
- Extracting a column of numbers from a table
- Components are user-configurable
- Some very specific, some very generic

Connections represent data interchange and control flow

- A number or a path to a file
- An identifier for a shared memory segment
- *Connections are themselves configurable*

NGW Graphical Editor

Based on Eclipse IDE framework
- Graphiti / EMF
- Borrows some ideas from Triquetrum/ESWG

Data-driven
- XML file to describe available component types

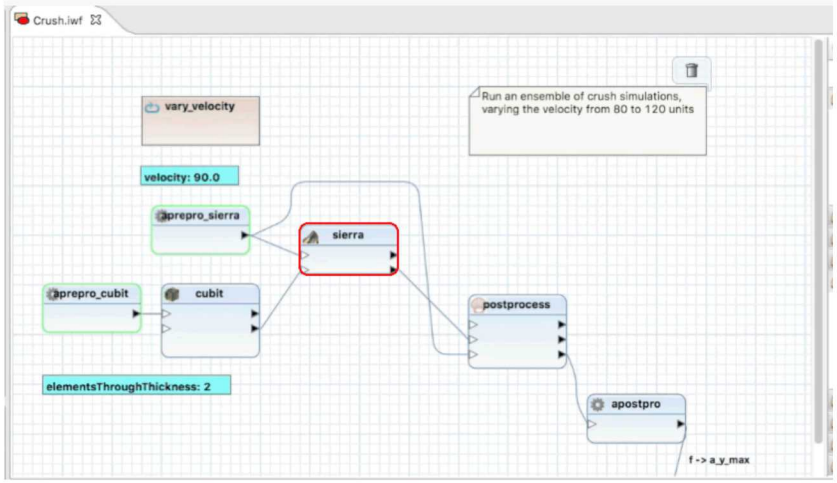
Easy to extend
- Can add component types
- Can add component-specific editing
- Can add special behaviors for embedded execution
- Programmers work with editor's EMF model

NGW Graphical Editor

Eclipse integration

Ease of use

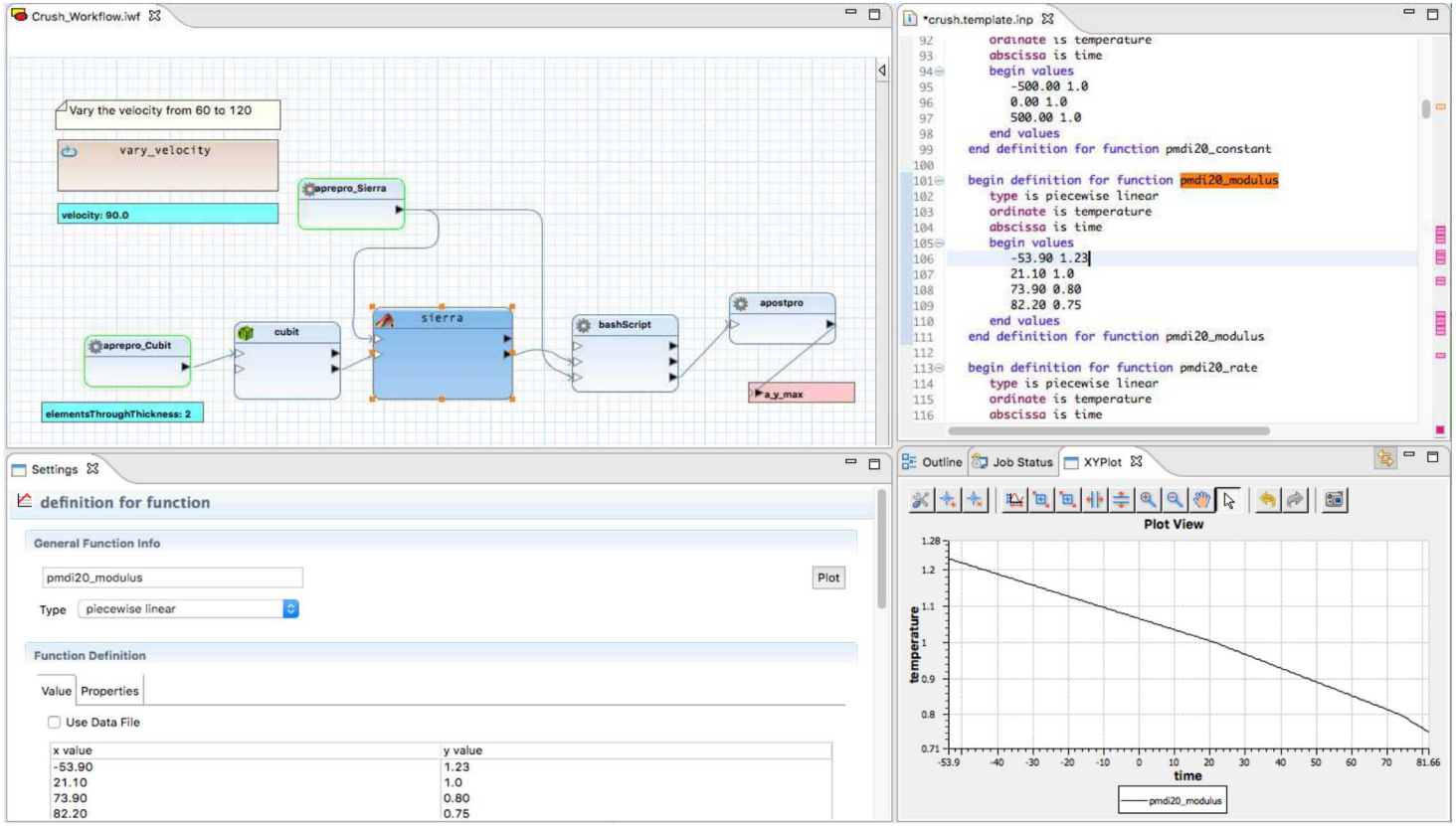
- Drag file from project, creates appropriate component to use that file
- File-type-specific editors automatically invoked



Integrates with other tools in SAW

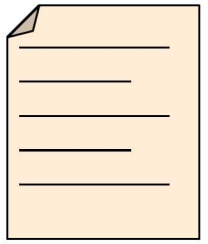
NGW Graphical Editor

Edit model components naturally using familiar tools



Workflow File Format

Based on EMF native format (XML)



Simple file format contains

- … component configuration
- … connectivity
- … optional graphical (layout) information

Does *not* contain component implementations

- Different runtime implementations can execute the same workflow definition

Does *not* contain rendering information

- Appearance of components easy to change

Can be generated or consumed by any code

- i.e., workflows can be defined by code or scripts
- Eclipse parser library not required
- No Eclipse code (EMF) in server

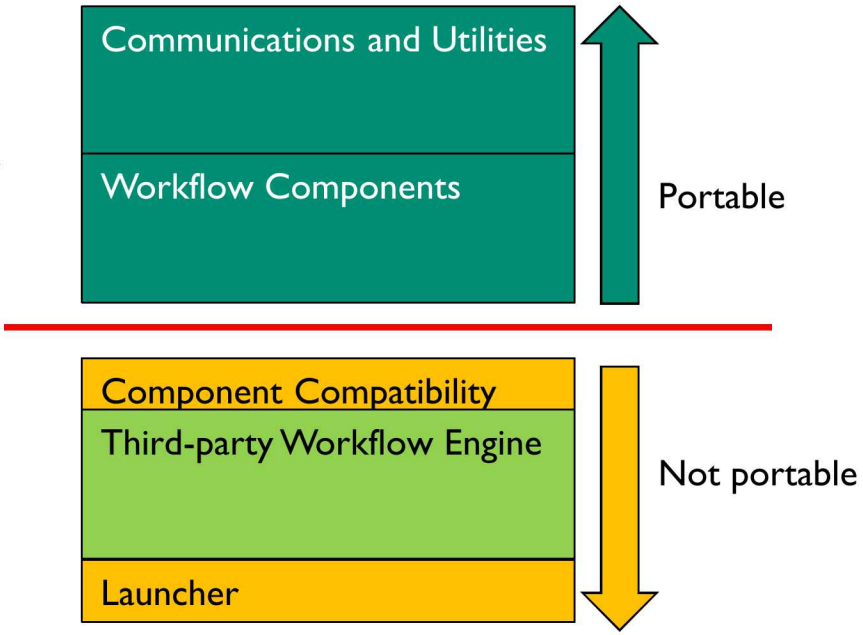
Workflow File Format

<gov.sandia.dart.workflow.domain:WFNode name="print" properties="/4 /5 /6 /7”
inputPorts="/2" outputPorts="/3" start="true" type="print" label="print"/>
<gov.sandia.dart.workflow.domain:InputPort name="x" type="default" node="/1"/>
<gov.sandia.dart.workflow.domain:OutputPort name="f" type="default" node="/1"/>
<gov.sandia.dart.workflow.domain:Property name="formatString" type="default" value="Hello, world!" node="/1"/>
<gov.sandia.dart.workflow.domain:Property name="async" type="boolean" value="false" node="/1"/>
<gov.sandia.dart.workflow.domain:Property name="privateWorkDir" type="boolean" value="false" node="/1"/>
<gov.sandia.dart.workflow.domain:Property name="clear private work directory”
type="boolean" value="false" node="/1"/>

NGW Engine

Layered Runtime Architecture

- NGW Components are written in Java to a vendor-neutral API. The compatibility layer adapts to a third-party rule engine
- Variant component implementations can be provided for different host environments

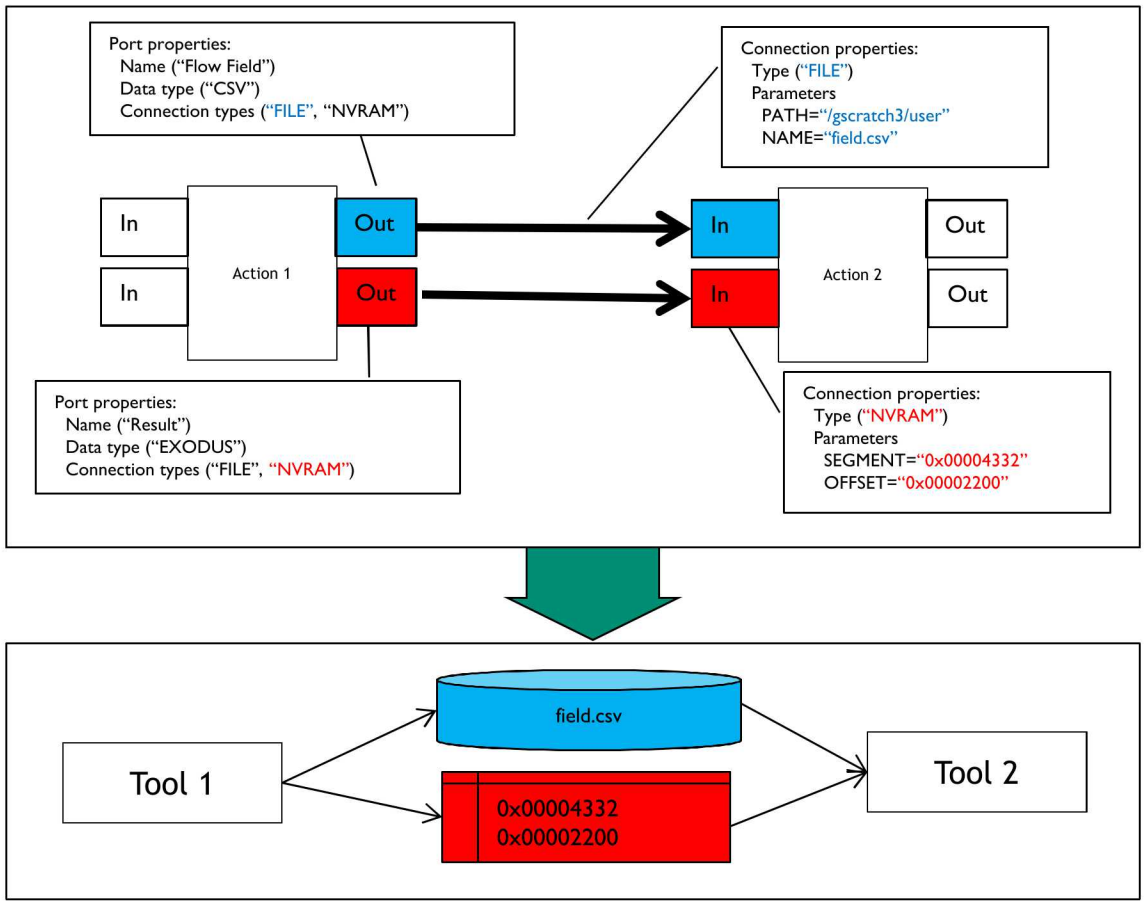


By using a thin compatibility layer, we can deploy on arbitrary third-party Java workflow engines with little effort

NGW Engine

Abstract Dataflow

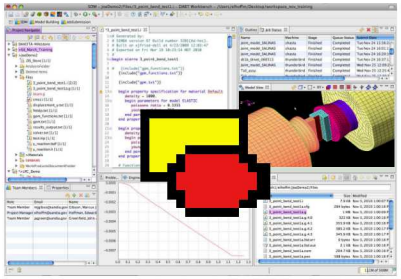
- Connections between components are configurable. Configuration options determine how data is exchanged at runtime
- Future work will involve adding support for more data exchange mechanisms
- In this notional diagram, the blue connection is configured to exchange data via a file, while the red is using a shared memory segment



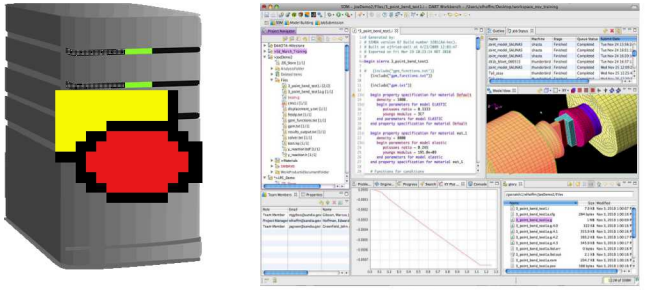
NGW Engine

Flexible Topology

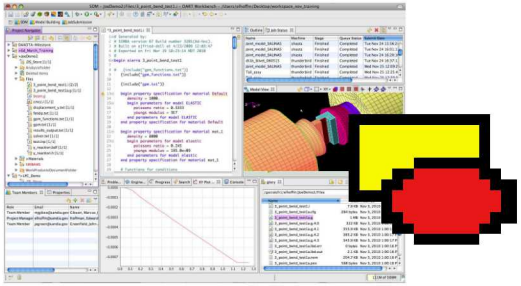
The same workflow can run in multiple environments. We can leverage our existing job submission and monitoring tools to implement this



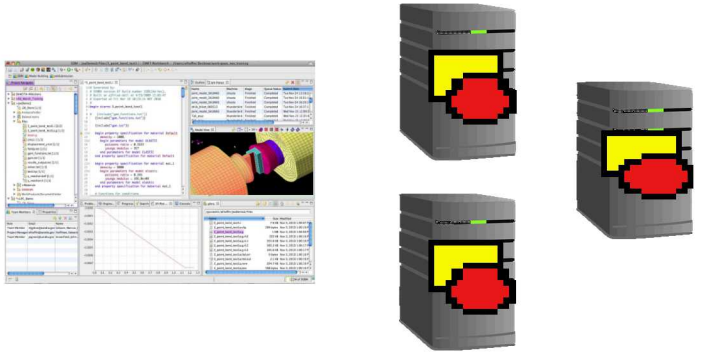
Interactive



Server



Batch



Distributed

Extending NGW

”Wrapping” an external code for runtime use

- *No programming required*
- Can be done in the workflow editor
- Configure a script node or external process node
- Save to palette for personal use
- Export to JAR file for sharing

Creating a more complex runtime node

- Requires Java programming
- Extend SAWCustomNode
- Implement (at minimum) one method
- Package as JAR file, in Eclipse plugin, or both

Extending NGW

Defining node types for editor

- Requires Java programming
- Implement one method in IWorkflowEditorNodeTypeContributor

Custom rendering for nodes in editor

- Requires Java programming
- Extend AbstractGARenderer and implement two methods
- Register with nodeRenderer extension point
- Package as Eclipse plugin

Extending NGW

Custom editors for specific node types
- Requires Java programming
- Implement ISettingsEditor and implement several methods
- Register with nodeTypeEditor extension point
- Package as Eclipse plugin

Custom images for nodes in editor
- Register icon with nodeIcon extension point
- Package as Eclipse plugin

Providing files and resources to workflow creator
- Register file with resourceContributor extension point
- Package as Eclipse plugin

Impact

- Best Practices and New Capabilities
  - Workflows capture the best way to complete a task
- 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
- Archival Information
  - Automatically preserve what was done and why

Future work

Façades

Web client

Alternate servers

- Python
- C++
- Other Java?

In situ workflow