Cyberintegrator

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Outline

- Definitions
  - Scientific Workflow
  - Cyberintegrator
- Examples
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  - TX Water Management (RAPID)
  - WSSI (RHESsys)
- Cyberintegrator
  - Architecture
  - Technologies used
  - Rest interface
- PAW
- Deployment, how to get it
- Future work
  - Integration with Medici

Scientific Workflow

- A scientific workflow system is a specialized form of a workflow management system designed specifically to compose and execute a series of computational or data manipulation steps, or a workflow, in a scientific application

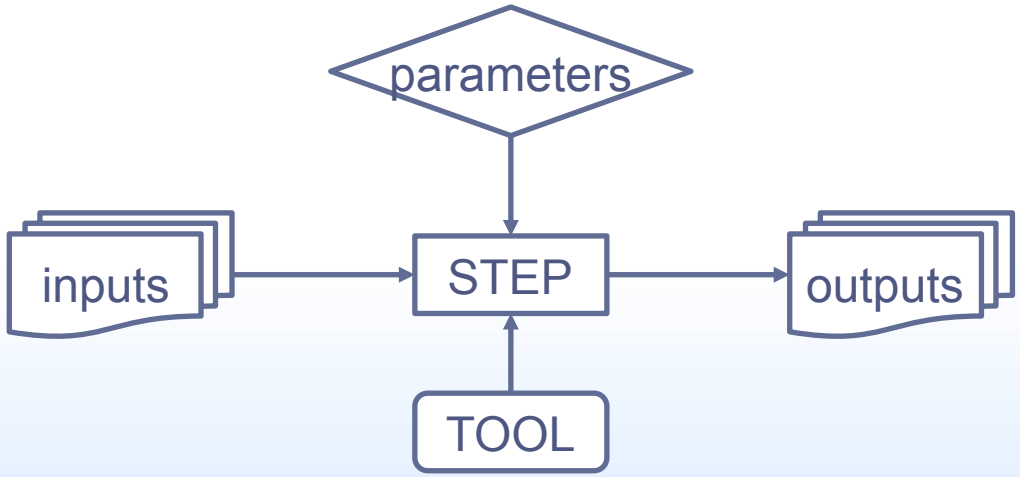
- A workflow consists of a sequence of connected steps where each step follows without delay or gap and ends just before the subsequent step may begin. It is a depiction of a sequence of operations, declared as work of one or more simple or complex mechanisms.

Cyberintegrator

- Workflows as a communication mechanism
  - Make workflows documented and sharable
  - Separate science from ‘logistics’
- Enable integration of independent tools
  - Keep models, algorithms, data in open formats accessible from outside the scientific workflow system
- Expose workflow as a service
  - The model encapsulated by a workflow can be exposed a restful service

Definitions

- Input = data that is used by algorithm
- Output = data that is created by algorithm
- Parameter = controls the algorithm executed
- Tool = the encapsulation of the algorithm
- Step = a single execution of a tool



Definitions

- Workflow = a sequence of steps
- Executor = code to execute a type of tool
- Engine = code to execute a workflow

USE CASES

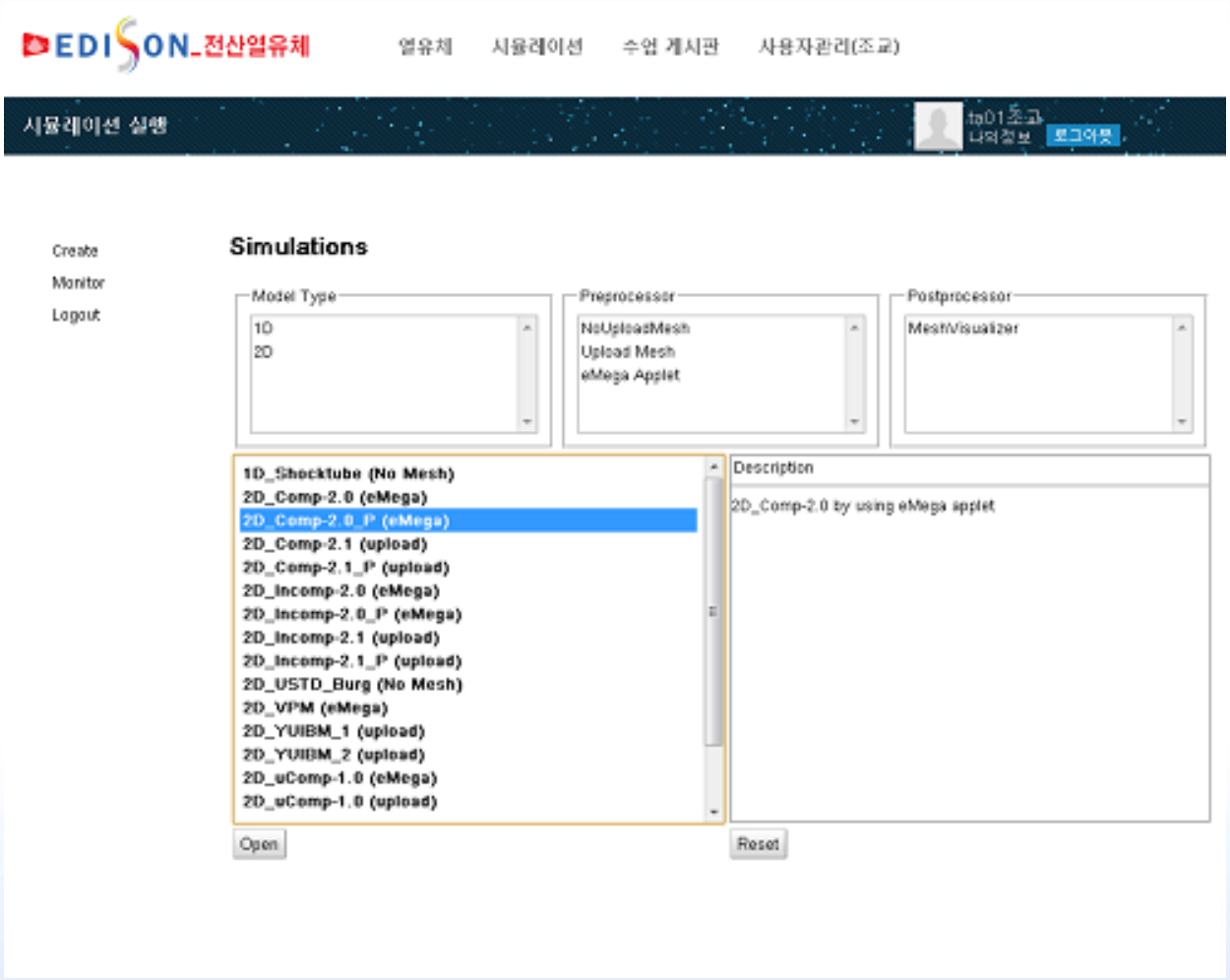
Cyberintegrator Use Cases

- KISTI
  - Execute complex CFD on HPC systems
  - Used in university courses with hundreds of students
- Texas Water Management
  - Execute RAPID model
  - Uses Cyberintegrator service from inside ArcGIS
  - Used by Microsoft as a demo at AGU
- WSSI
  - Execute RHESsys model

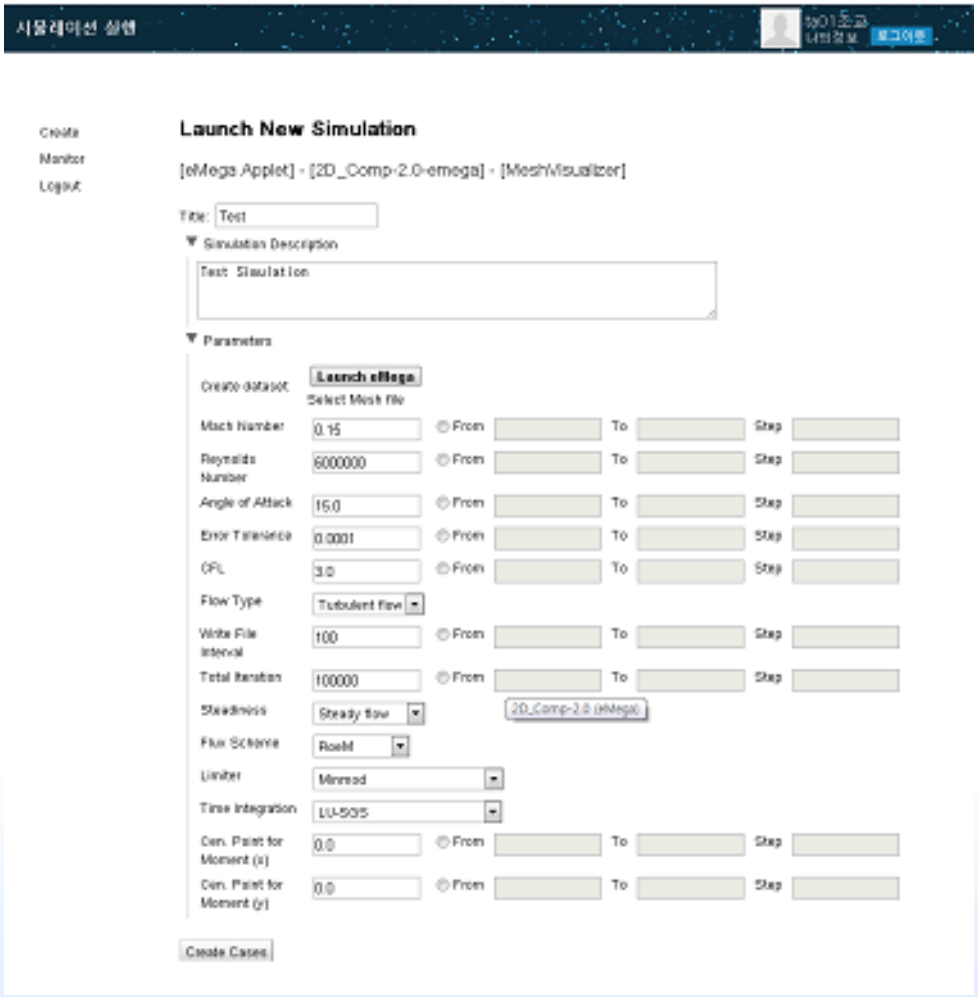
KISTI Use Case

- Working with KIST super computer center in Korea
- Allow users to run complex solvers
- Upload their models
- Run solvers on HPC
- Parameter sweeps
- Visualize results

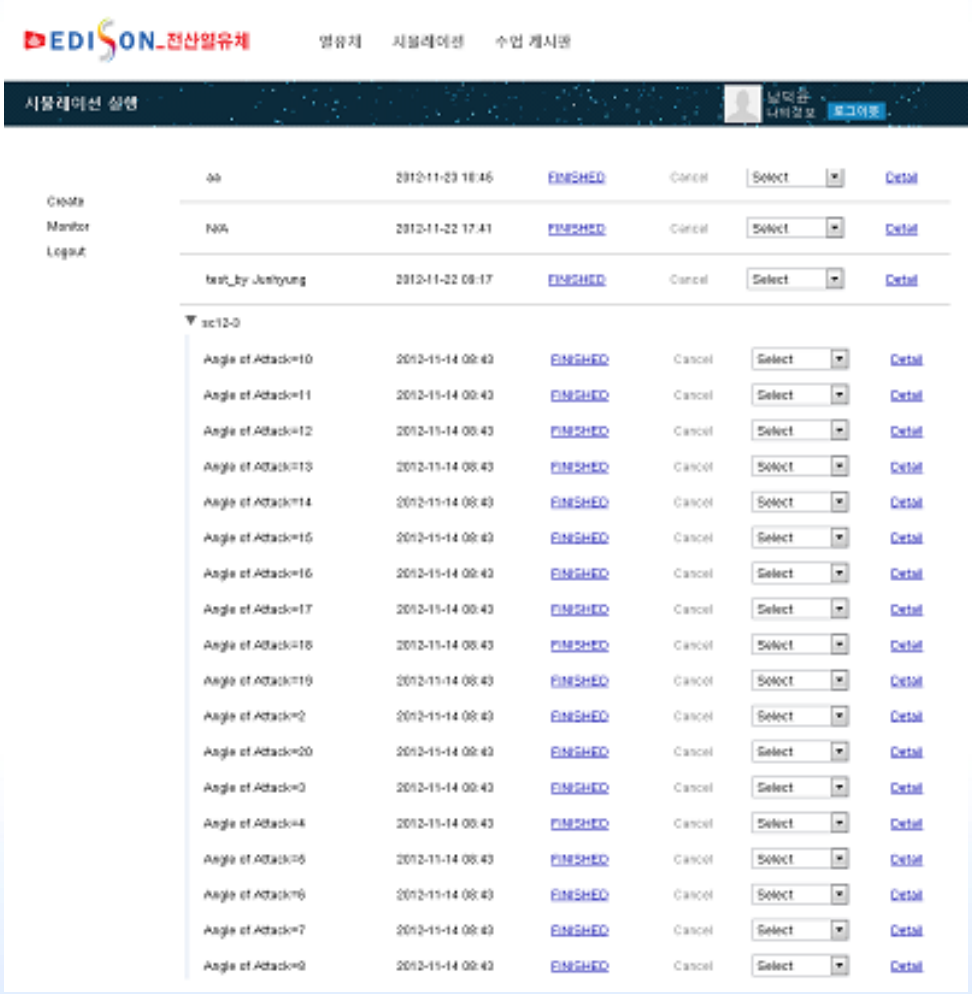
Solver Selection



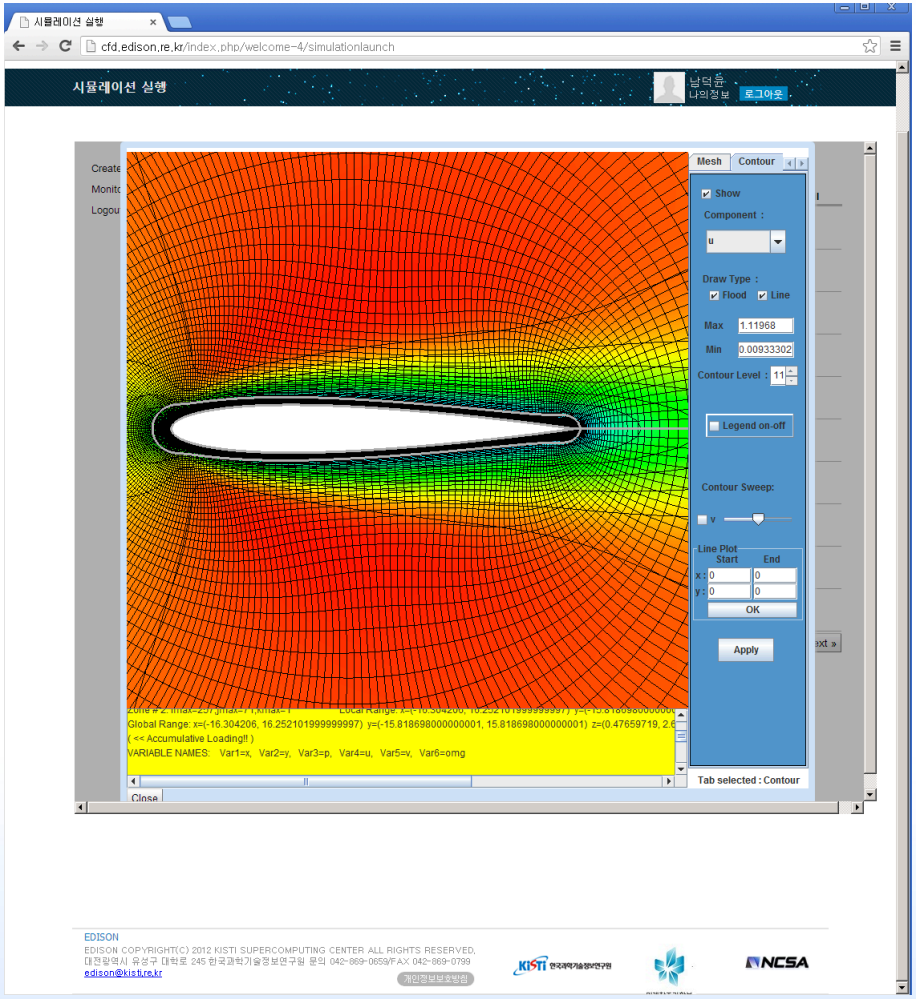
Parameter Selection



Execution List



Visualization

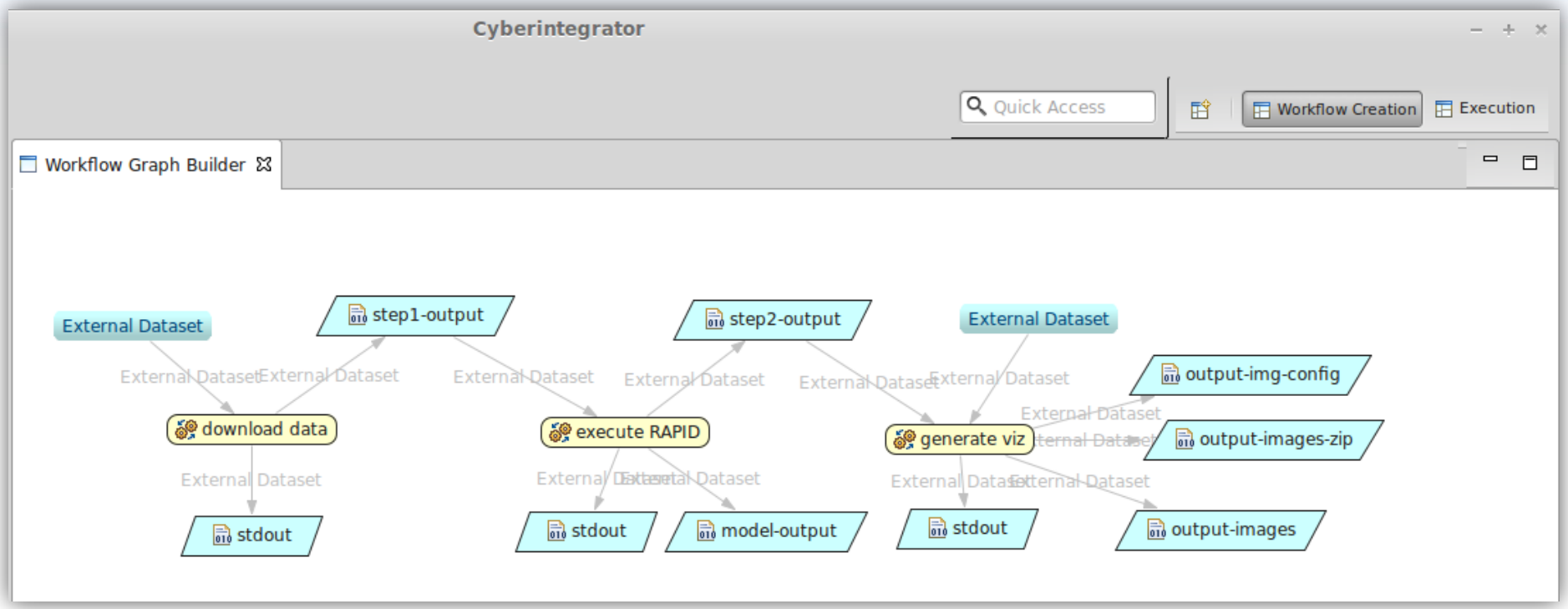


TEXAS WATER MANAGEMENT

Texas Water Management

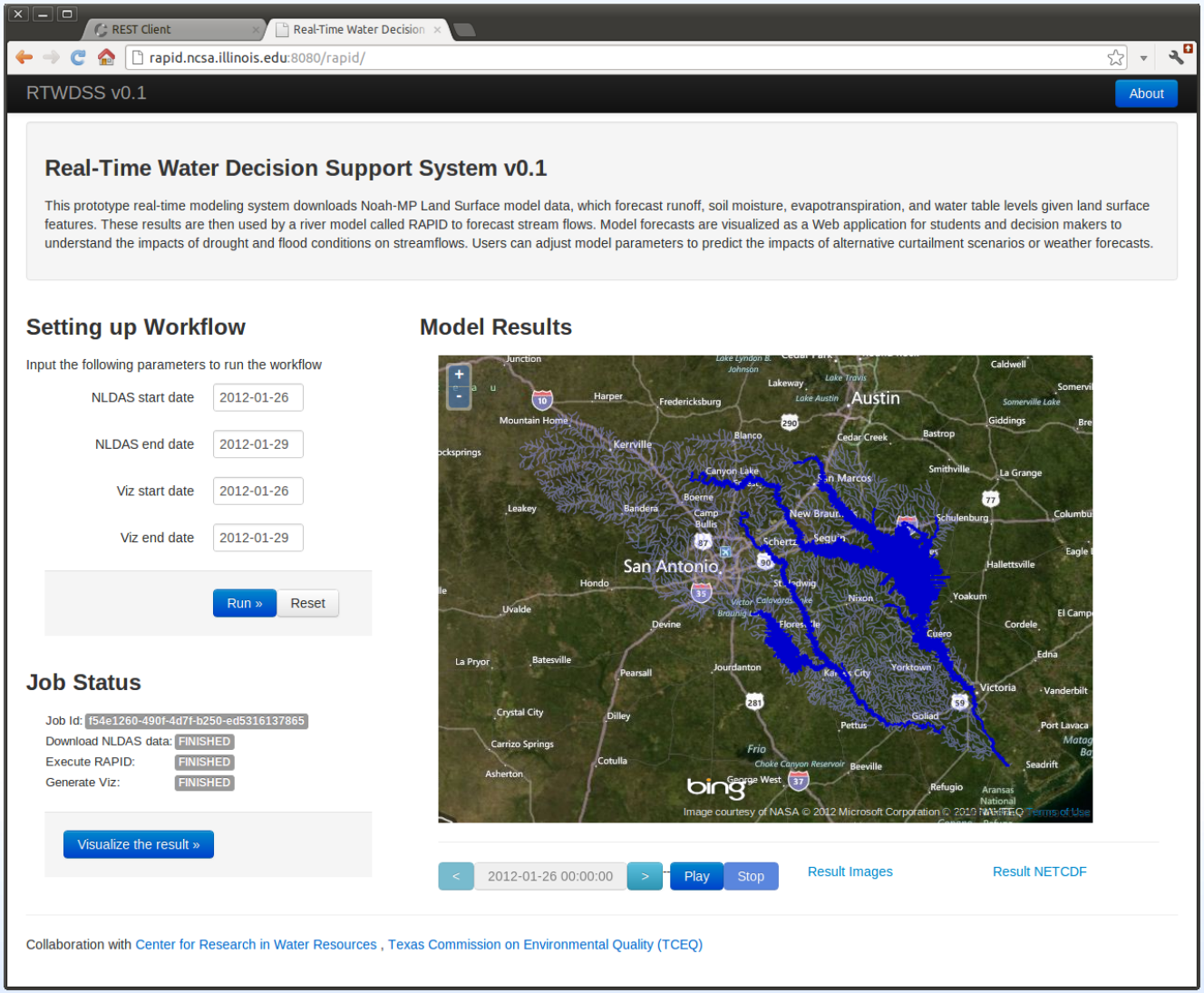
- Working with UT-Austin and Texas Commission on Environmental Quality (TCEQ)
- Goal: Building a decision support system for water management
- Utilizing the river flow model called RAPID

Building a Cyberintegrator Workflow for RAPID



- Download NLDAS data
- Execute RAPID model
- Generate visualization (images) of the model results

Web Application



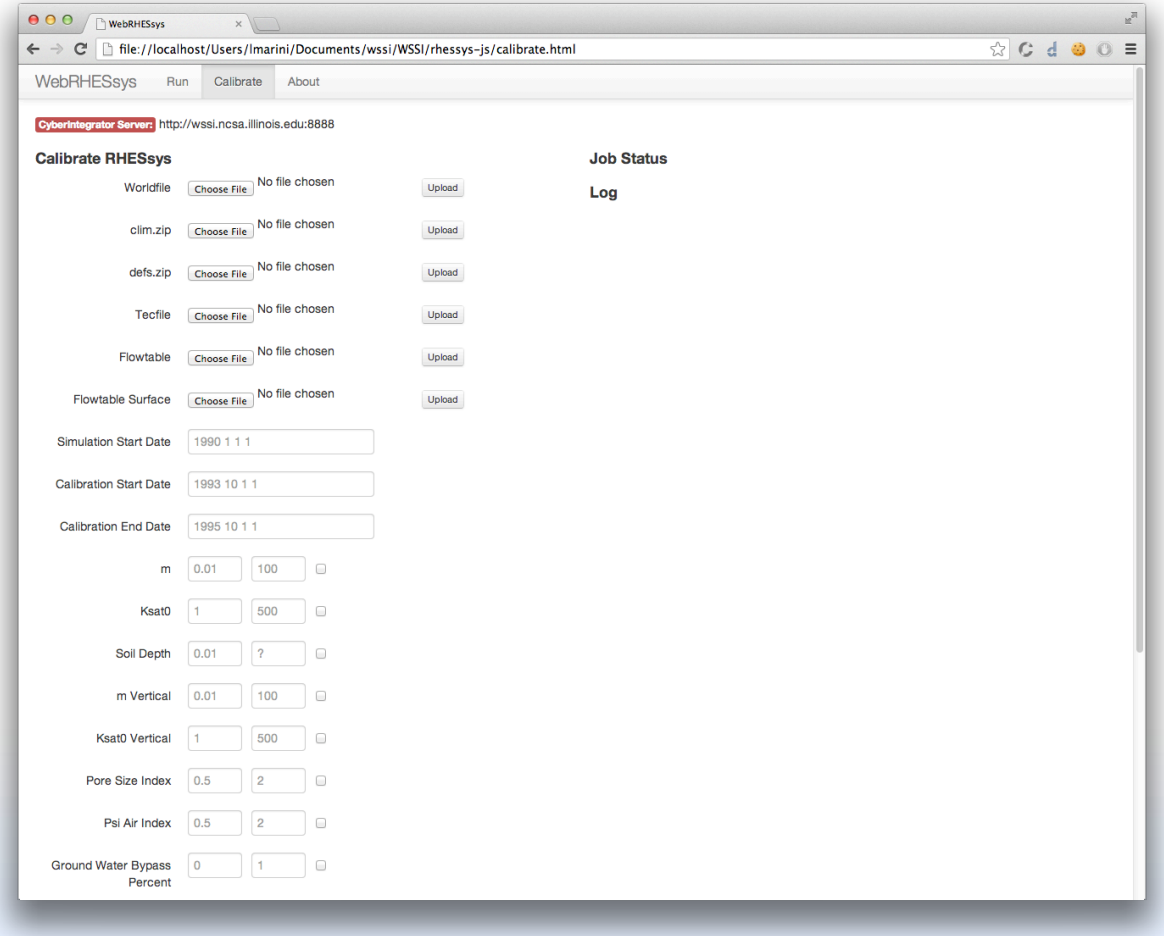
USE CASE: WSSI

Creating CI Workflow

- You can create a CI workflow by using CI Desktop
- CI workflow can wrap the command line tools
- Example: simplified **run.sh** script to run RHESsys
  - 3 inputs: worldfile.zip, tecfile, flowfile
  - Unzip worldfile.zip, Run RHESsys, Zip the results

```
#!/bin/bash
unzip $1
/home/jonglee/rhessys/rhessys -st 1990 1 1 1 -ed 1993 10 1 1 \
   -b -t $2 -w ./worldfile -r $3 -s 12.0880 14.2677 \
   -sv 2.1529 83.7472 -gw 0.4108 0.0823
zip results.zip result_*
```

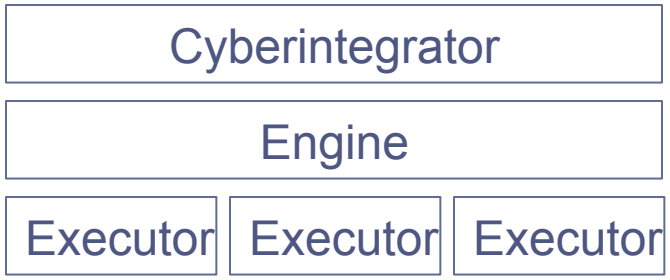
Simple Web Application



CYBERINTEGRATOR

Cyberintegrator Architecture

- Plugin based
- Executor types
  - Local (on local machine)
  - Remote (remote service)
- Example executors
  - Java (local)
  - Command Line (local)
  - HPC (remote)



Technologies Used

- JAVA
- Spring Framework, especially spring-data, well established, been around long time.
- Hibernate, used as ORM
  - Data is stored in MySQL (tested), but can be any relational database.

Local vs Remote Executors

- Local Executors
  - Run on same machine as Cyberintegrator
  - Cyberintegrator controls what executors is running
  - Limited number of parallel processes

- Remote Executors
  - Run on different machine
  - Process Management is done outside of Cyberintegrator
  - All executors are started if possible

JAVA Executor

- Local executor
- JAVA code is run in Cyberintegrator VM
- Need implementation of JAVA interface
  - setInput
  - setParameter
  - Execute
  - getOutput

- System.exit() is a bad call!

Java Wizard

- Add JAR files with tools
  - Including any additional jar files needed
- Select tools that needs to be imported

- Wizard will use interface to get
  - Name and description
  - Inputs and outputs
  - Parameters

Command Line Executor

- Local executor
- Execute command line tool
- Sets working folder to a temp folder
- Can capture stdout and stderr
- Will add copy of inputs in temp folder
  - Prevents modification
- Will copy outputs back to database

Command Line Wizard

- Point to executable
- What inputs, outputs are needed
- What parameters are needed
  - Flags, options etc.
- Any additional files needed
- Set environment variables

HPC Executor

- It is a RemoteExecutor that uses SSH Channels to communicate with various queuing systems
- Similar to Command Line Executor except the execution line (executable, flags, inputs, etc) for the tool are appended to a script and submitted to a queuing system
- An XML definition file must be provided to the tool with information about the HPC (e.g. location of submit, terminate, status commands), a script to append the execution line to, and the regex for parsing job status messages
- Queuing systems tested
  - PBS
  - Loadleveler
  - SGE (minimally tested)

HPC Tool

- A Wizard guides users through tool creation process
- User provides XML host definition file and executable
- The wizard allows user to specify program arguments and inputs that will be used to build the tool's User Interface
- Each HPC Tool requires the following information, which is added dynamically to the tool definition and will be part of the tool's UI
  - Username on target machine
  - Userhome on target machine
  - SSH URI for target machine

Cyberintegrator Applications

- Server Application
  - Exposes Cyberintegrator as restful service
  - Allows uploading/downloading workflows/data
  - Allows execution of workflows on server
- Workflow Editor
  - Web based
  - Work online/offline
  - Allows for creation/editing of workflows on server
- Tool creator
  - Temporary tool to allow creation of tools on server

Cyberintegrator Server

- Standard REST endpoint
  - Results are JSON
- Same engine/executors as Desktop
- Can execute workflows on demand
  - Workflows as a service!
- Can upload datasets for workflow
- Can specify parameters for workflow

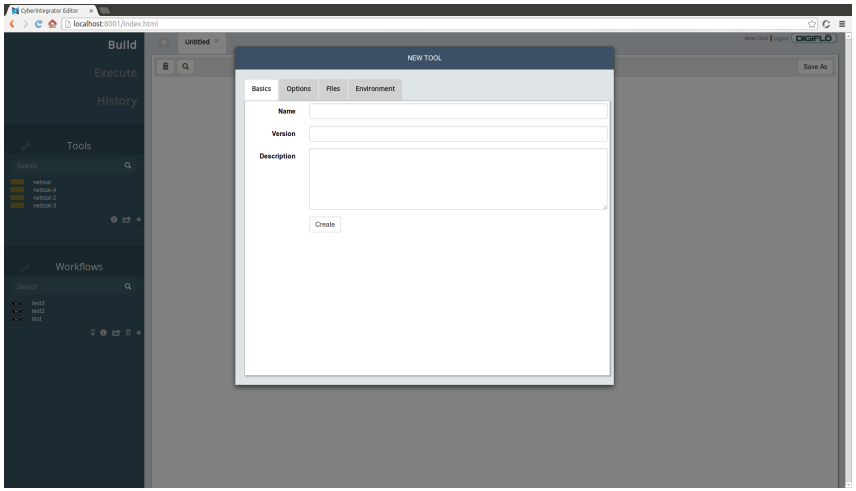
Cyberintegrator REST

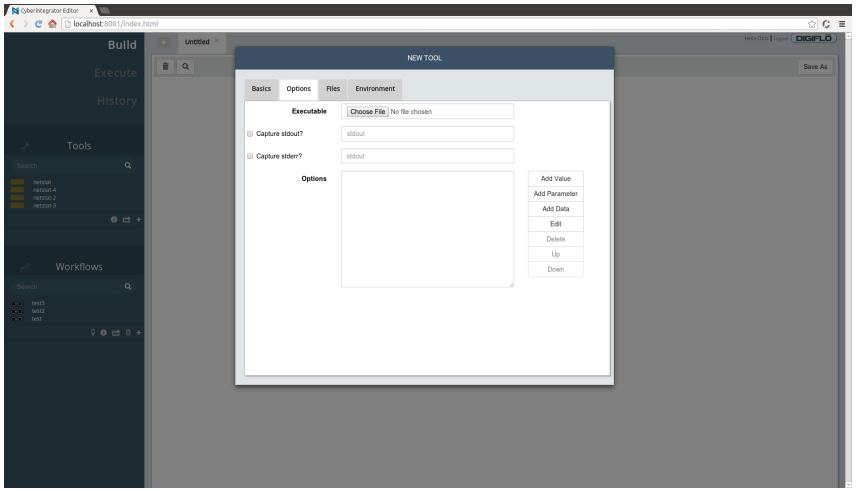
- People [GET, POST]
  - http://<host:port>/persons/{pid}
- Workflows [GET, POST]
  - http://<host:port>/workflows/{wid}/
  - http://<host:port>/workflows/{wid}/zip
  - http://<host:port>/workflows/{wid}/executions/{eid}
- LogFiles [GET]
  - http://<host:port>/logfiles/{lid}/
- Datasets [GET, POST]
  - http://<host:port>/datasets/{did}/
  - http://<host:port>/datasets/{did}/zip
  - http://<host:port>/datasets/{did}/{fid}
  - http://<host:port>/datasets/{did}/{fid}/zip

Workflow Editor

- Web based
- Create tools
- Create workflows
- Execute workflows
- View past executions
- Upload/download datasets/results

Workflow Editor





PAW

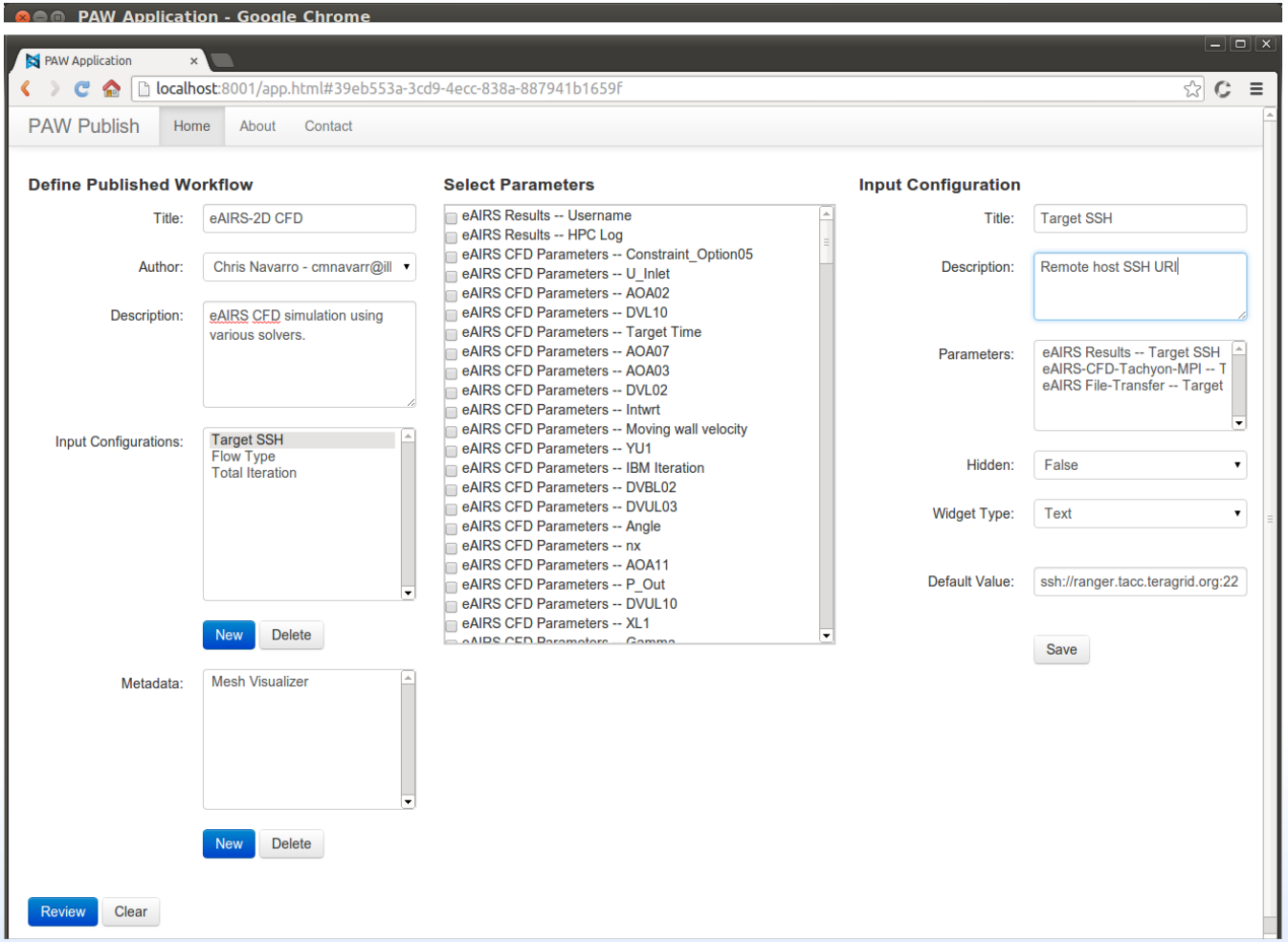
PAW

- Published Active Workflow
- Workflows can have many steps, many inputs and many parameters, not all should be exposed to user or as service.
- Allows single widget to control multiple parameters
- Associates UI widgets with parameters.

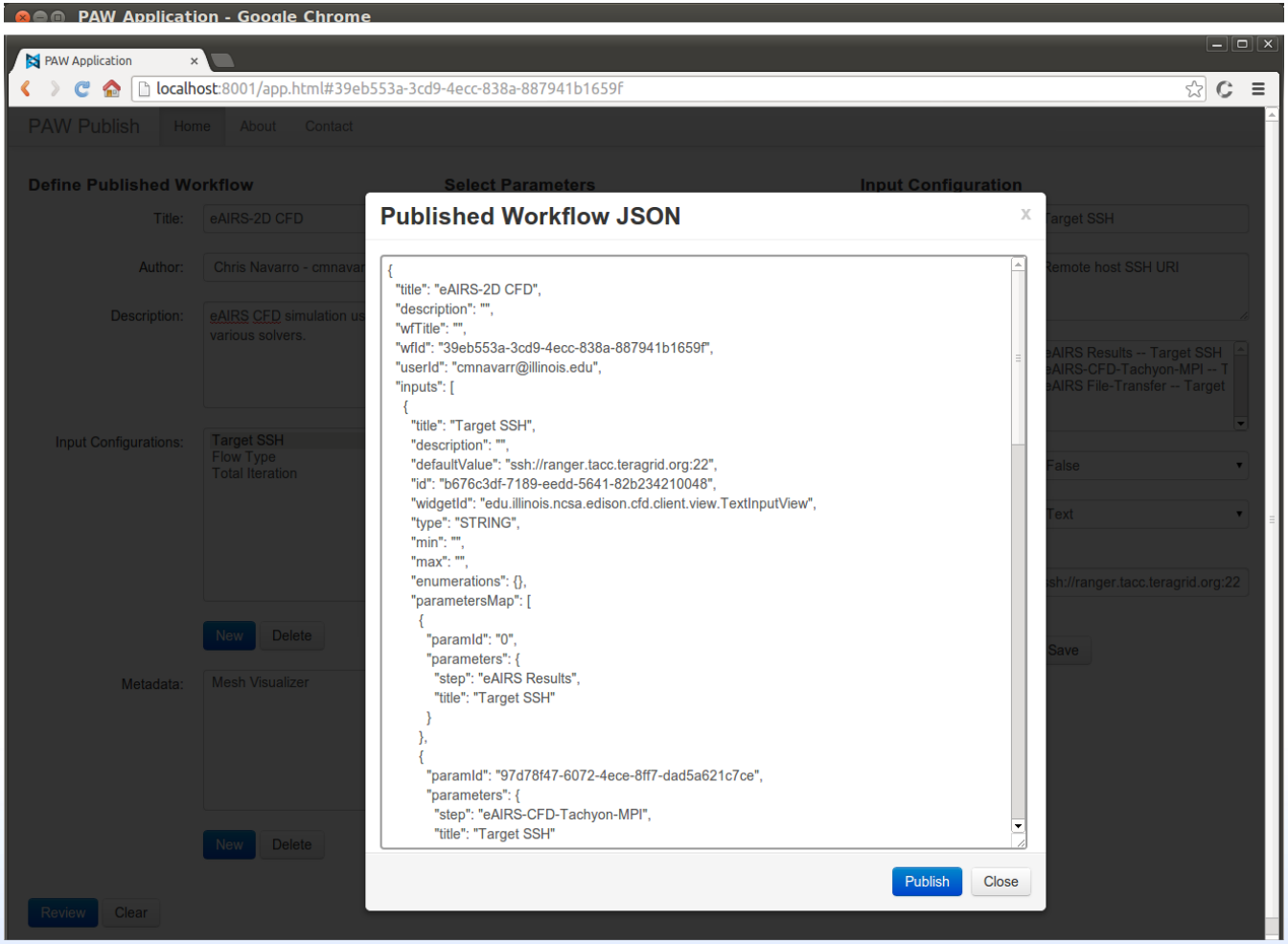
PAW Editor

- Web based (HTML5) tool for interactively publishing workflows. The tool allows you to:
  - Publisher can specify which workflow fields to expose to users
  - Guides user through process of mapping Web UI widgets (Text, Int, Float, Custom) to one or more exposed workflow fields
  - Add Metadata about workflow tools
- Review panel allows user to review/modify JSON before publishing

PAW Editor – Field Mapping



PAW Editor – Review JSON



Getting Started with Cyberintegrator

- Download Cyberintegrator app

- Create tools
  - Use toolcreator for now
- Create workflow
- Execute workflow on server
- Check results

Future Work

- Finish Web based editor
  - Allow for tool creation
  - Add authentications (openID)
- Data integration with Medici
  - Right now data stored in filesystem
  - Data can be stored in Medici
- More executors for Cyberintegrator
  - MATLAB
  - R
- PAW editor
  - Allow selection of widgets
  - Publish PAW as a web application

Cyberintegrator FAQ

- Source Code
  - https://opensource.ncsa.illinois.edu/stash/projects/CBI
- Bugs
  - https://opensource.ncsa.illinois.edu/jira/browse/CBI
- Documentation
  - https://opensource.ncsa.illinois.edu/confluence/display/CBI
- Application Downloads
  - http://isda.ncsa.illinois.edu/download/index.php?project=Cyberintegrator&sort=version

Questions

- Feel free to contact us
- http://isda.ncsa.illinois.edu
- isda@ncsa.illinois.edu

DEMO

Cyberintegrator Demo

- Software URLS:
  - https://opensource.ncsa.illinois.edu/bamboo/browse/CI-SERVER
  - Download latest build:
    - cyberintegrator-webapp-all.zip
    - cyberintegrator-tool-creator.zip
- Source URL:
  - https://opensource.ncsa.illinois.edu/stash/scm/~cnavarro/grep-demo.git

Cyberintegrator Start

- Unzip cyberintegrator-webapp-all.zip
- Launch bin/cyberintegrator-service
- Open webbrowser
  - http://localhost:8888/persons (Should return [])

- Unzip cyberintegrator-tool-creator.zip
- Launch bin/tool-creator

Create First Tool

- Add Person
- Add Command-Line tool
  - netstat
    - Executable is netstat
    - Capture stdout
    - Add parameter
      - Name is options
      - Default value is –an
      - Can be empty

Create Second Tool

- Build in eclipse
  - Clone git repository
    - https://opensource.ncsa.illinois.edu/stash/scm/~cnavarro/grep-demo.git
  - Import projects
  - Run->As Maven package

- Build in command line
  - git clone https://opensource.ncsa.illinois.edu/stash/scm/~cnavarro/grep-demo.git
  - cd grep-demo/grep-tool
  - mvn package

Add Second Tool

- Add Java tool
  - Add files point to target/grep-tool-example-0.0.1-SNAPSHOT.jar
  - Select GrepTool

Create Workflow

- In browser go to http://localhost:8888/editor
  - Login is email address of user created
  - Password can be blank (for now)
  - Editor should show 2 tools
  - Create new workflow
    - Either plus under workflows or on tab page
    - (known bug of invalid first workflow page CBI-468)
  - Drag netstat and grep on canvas
    - Connect stdout of netstat to input file of grep
  - Save workflow
    - http://localhost:8888/workflows

Execute Workflow

- Click on Execute
- Open workflow just created
- Fill in workflow
  - Title, description
  - Options = -an
  - Regex = .*LISTEN.*

Workflow History

- Click on History
- Select on execution just created
  - See how long a step took (milliseconds)
  - Download results