CCSI
Carbon Capture Simulation Initiative

Data Management and Simulation Support Accelerating Carbon Capture through Computing

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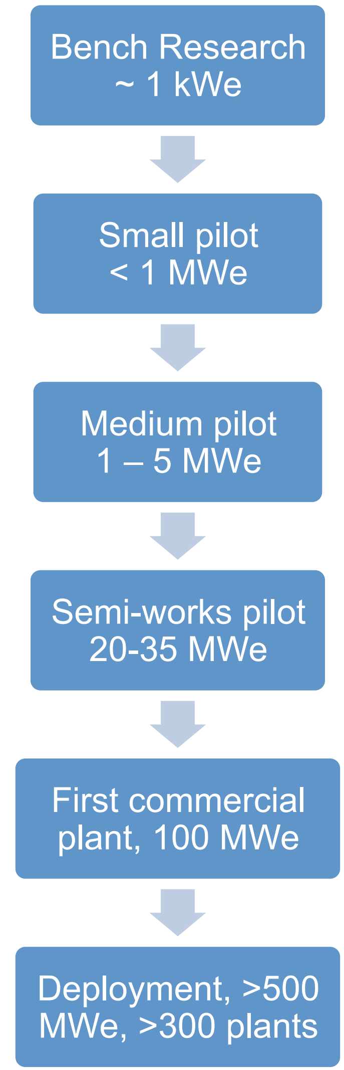
NETL BERKELEY LAB Lawrence Livermore National Laboratory Los Alamos NATIONAL LABORATORY EST.1943 Pacific Northwest NATIONAL LABORATORY U.S. DEPARTMENT OF ENERGY

Carbon Capture Challenge

- The traditional pathway from discovery to commercialization of energy technologies is long[1], i.e., ~ 20-30 years
- President's plan[2] requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years
- To help realize the President's objectives, new approaches are needed for taking concepts from lab to power plant, quickly, at low cost and with minimal risk
- Carbon Capture Simulation Initiative (CCSI) designed to accelerate the development of CCS technology, from discovery through deployment, with the help of science-based simulations



1. *International Energy Agency Report: Experience Curves for Energy Technology Policy," 2000*
2. *http://www.whitehouse.gov/the-press-office/presidential-memorandum-a-comprehensive-federal-strategy-carbon-capture-and-storage*

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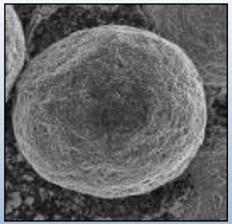
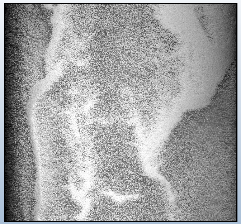
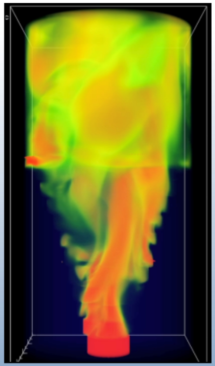


Identify promising concepts → **Reduce the time for design & troubleshooting** → **Quantify the technical risk, to enable reaching larger scales, earlier** → **Stabilize the cost during commercial deployment**

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory EST. 1943
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Virginia Tech
- Penn State 1855
- Princeton University
- West Virginia University
- University of Pittsburgh

Industry

- ADA Environmental Solutions
- Ameren
- B&W the babcock & wilcox company
- Babcock Power Inc.
- Air Products
- Alstom
- Fluor
- Ramgen Power Systems USA
- AEP American Electric Power
- Duke Energy
- GE
- PG&E
- Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
- Southern Company
- Chevron
- Eastman
- EPRI Electric Power Research Institute
- WorleyParsons resources & energy
- URS

Essential for accelerating commercial deployment

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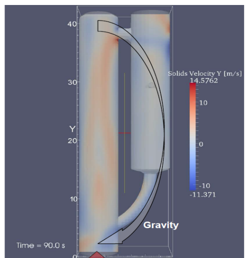
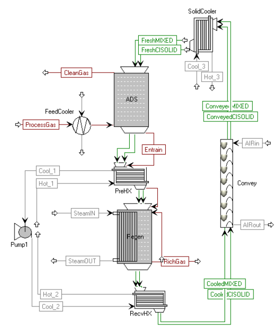
CCSI Integrated Process Design Environment

Bench-scale Experiments

Particle-scale Simulations



Process Simulations



Small-scale Deployments

Uncertainty Quantification, Decision Support, Optimization, etc

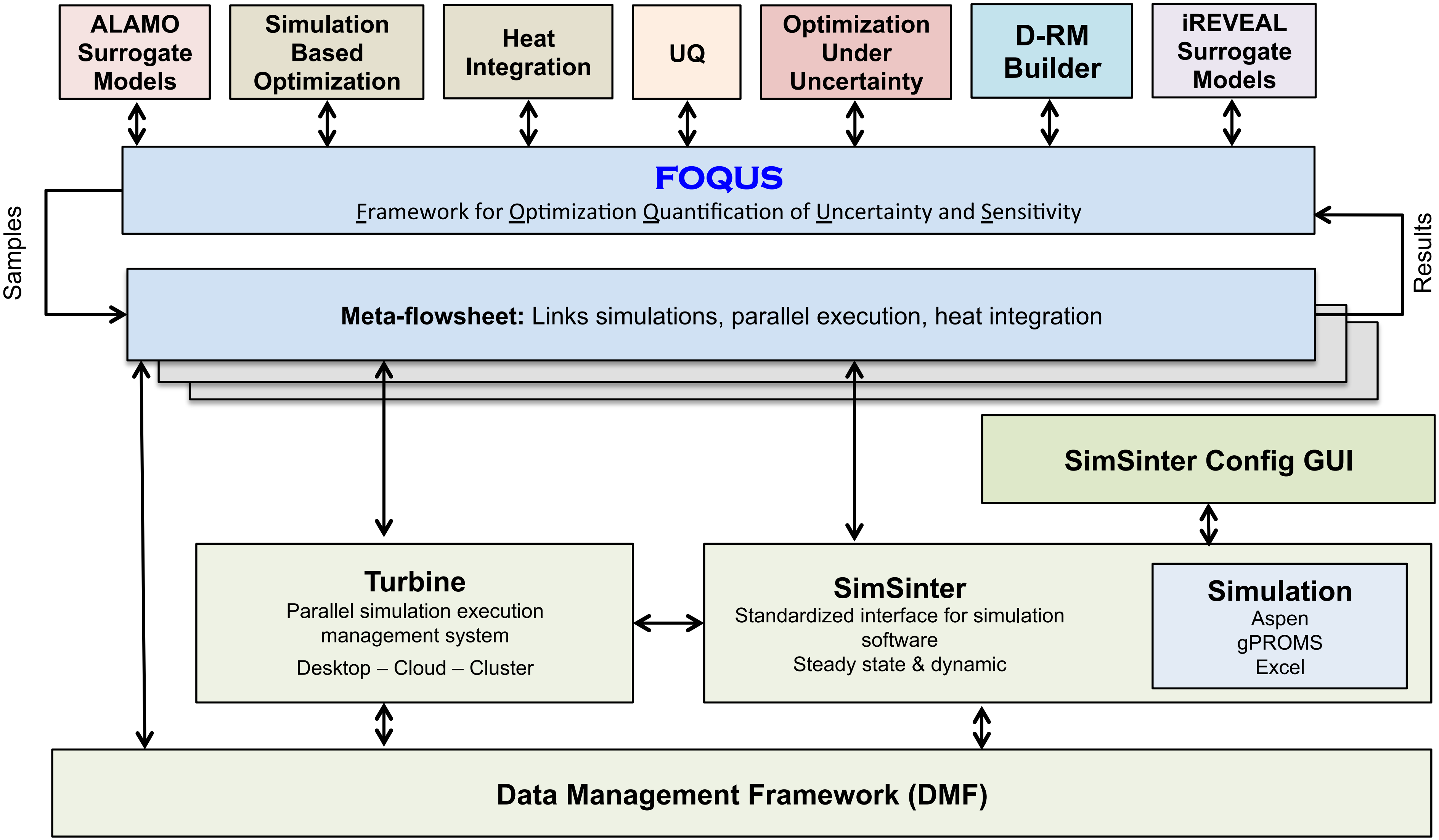
Knowledge, Information, & Integrated User Environment

Decision Makers

CCSI Toolset

- Comprehensive, integrated suite of validated science-based computational models
- Modular design that leverages existing software components
- Simulation and data management support provided through CCSI Integration Framework
- Components:
  - Core capabilities for optimization, modeling and uncertainty quantification
  - Orchestration: FOQUS
  - Process simulation framework: Turbine, SimSinter, DMF

CCSI Toolset Architecture



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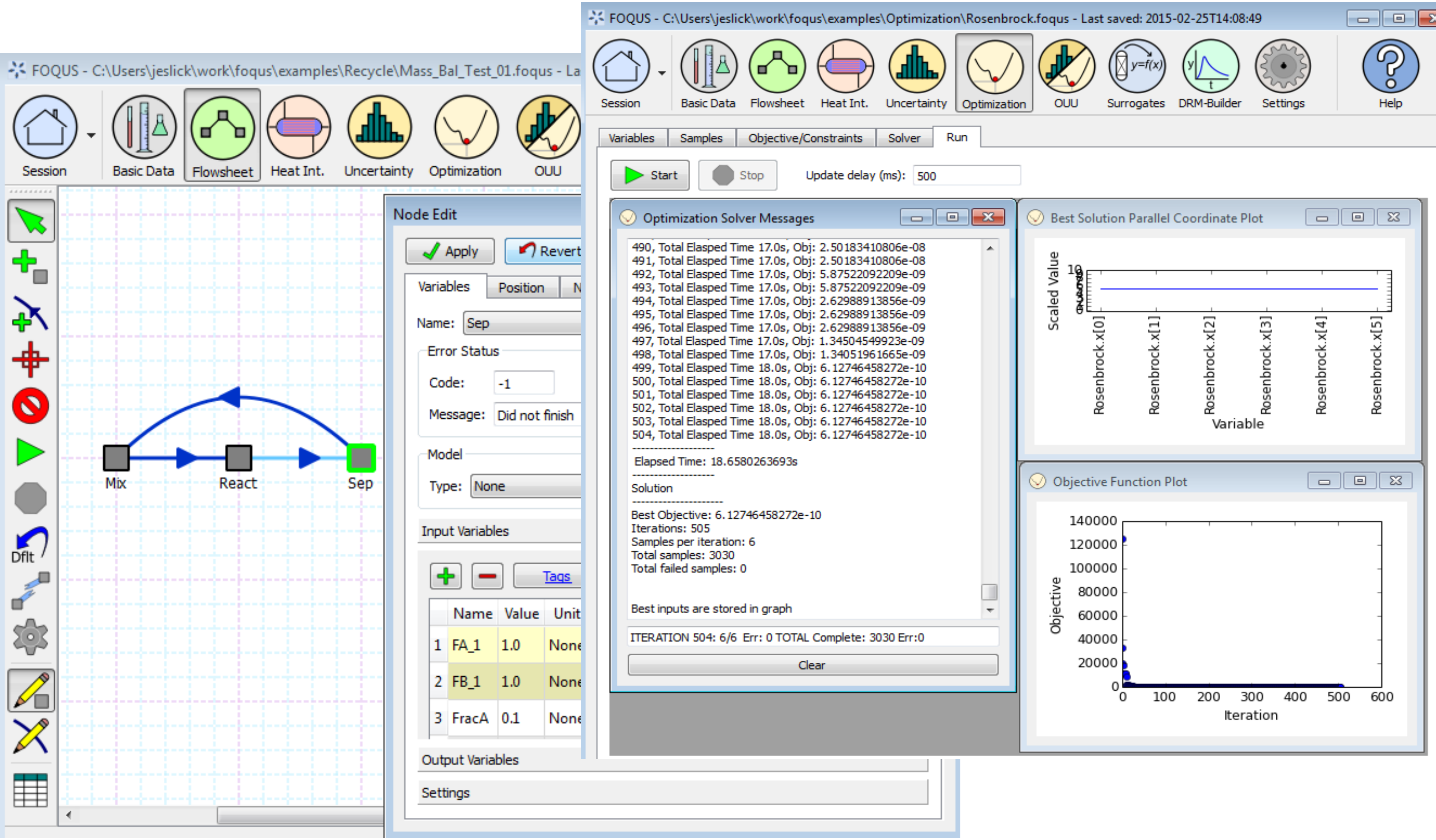
FOQUS

- Framework for Optimization and Quantification of Uncertainty and Sensitivity
- Serves as the primary computational interface in the CCSI Toolset.
- Interface to simplify running complex modeling and UQ studies
- Modular design involving plugin system
- *Flowsheet*: Composite model, *Meta-Flowsheet*: Combination of flowsheets
- Provides GUI and platform for flowsheet analysis tools
- Developed in Python/PyQt/PySide

FOQUS: GUI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Basic Data
Flowsheet
Heat Int.
Uncertainty
Optimization
OUU
Dflt
Mix
React
Sep
Node Edit
Apply
Revert
Variables
Position
Name:
Sep
Error Status
Code:
-1
Message:
Did not finish
Model
Type:
None
Input Variables
Tags
Name
Value
Unit
1 FA_1 1.0 None
2 FB_1 1.0 None
3 FracA 0.1 None
Output Variables
Settings
FOQUS - C:\Users\jeslick\work\foqus\examples\Optimization\Rosenbrock.foqus - Last saved: 2015-02-25T14:08:49
Session
Basic Data
Flowsheet
Heat Int.
Uncertainty
Optimization
OUU
Surrogates
DRM-Builder
Settings
Help
Variables
Samples
Objective/Constraints
Solver
Run
Start
Stop
Update delay (ms):
500
Optimization Solver Messages
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503, Total Elasped Time 18.0s, Obj: 6.12746458272e-10
504, Total Elasped Time 18.0s, Obj: 6.12746458272e-10
Elapsed Time: 18.6580263693s
Solution
Best Objective: 6.12746458272e-10
Iterations: 505
Samples per iteration: 6
Total samples: 3030
Total failed samples: 0
Best inputs are stored in graph
ITERATION 504: 6/6 Err: 0 TOTAL Complete: 3030 Err:0
Clear
Best Solution Parallel Coordinate Plot
Scaled Value
Rosenbrock.x[0]
Rosenbrock.x[1]
Rosenbrock.x[2]
Rosenbrock.x[3]
Rosenbrock.x[4]
Rosenbrock.x[5]
Variable
Objective Function Plot
Objective
140000
120000
100000
80000
60000
40000
20000
0
0
100
200
300
400
500
600
Iteration

Turbine Science Gateway

- Scaling up experiments
  - Solving large scale simulations (particles, CFD)
    - Dense phase, reactive flows with complex submodels
  - Multiple simulation runs (optimization, UQ)
    - Multiple scales (Particle, Device, System)
- Batch system providing staging of input and output files
- Generic solution that can be extended to process modeling and simulation packages
- Integrated with FOQUS to schedule and scale-up simulation runs

Turbine Science Gateway: Components

- Designed to operate primarily in Windows
- Turbine Web application:
  - Windows service
  - RESTful, HTTP API
  - Five resources in API: Application, Simulation, Job, Consumer, Session
  - Python library for interfacing with other tools
- Turbine Client
  - Platform independent
- Turbine Database
  - SQLite
  - Stores state and results
- Turbine Server
  - Executes and manages simulation process through use of SimSinter through Turbine Workers
  - Multiple workers can be used to form Turbine Cluster

Turbine Server Experiences

- Framework can be used with single machines, clusters, Cloud computing resources
- Scale simulations to allow computations in thousands
- Successfully executed 400 instances of Aspen Plus simulations using Amazon EC2
- Harnesses Amazon EC2 spot instances vs owning a cluster of computers
- Parallelization increases application throughput and decreases time to solution
- Integrated Mass Transfer Model
  - Local optimization (single processor) 12 hours
  - Cloud optimization (4-6 consumers) 2.75 hours

Turbine Science Gateway: Use case

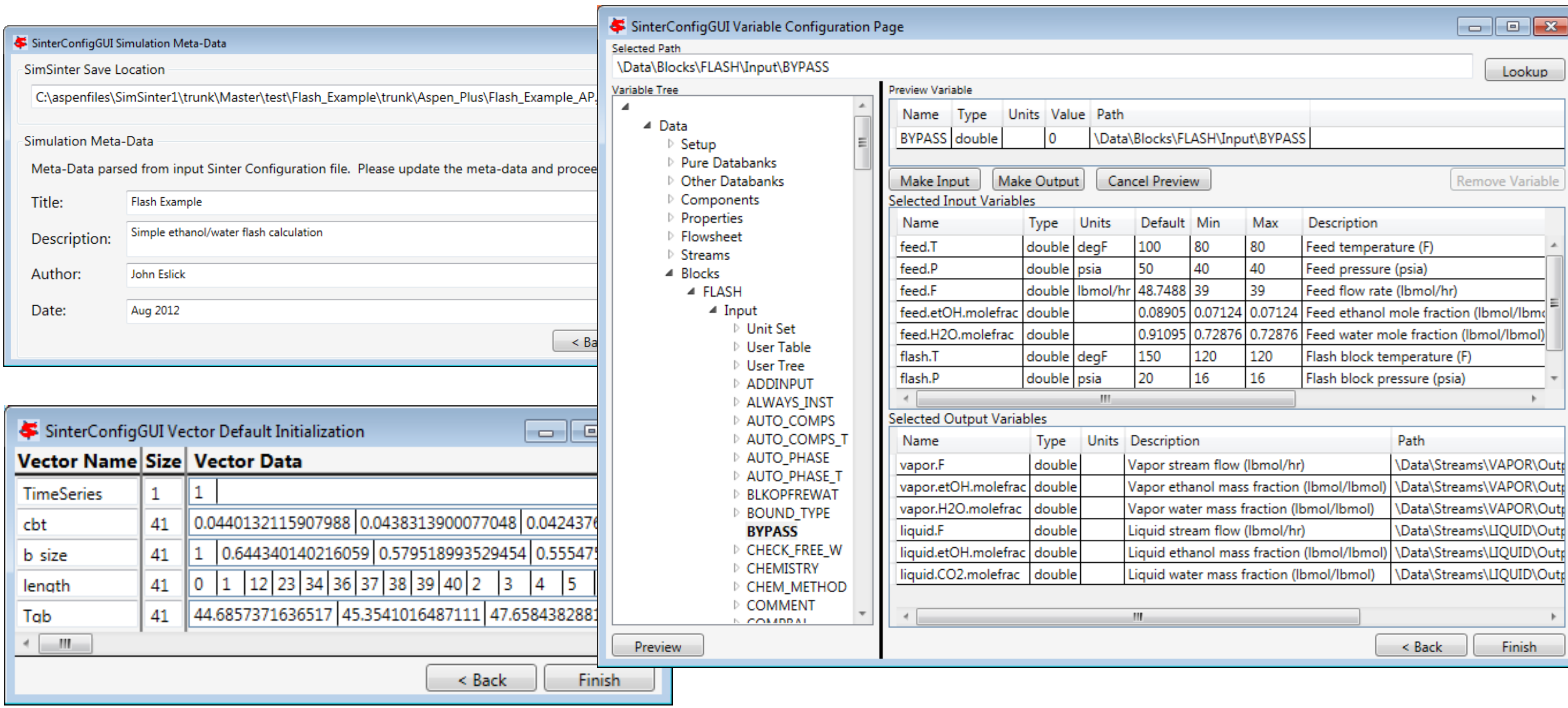
Plot of simulation runtime versus start time of simulation execution

SimSinter

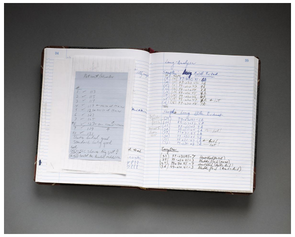
- Provides extensible support with various commercial simulation tools
  - Aspen Custom Modeler, Aspen Plus, gProms, Microsoft Excel
- Standard Interface library for driving single-process Windows based process simulation software
- Based on .NET and Microsoft COM interface
- Connects Turbine Science Gateway with process simulation tools
- Sinter configuration files:
  - Created by model creators
  - Identify simulation input and output variables
  - JSON format

Simsinter Config GUI

- SimSinter Config GUI: Allow easier creation and editing of Sinter configuration files



DMF: Motivation



- Recognition that computational experiments are an important resource
- Financial decisions based on computational experiments
- Need for system to permanently store information about computational experiments:
  - Complete specification of the computational experiment (all the inputs)
  - Significant results files (outputs)
  - Metadata (who, when, what)
  - Dependencies of inputs and results (provenance)

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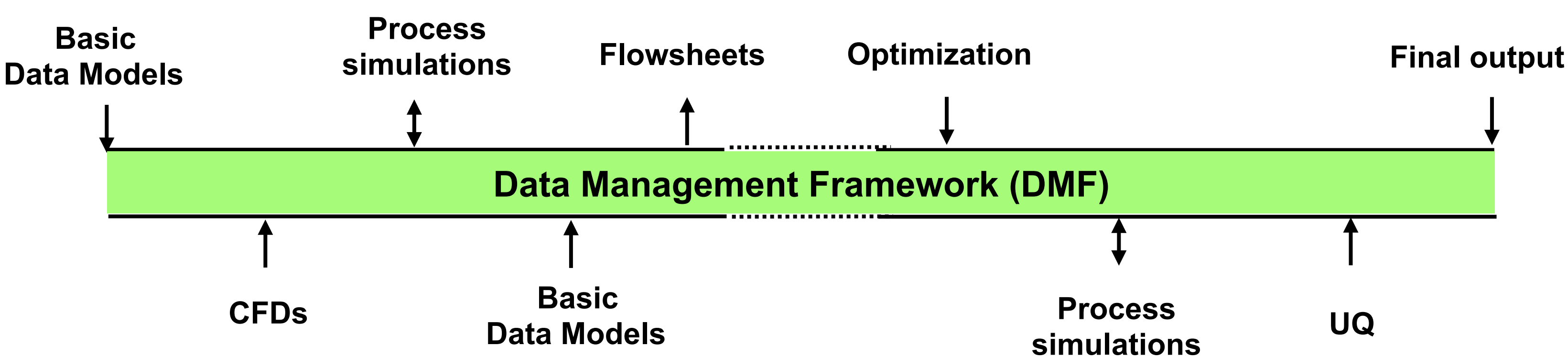
Pacific Northwest National Laboratory

U.S. Department of Energy

DMF: Requirements and Impact

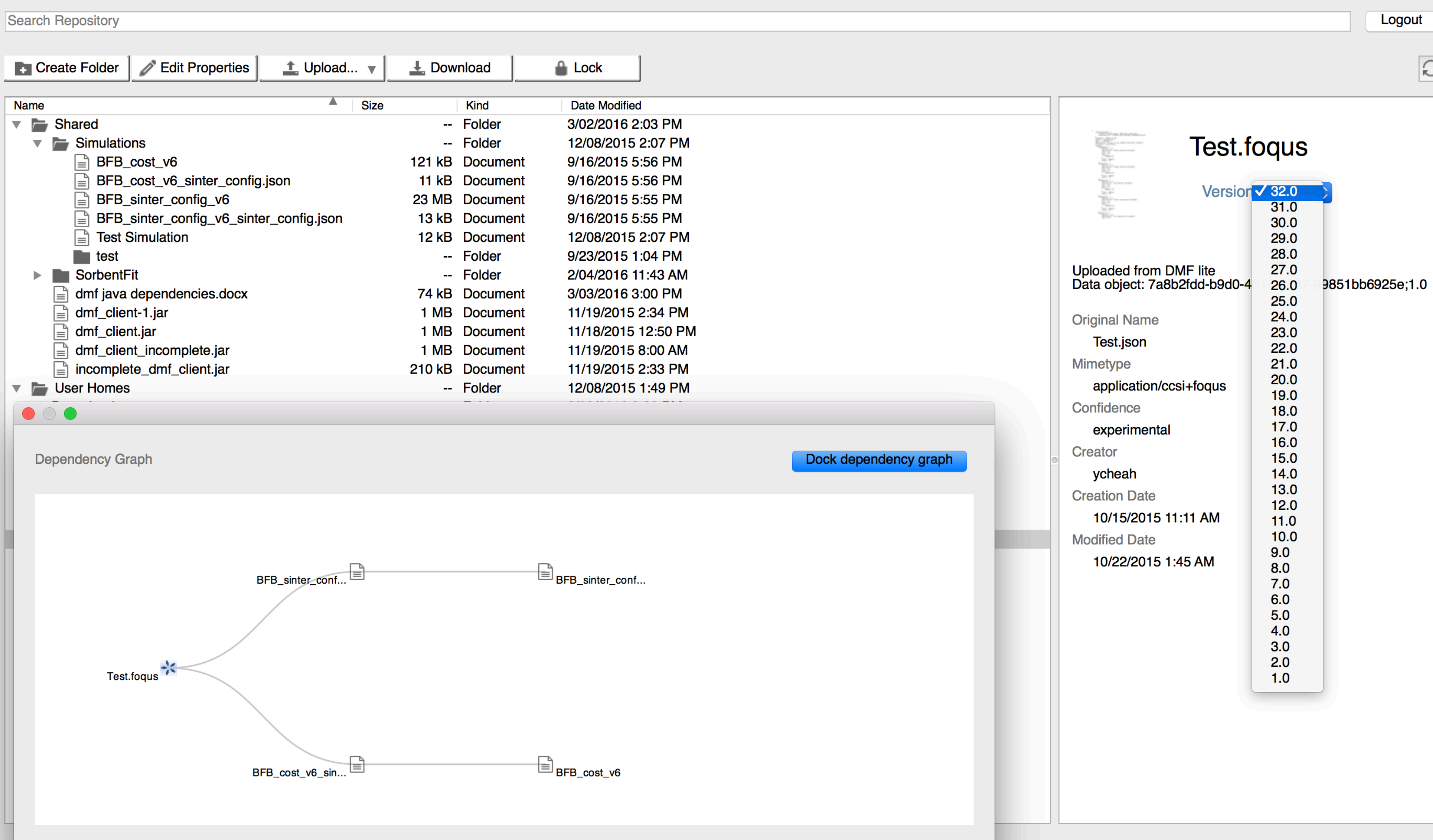
- Data management capabilities for CCSI data:
  - Browsing
  - Searching
  - Versioning
  - Metadata tracking
  - Dependency/Provenance tracking
  - Facilitate sharing
- Integration with other CCSI tools to provide better workflow



DMF: Components

- Developed in Python 2.7
  - Needs to run on both Windows & Linux platforms
- Two versions of the DMF:
  - DMF Lite: Git backend http://git-scm.com/
  - DMFServ: Alfresco repository backend http://www.alfresco.com/
- DMF Browser
  - GUI supporting both versions of DMF
  - Developed using PyQt / PySide
  - D3 for provenance visualization
- Command line tools
  - Basic Data uploader
  - Simulation uploader

DMF Browser: Provenance



Conclusions & Future Work

- Traditional end-to-end process for carbon capture takes decades
- The CCSI toolset integration framework is designed and deployed to scale simulations and facilitate the science for carbon capture simulation
- CCSI Phase I is completed
- Augmenting existing CCSI Toolset with tools to help
- Implementation of dashboard to present and integrate existing data in an effective manner

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