CCSI

Carbon Capture Simulation Initiative

Simulation-Based Optimization Framework with Heat Integration

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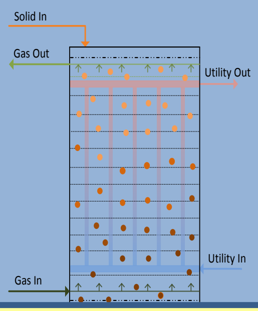
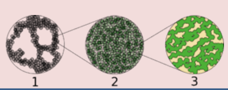
Tools to Develop an Optimized Process using Rigorous Models

Process Models



Uncertainty

Basic Data Submodels



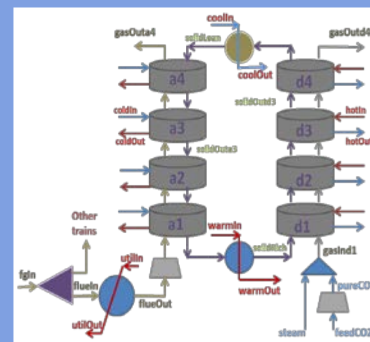
Uncertainty

Algebraic Surrogate Models

ALAMO

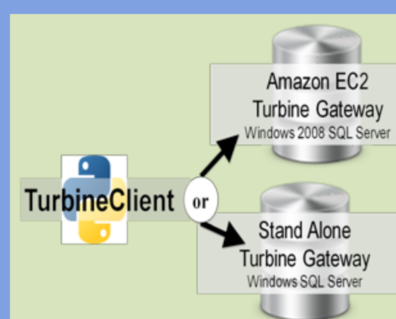
Uncertainty

Superstructure Optimization (Determine Configuration)



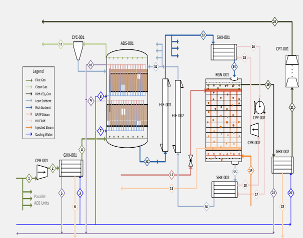
Uncertainty

Simulation-Based Optimization



Uncertainty

Optimized Process



Uncertainty

- **Uncertainty Quantification**
- **Process Dynamics and Control**
- **CFD Device Models**
- **Risk Analysis**

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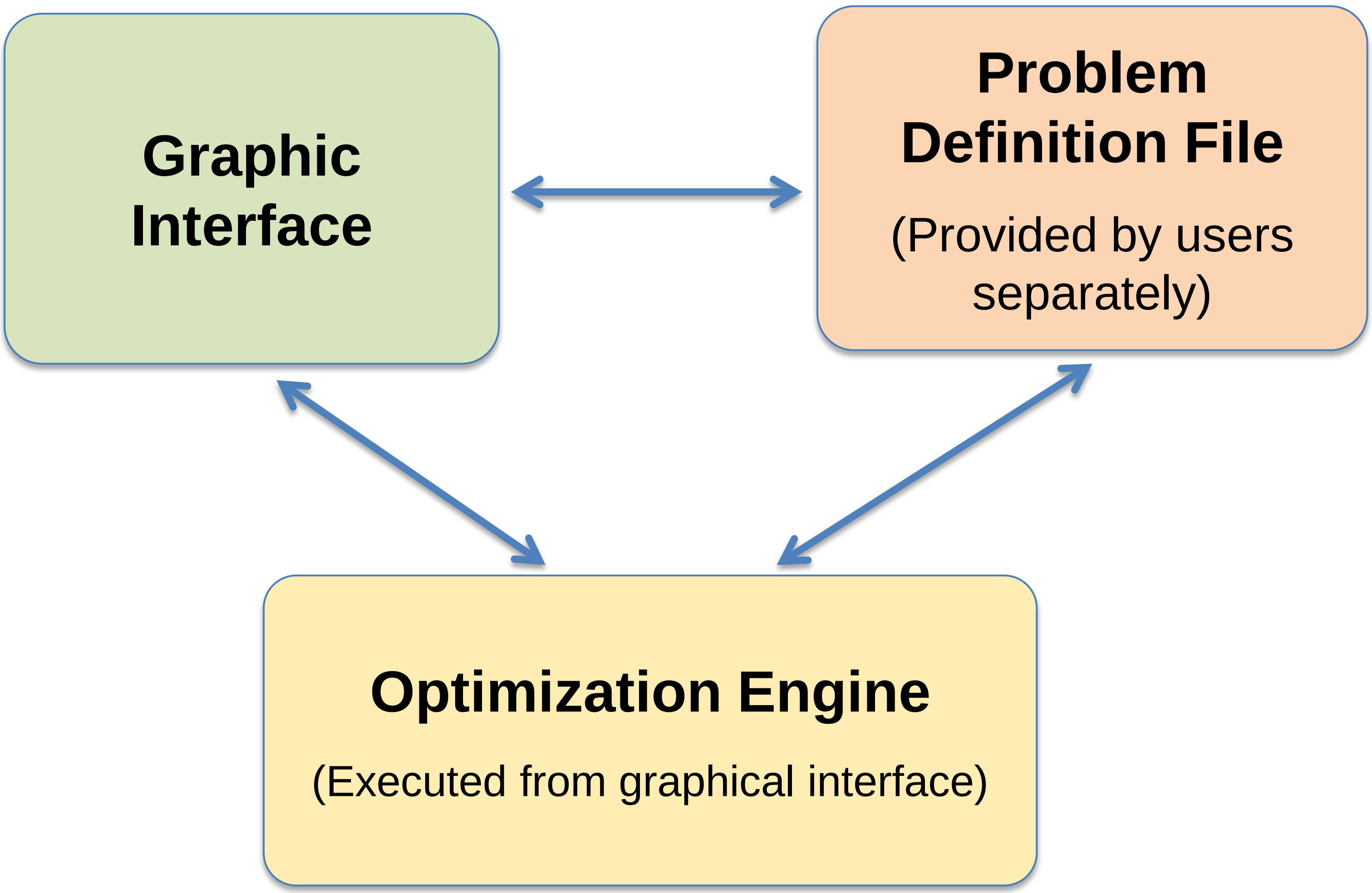
Simulation-Based Optimization

+ Treats simulation as black box (does not require mathematical details of model)
  → **Easy to implement**
+ Does not require simplification of the process model
  → **High-fidelity models applied**
+ Readily adapted for parallel computing
  → **Computational time reduced**
− Not well suited for problems with many variables such as heat integration, and superstructure optimization
  → **Heat integration is a separate module in optimization**
  Superstructure optimization pre-determines best topology

Goal: Develop a simulation-based optimization framework with heat integration for large-scale high-fidelity process models.

Simulation-Based Optimization Framework



Problem Definition File (Session File)

Optimization Settings

Black-Box optimization parameters, bounds, variable scaling

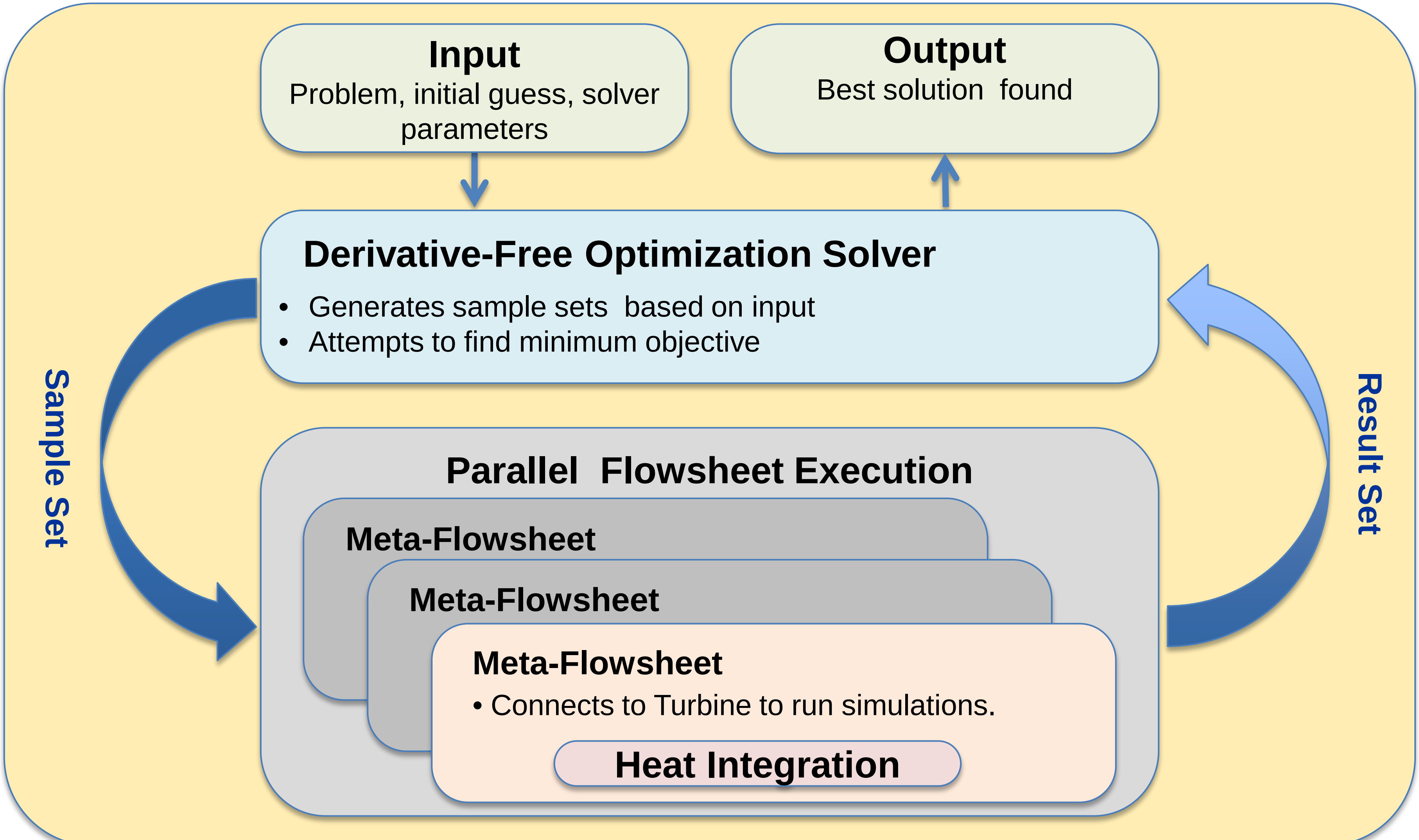
Model Settings

- Define input and output variables for simulations
- Specifies simulation files and metadata

Meta-Flowsheet

- Connect Multiple simulations and calculations
- Recycle loops are allowed

Optimization Engine



Derivative-Free Optimization Methods

- CMA-ES
  - Covariance Matrix Adaptation Evolution Strategy
  - For difficult non-linear non-convex optimization problems in continuous domain
- SNOBFIT
  - Stable Noisy Optimization by Branch and FIT
  - For the robust and fast solution of noisy optimization problems with continuous variables
- Global-OPT (DOES)
  - Uses design of experiments to determine the global optimum
  - Can optimize smooth and not-smooth, continuous and discrete variable problems

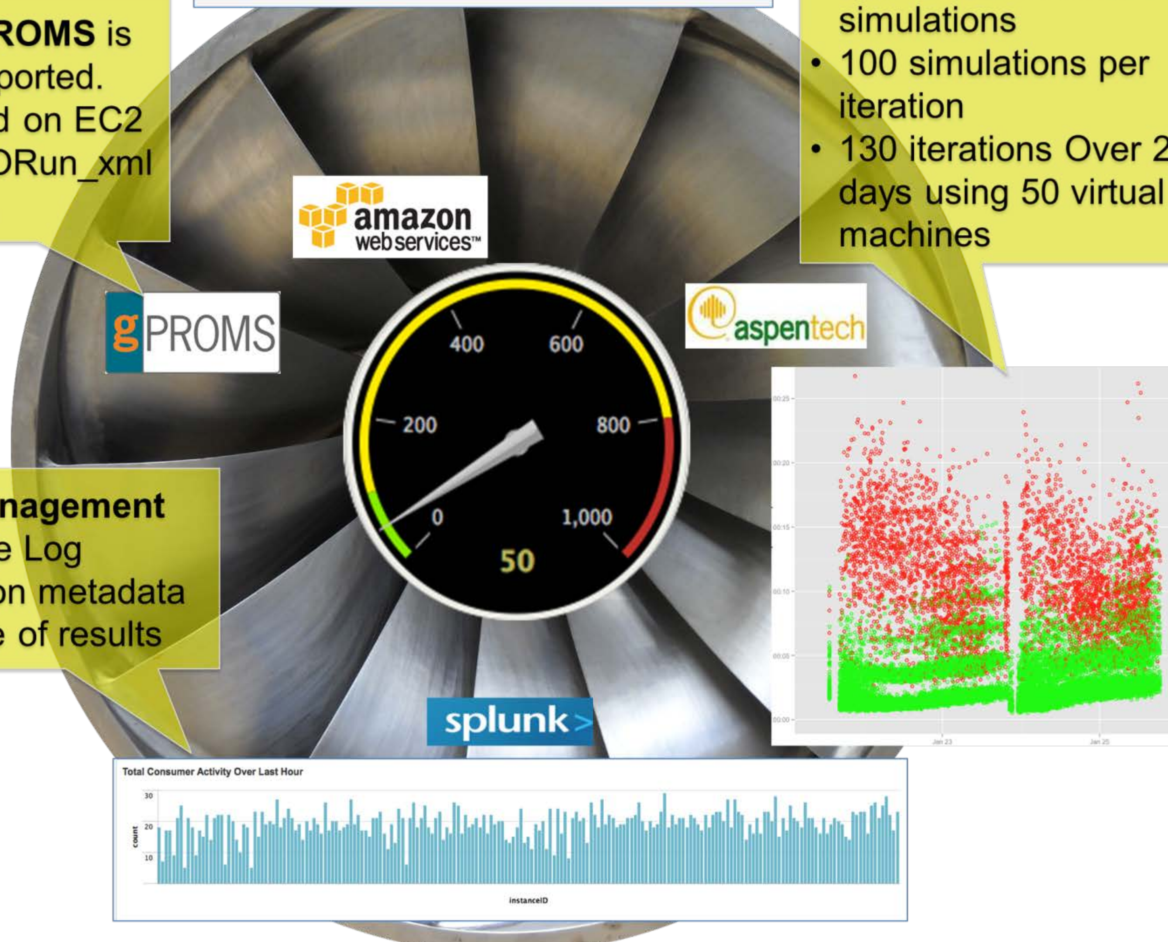
Software Integration

Turbine Science Gateway
Parallel Simulation Execution
Available for local use and
Amazon EC2 Cloud

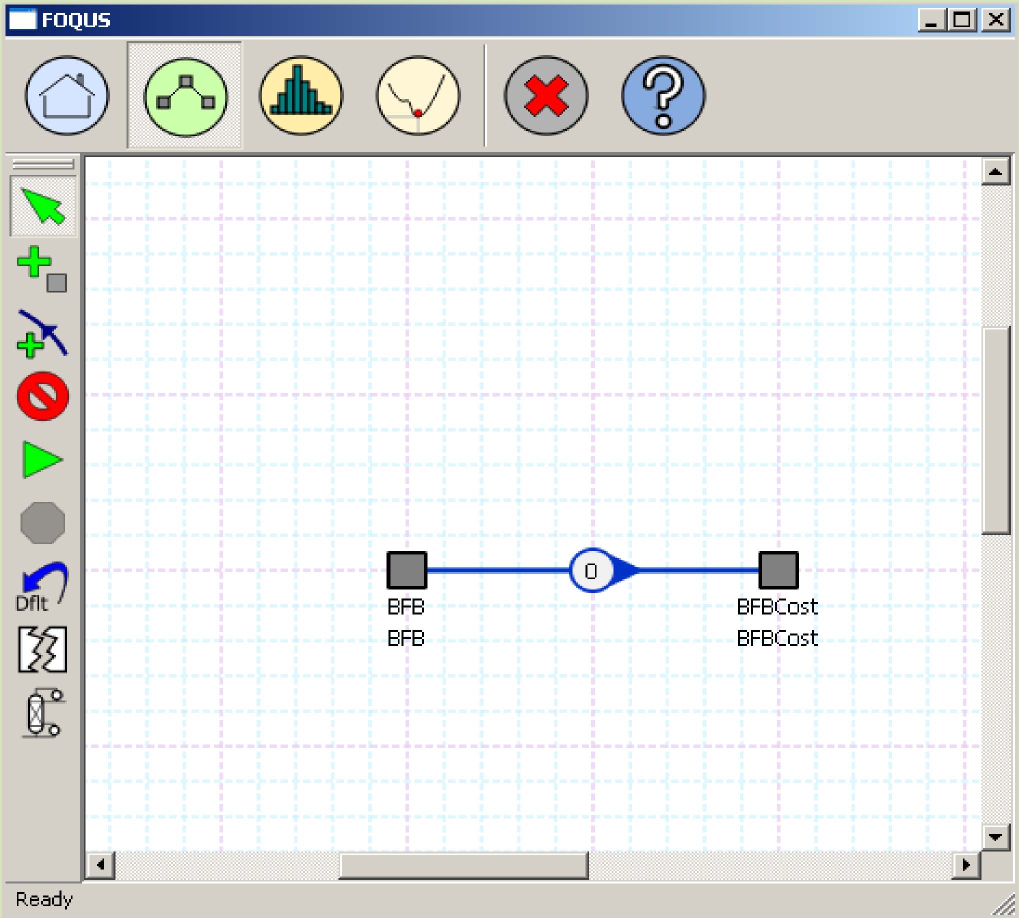
PSE gPROMS is now supported. Deployed on EC2 with 5 gORun_xml licenses

ACM Hybrid Split Optimization
- Experiment ran 13000 simulations
- 100 simulations per iteration
- 130 iterations Over 2 days using 50 virtual machines

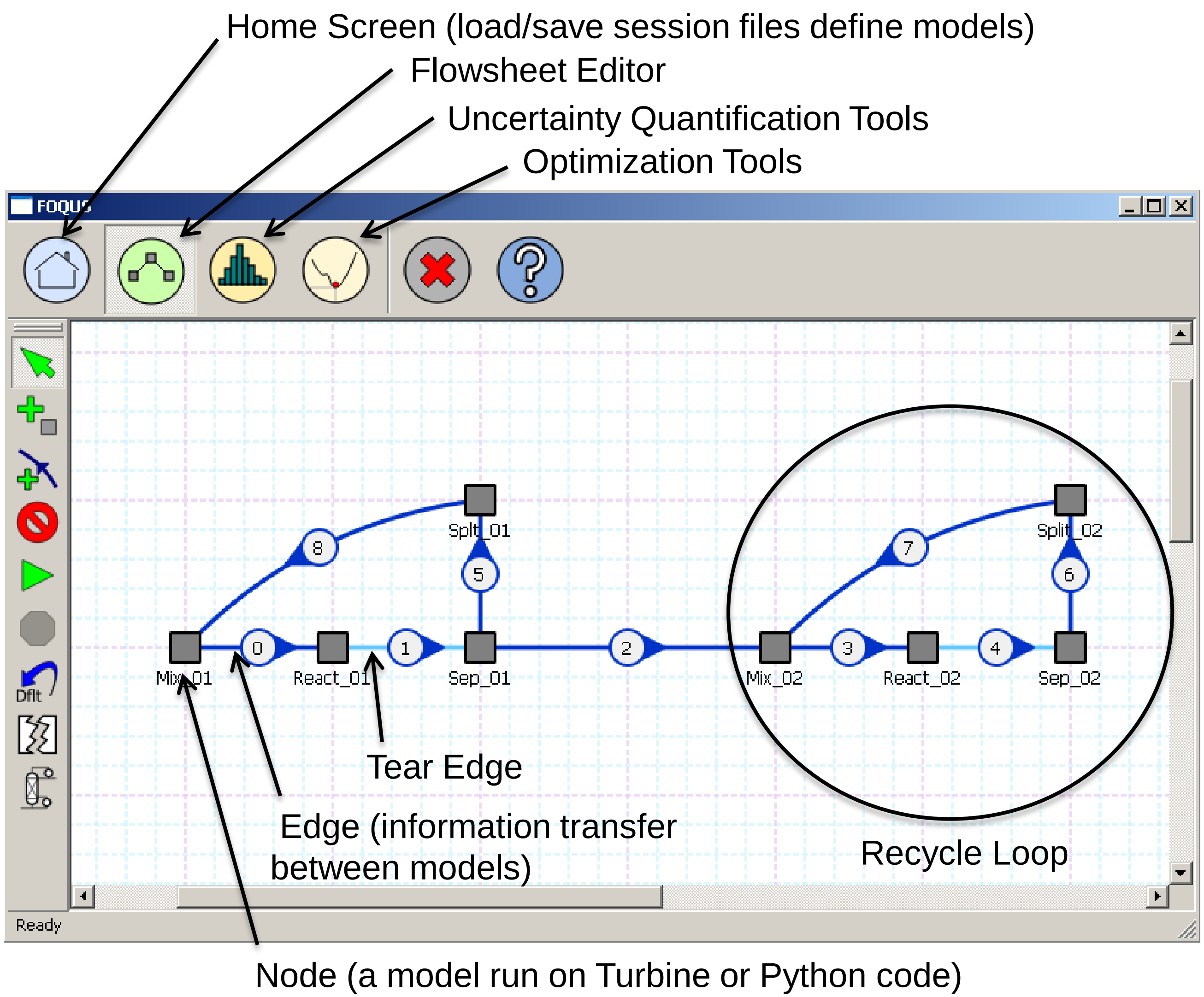
Data Management
Real-time Log
Simulation metadata
database of results



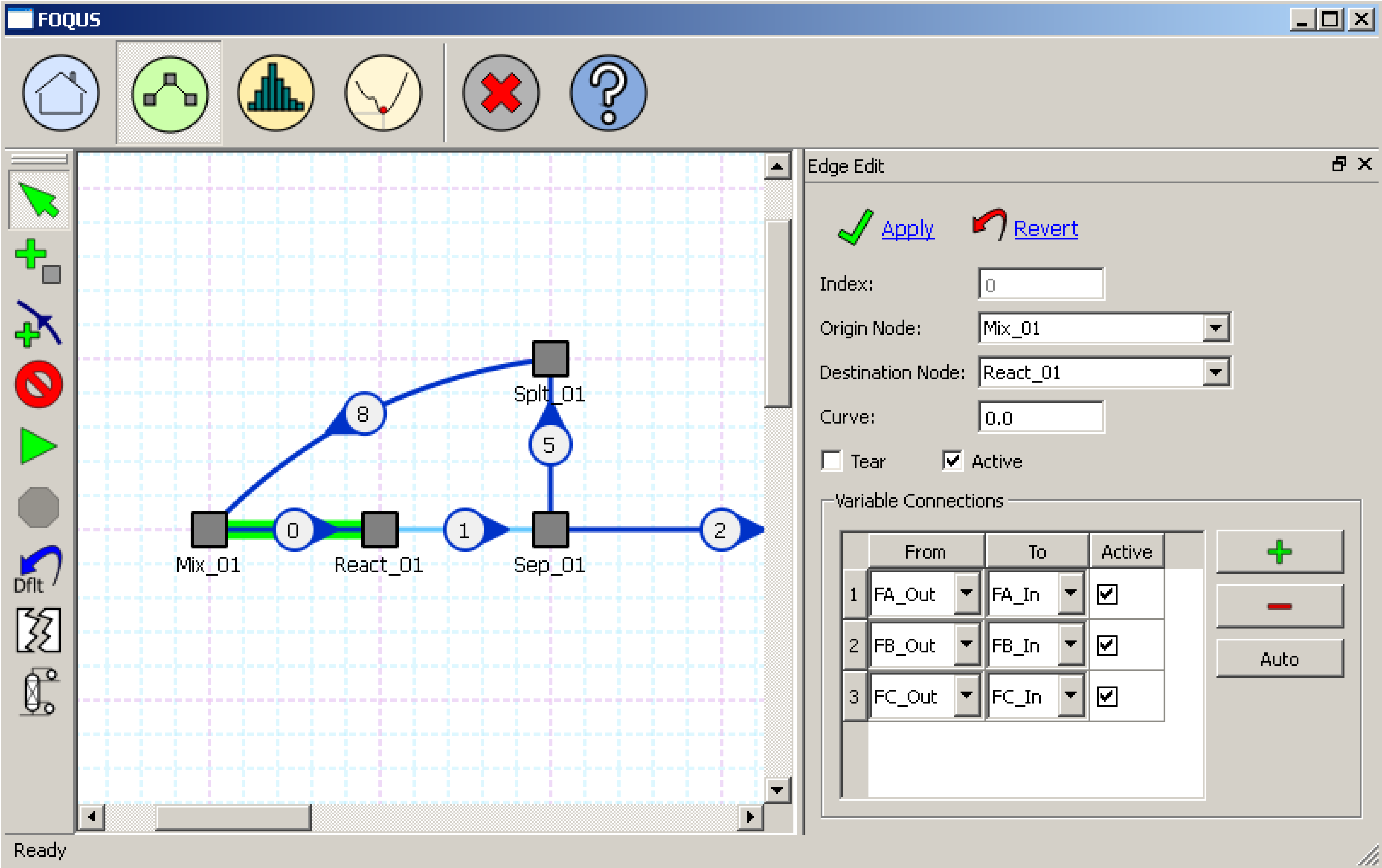
Graphic Interface



Meta-Flowsheet Editor



Information Flow



Optimization Problem Setting

Solver selection and parameters

Select decision variables

Variable Scaling Method
input variables are scaled
to be 0 at min and 10 at max

Min/Max constraints

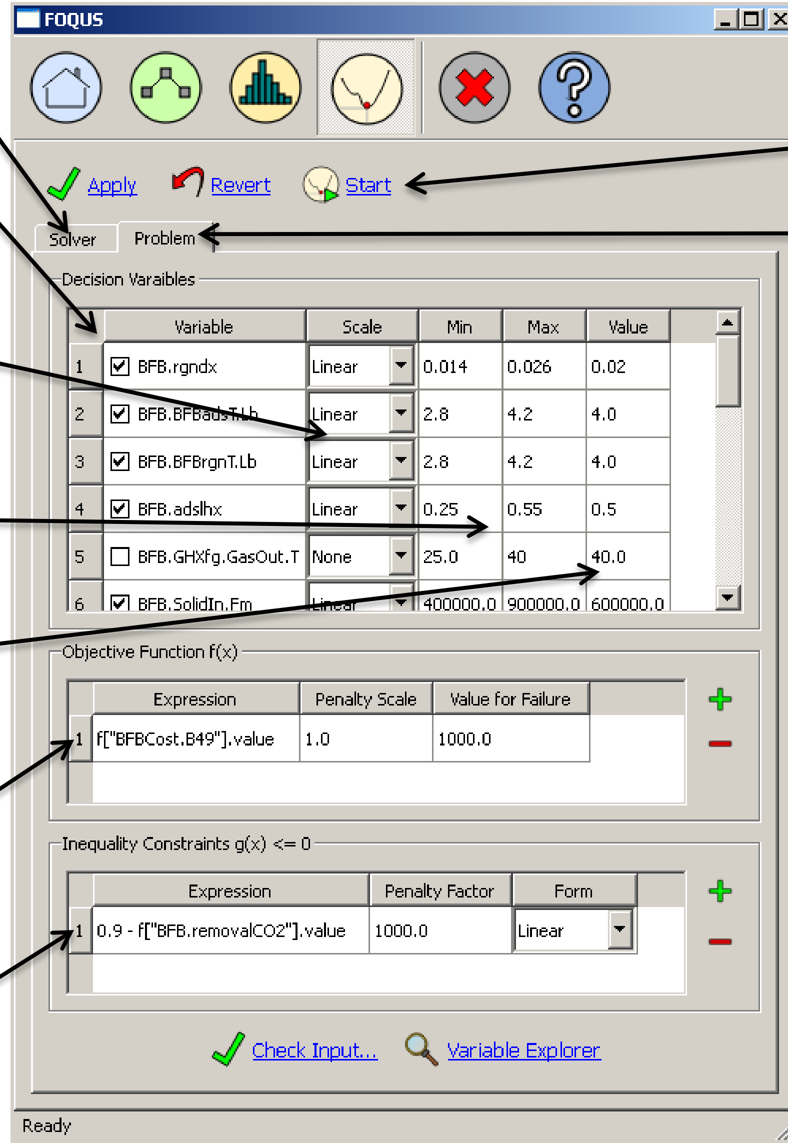
Current Value
(initial guess)

Objective function
Python expression

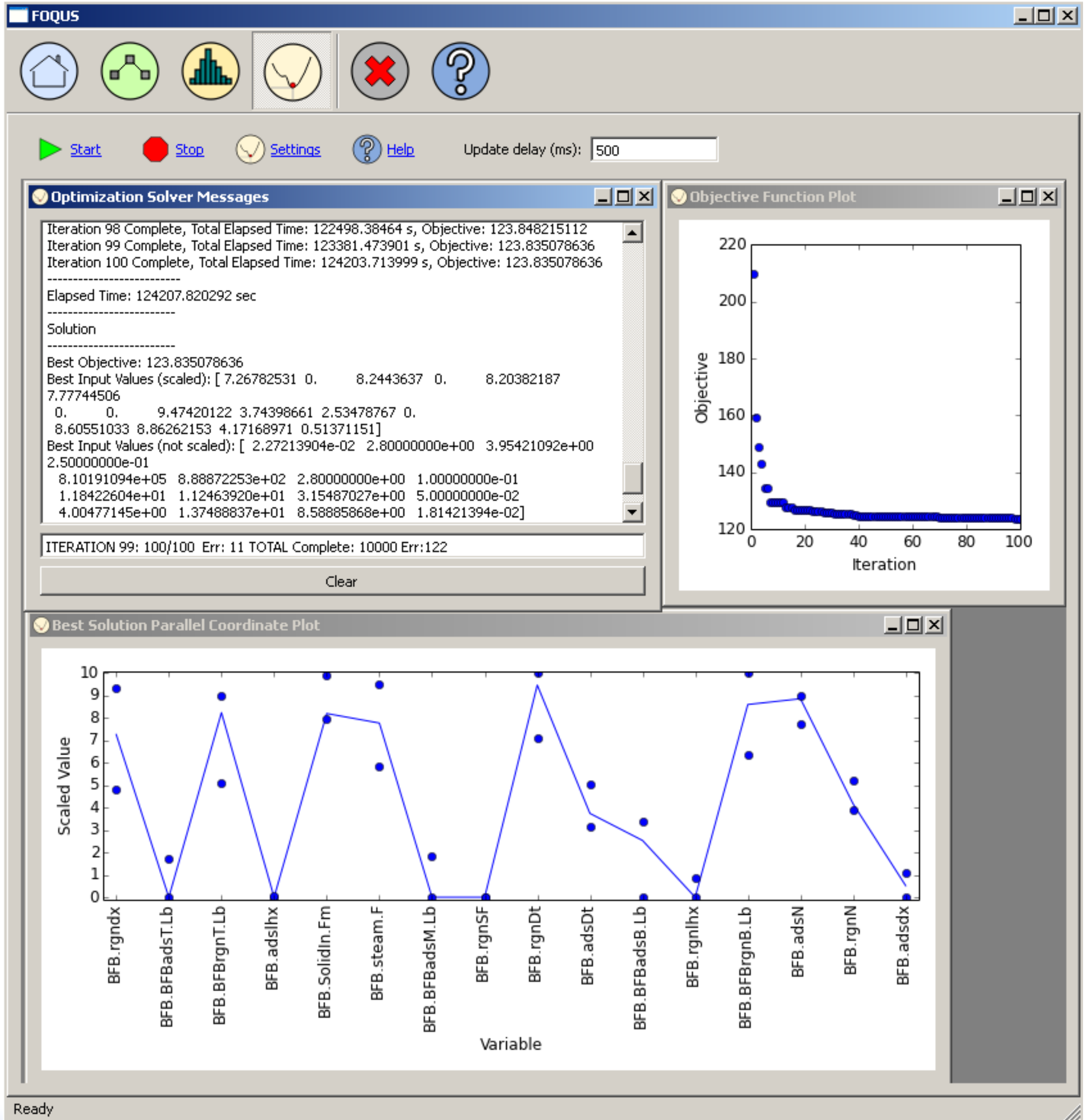
Inequality constraint
Python expression
(enforced with penalty)

Start/Monitor Optimization

Problem Definition



Optimization Monitor



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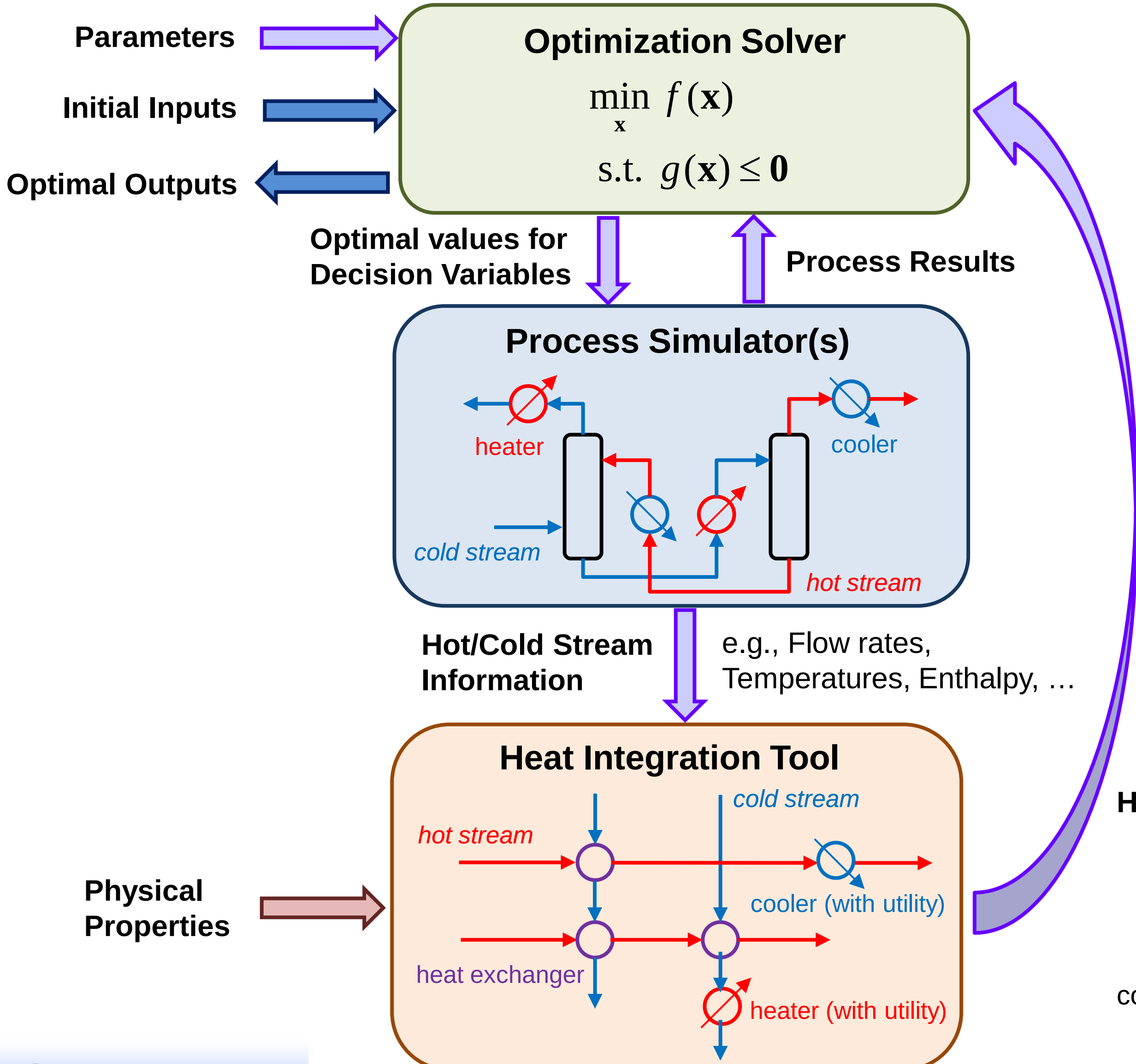
Simulation-Based Optimization with Heat Integration



Simultaneous process optimization and heat integration are achieved in this framework

Heat Integration Results:

- Hot/cold utility consumptions
- Minimum utility cost
- Minimum number of heat exchangers
- Optimal matches between hot and cold streams

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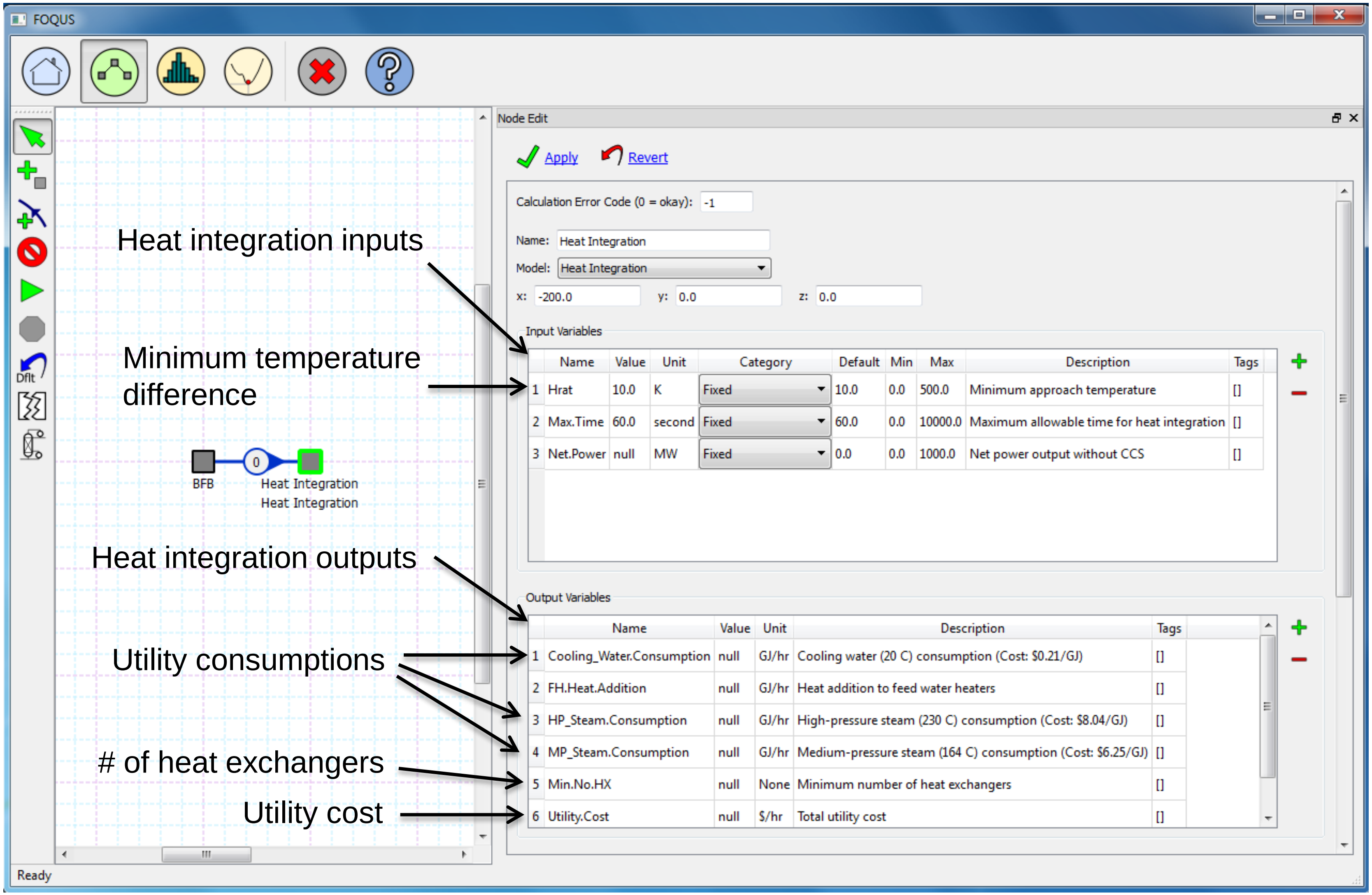
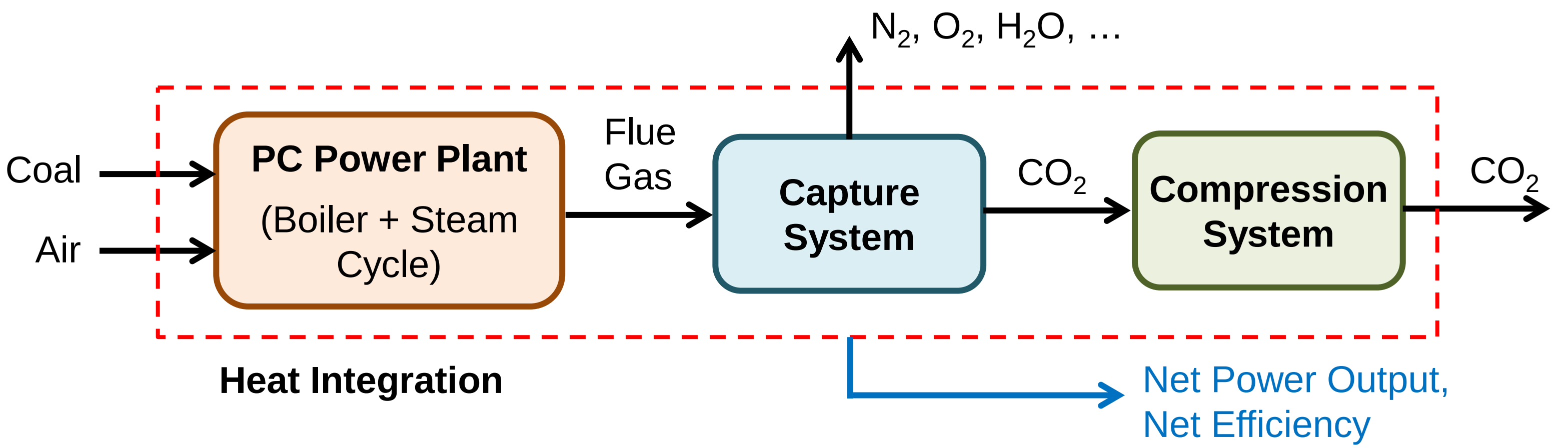
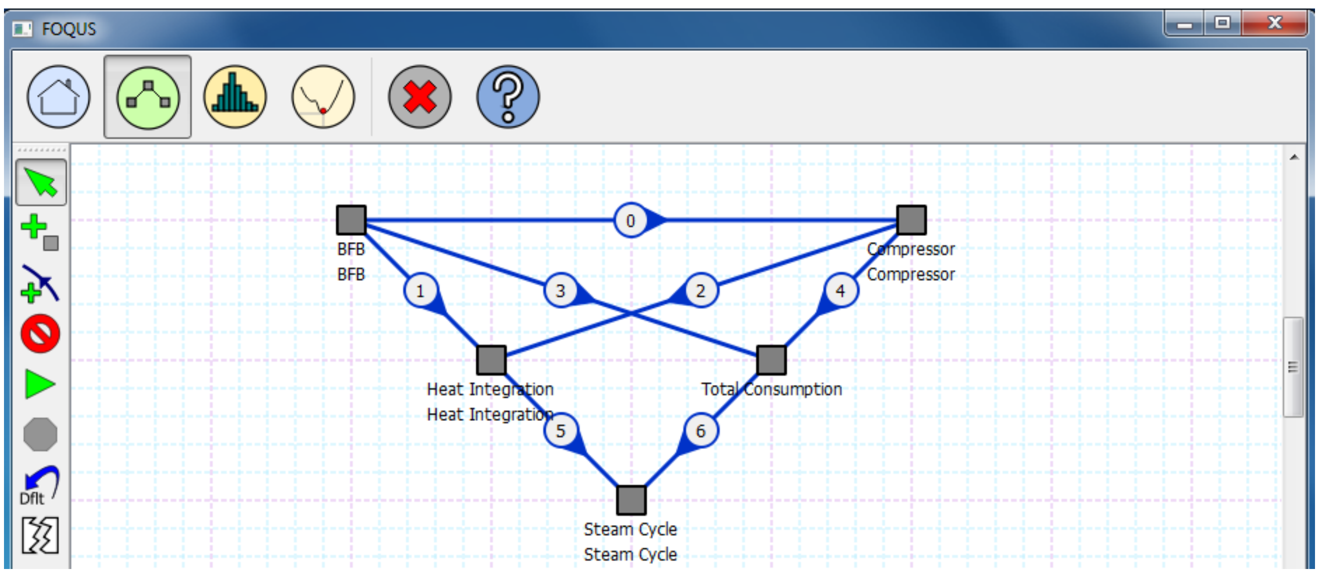
Heat Integration Interface



Case Study



N_2, O_2, H_2O, …
Coal
Air
PC Power Plant
(Boiler + Steam Cycle)
Flue Gas
Capture System
CO_2
Compression System
CO_2
Heat Integration
Net Power Output,
Net Efficiency



FOQUS
BFB
BFB
Compressor
Compressor
Heat Integration
Heat Integration
Total Consumption
Steam Cycle
Steam Cycle
Dflt
0
1
2
3
4
5
6

Case Study Results

Objective Function: Maximizing Net Efficiency

Constraint: CO_2 Removal Ratio ≥ 90%

	Net Efficiency (%)	CO_2 Removal Ratio (%)
w/o CCS		
Base Case	42.1	0.0
with CCS but w/o Heat Integration		
Base Case	26.7	91.3
Optimal Solution	28.6	90.9
with CCS and Heat Integration		
Base Case	28.7	91.5
Optimal Solution	**29.9**	91.0

Optimization and heat integration significantly increased net efficiency of power plant with CCS.

Software: FOQUS

Framework for Optimization and Quantification of Uncertainty and Sensitivity

- Builds on Sinter and the Turbine Gateway
- Common framework for model execution
  - simulation based optimization
  - uncertainty quantification (UQ)
  - steady state reduced model building (coming soon)

More information: https://www.acceleratecarboncapture.org

Conclusions and Future Work

Conclusions

- Simulation-based optimization framework is a suitable tool for optimization of large-scale high-fidelity process models.
- Multiple simulation and optimization software are incorporated so that different units or subsystems in the process can be modeled in different simulators.
- Performance of power plant with CCS can be significantly increased by optimization and heat integration.

Future Work

- Add more process simulators and optimization solvers into the framework.
- Allow parallel computing for heat integration.

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DOE: Carbon Capture Simulation Initiative (CCSI)

Disclaimer