

CCSI

Carbon Capture Simulation Initiative

Simulation-Based Optimization Framework with Heat Integration

Yang Chen^a, John Eslick^a, Ignacio Grossmann^a, David Miller^b

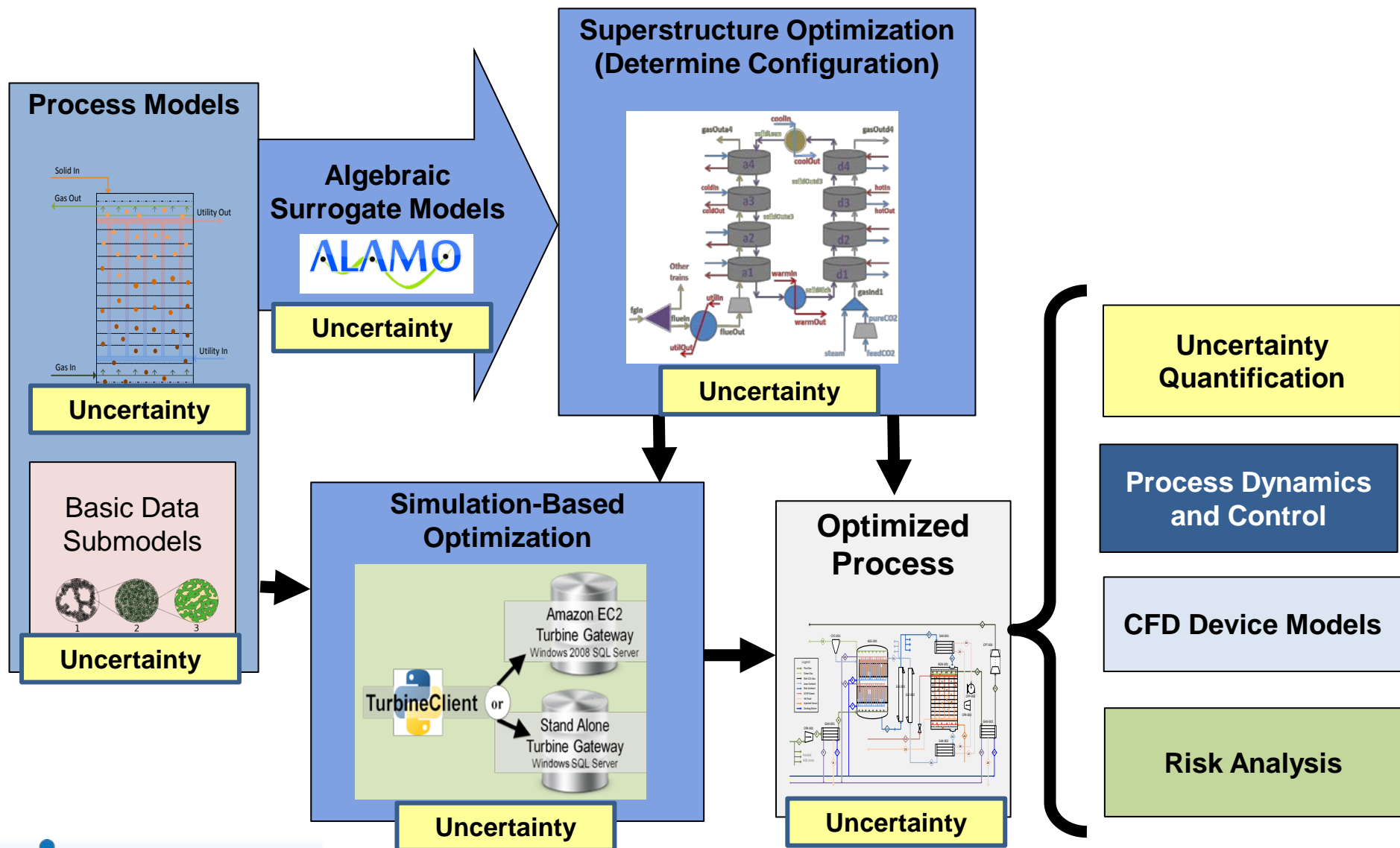
a. Dept. of Chemical Engineering, Carnegie Mellon University

b. DOE, National Energy Technology Laboratory

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Tools to Develop an Optimized Process using Rigorous Models

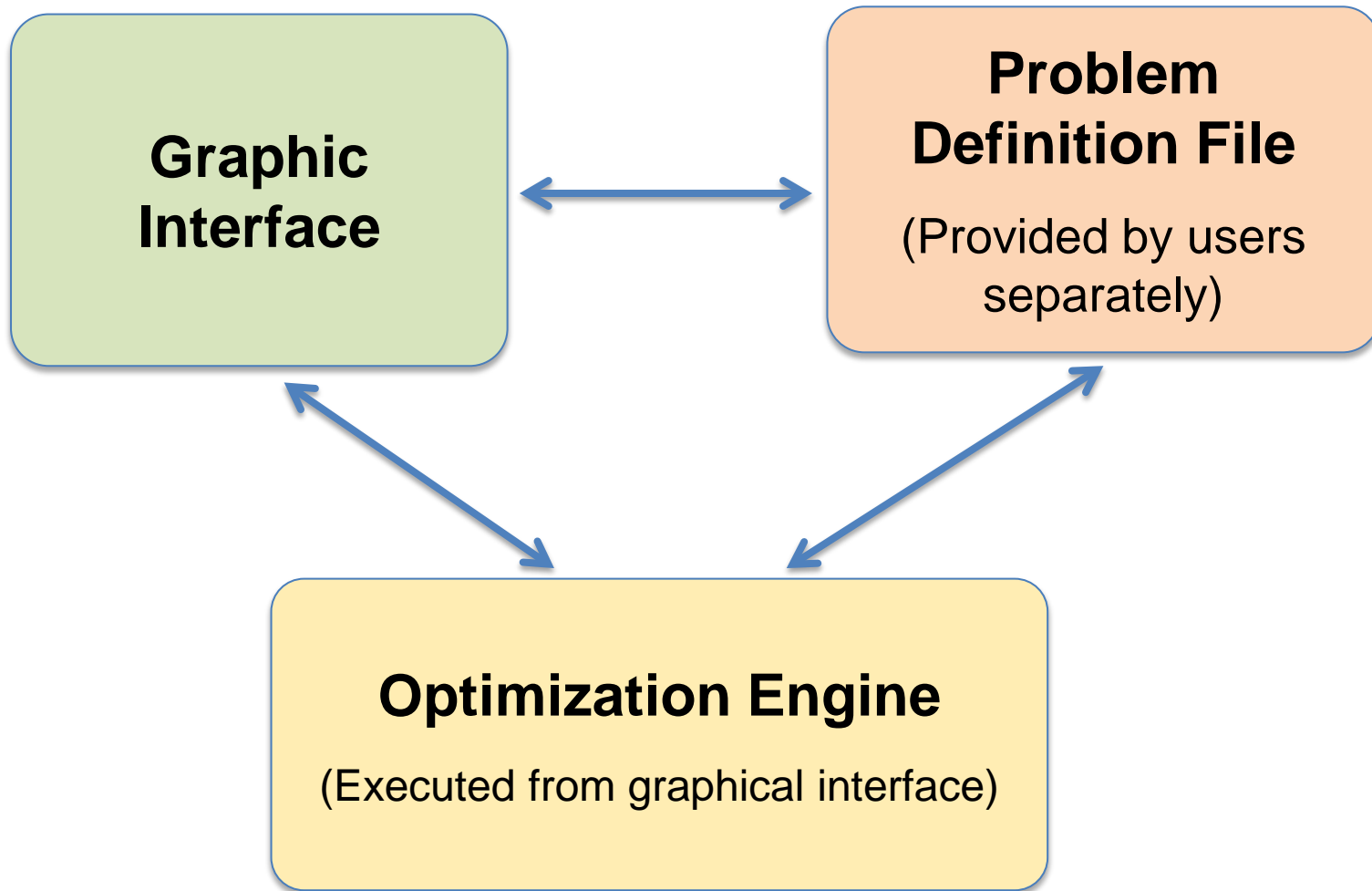


Simulation-Based Optimization

- + 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

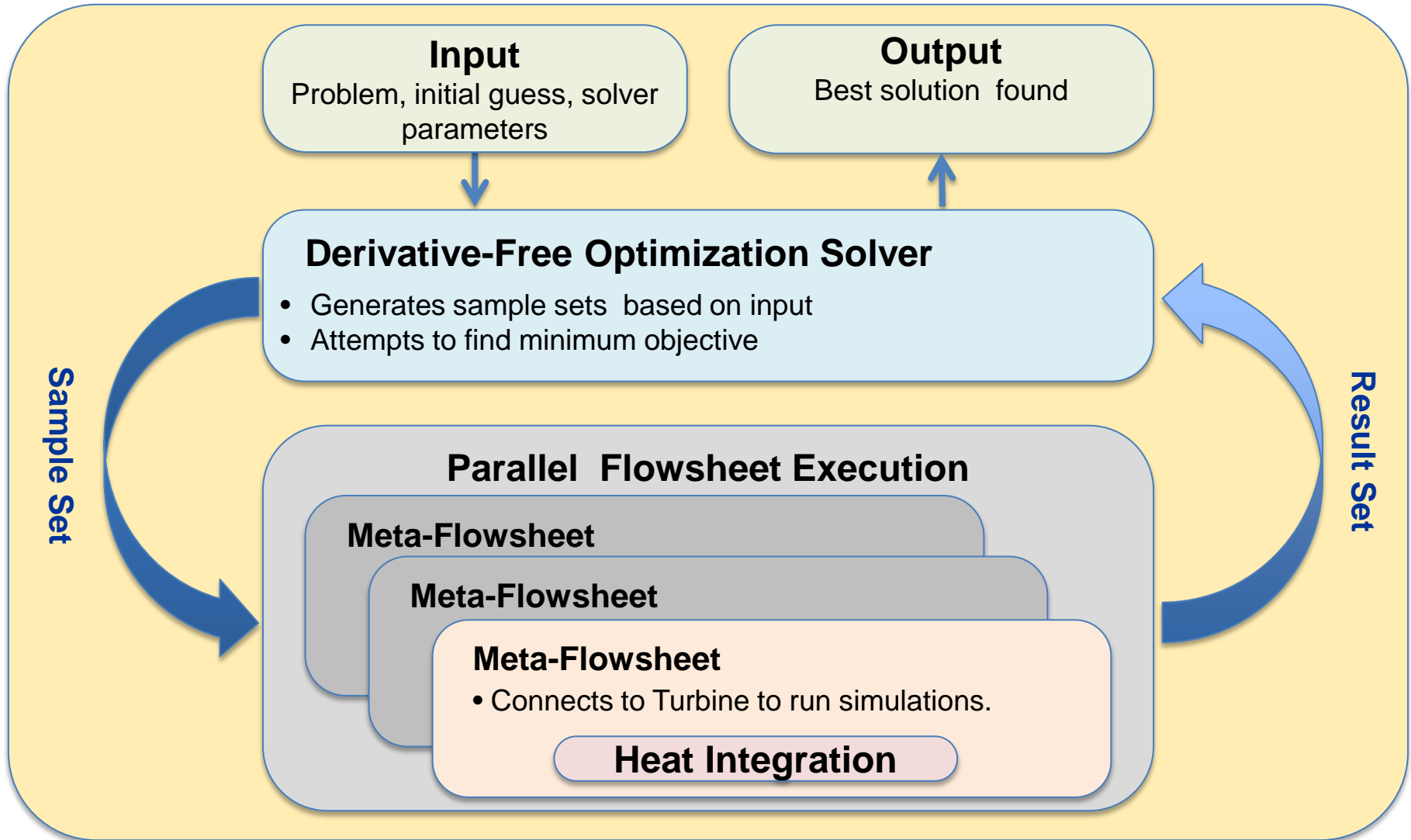
Model Settings

- 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

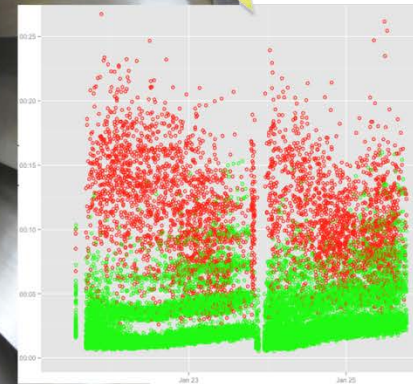
ACM Hybrid Split Optimization

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

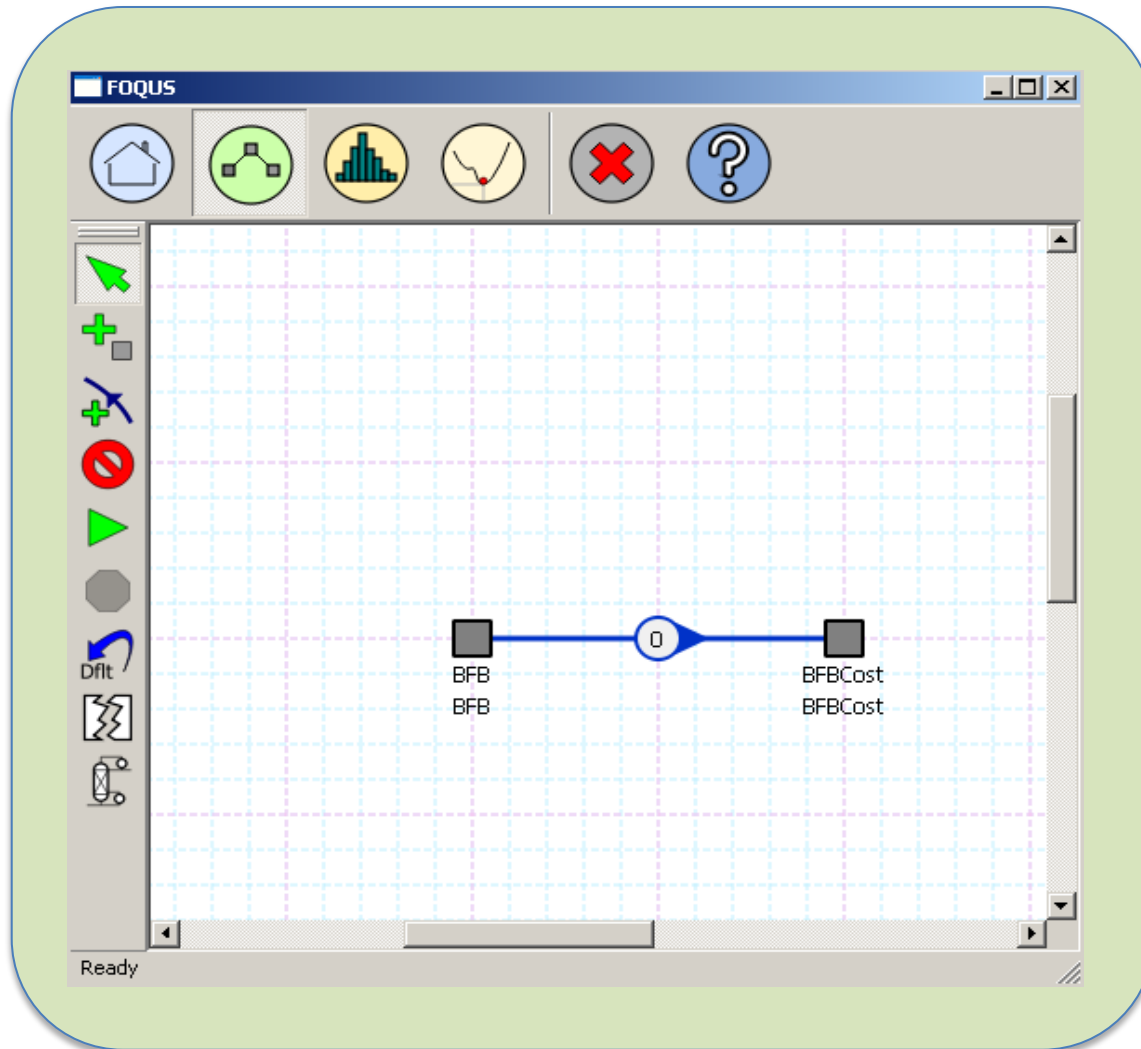
PSE gPROMS is now supported.
Deployed on EC2 with 5 gORun_xml licenses



Data Management
Real-time Log
Simulation metadata
database of results



Graphic Interface



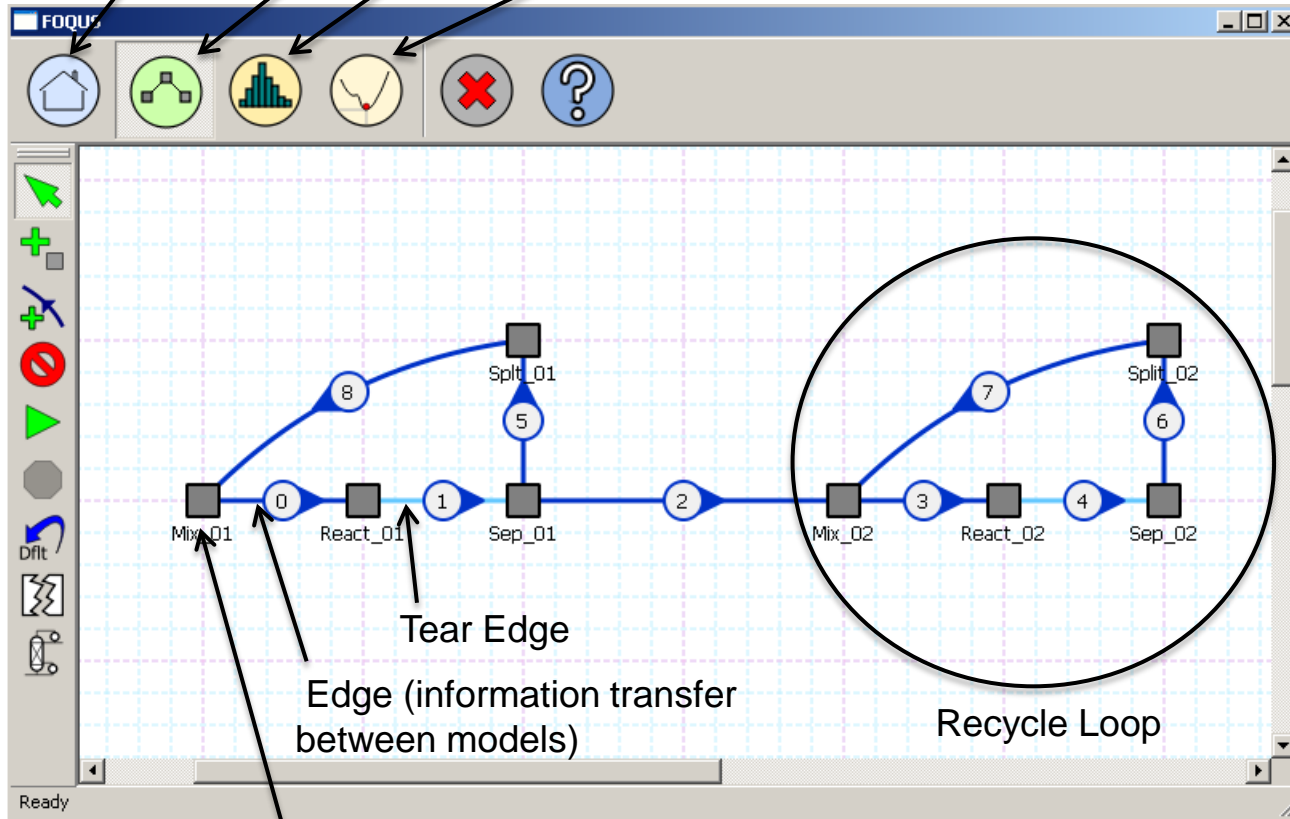
Meta-Flowsheet Editor

Home Screen (load/save session files define models)

Flowsheet Editor

Uncertainty Quantification Tools

Optimization Tools



Node (a model run on Turbine or Python code)

Information Flow

The screenshot displays the FOQUS software interface. The main workspace shows a process flow diagram on a grid background. The diagram includes several nodes: Mix_01, React_01, Sep_01, and Splt_01. Edges connect these nodes, with some edges labeled with numbers (0, 1, 2, 5, 8). The status bar at the bottom left indicates 'Ready'.

The 'Edge Edit' panel on the right side of the interface is active, showing the following configuration:

- Apply** (checked) and **Revert** (unchecked) buttons.
- Index:** 0
- Origin Node:** Mix_01
- Destination Node:** React_01
- Curve:** 0.0
- Tear:** (unchecked)
- Active:** (checked)

The 'Variable Connections' table in the Edge Edit panel is as follows:

	From	To	Active
1	FA_Out	FA_In	<input checked="" type="checkbox"/>
2	FB_Out	FB_In	<input checked="" type="checkbox"/>
3	FC_Out	FC_In	<input checked="" type="checkbox"/>

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)

Variable	Scale	Min	Max	Value
<input checked="" type="checkbox"/> BFB.rgndx	Linear	0.014	0.026	0.02
<input checked="" type="checkbox"/> BFB.BFBads.T.Lb	Linear	2.8	4.2	4.0
<input checked="" type="checkbox"/> BFB.BFBrgn.T.Lb	Linear	2.8	4.2	4.0
<input checked="" type="checkbox"/> BFB.adslhx	Linear	0.25	0.55	0.5
<input type="checkbox"/> BFB.GHXfg_GasOut.T	None	25.0	40	40.0
<input checked="" type="checkbox"/> BFB.SolidIn.Fm	Linear	400000.0	900000.0	600000.0

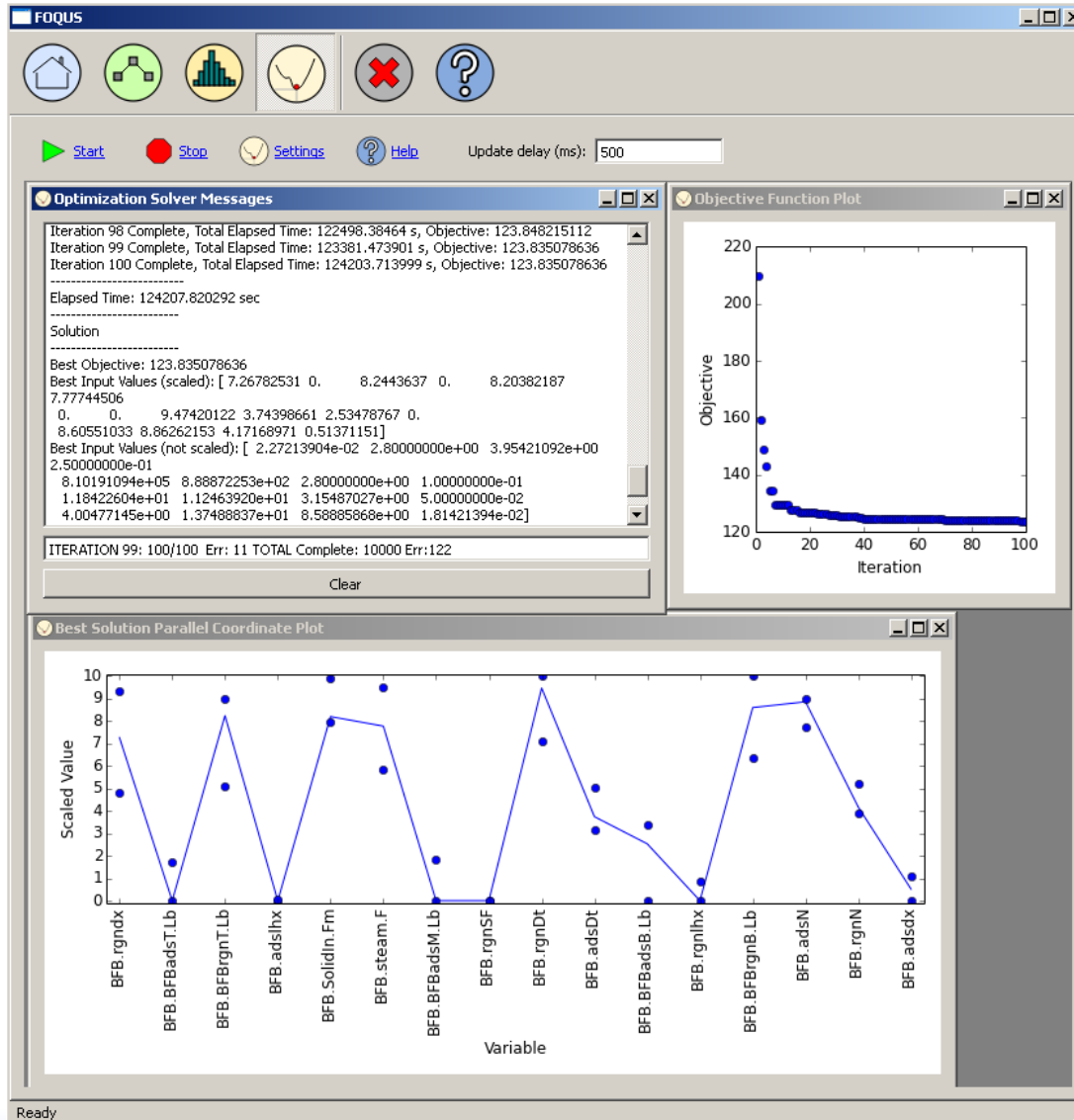
Expression	Penalty Scale	Value for Failure
1 f["BFBCost.B49"].value	1.0	1000.0

Expression	Penalty Factor	Form
1 0.9 - f["BFB.removalCO2"].value	1000.0	Linear

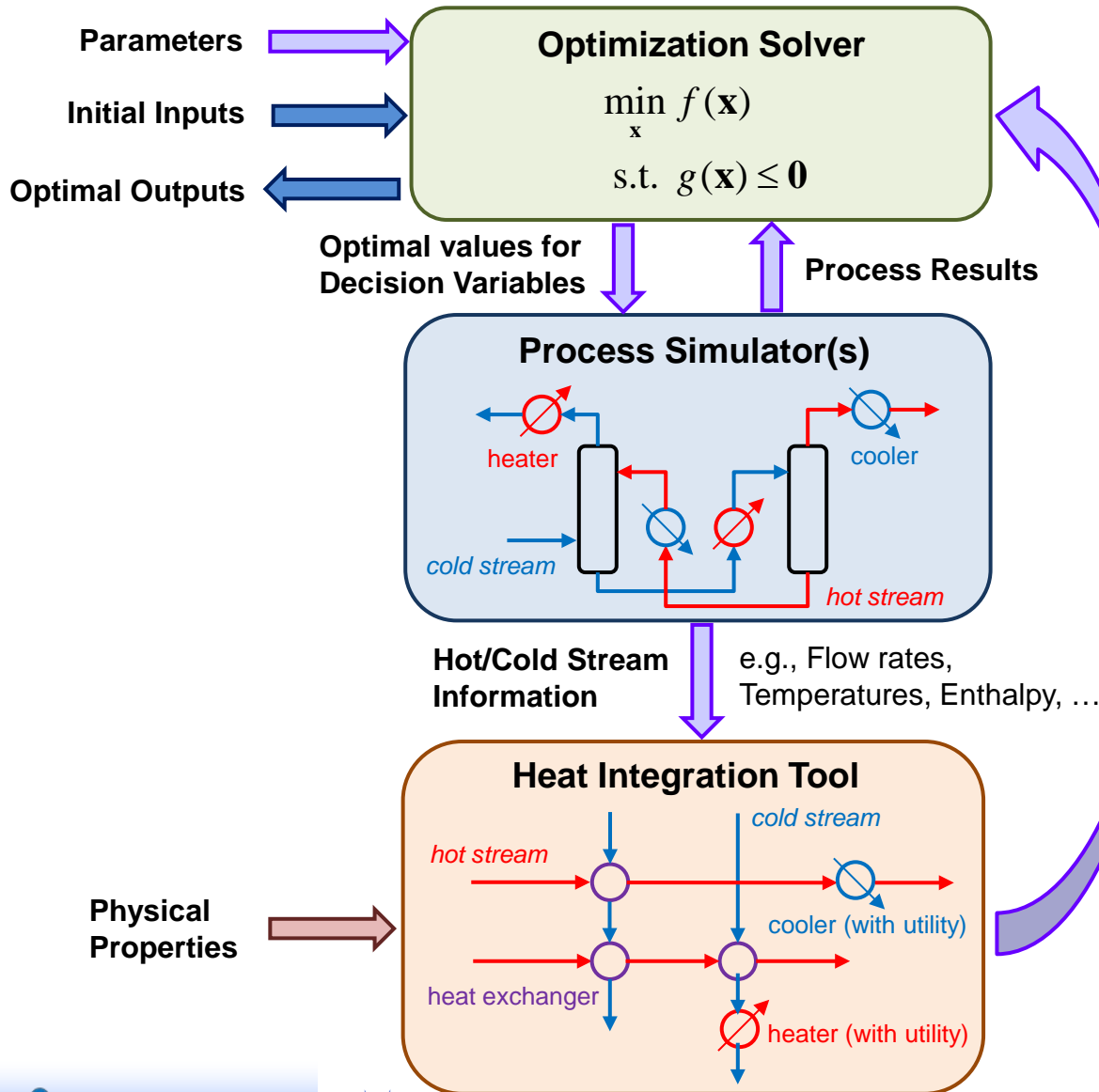
Start/Monitor Optimization

Problem Definition

Optimization Monitor



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

Heat Integration Interface

The screenshot shows the FOQUS software interface. On the left is a process flow diagram with a BFB unit and two Heat Integration units. On the right is the 'Node Edit' window for the 'Heat Integration' node. The window includes a 'Node Edit' title bar, 'Apply' and 'Revert' buttons, a 'Calculation Error Code' field, and two tables: 'Input Variables' and 'Output Variables'.

Heat integration inputs (indicated by an arrow pointing to the 'Input Variables' table)

Minimum temperature difference (indicated by an arrow pointing to the 'Hrat' row in the 'Input Variables' table)

Heat integration outputs (indicated by an arrow pointing to the 'Output Variables' table)

Utility consumptions (indicated by an arrow pointing to the 'Cooling_Water.Consumption' row in the 'Output Variables' table)

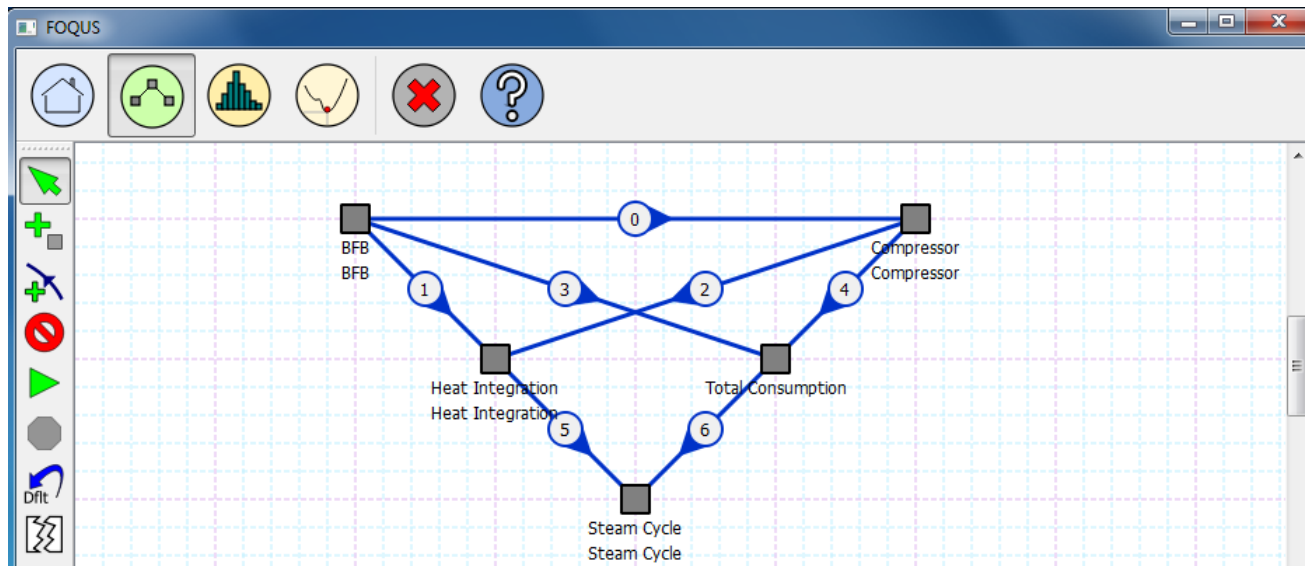
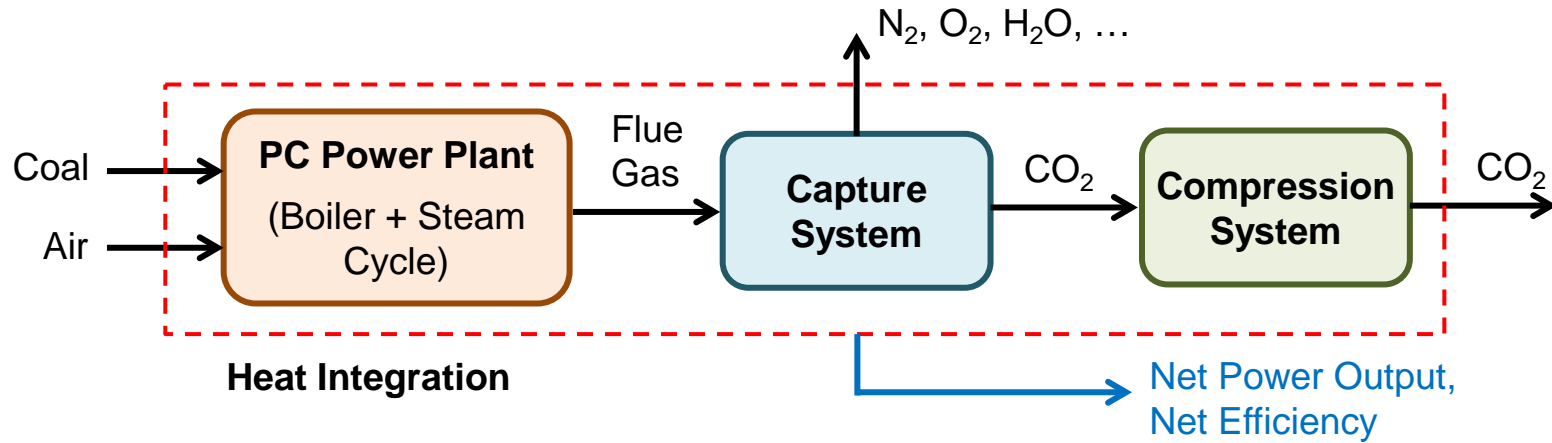
of heat exchangers (indicated by an arrow pointing to the 'Min.No.HX' row in the 'Output Variables' table)

Utility cost (indicated by an arrow pointing to the 'Utility.Cost' row in the 'Output Variables' table)

Name	Value	Unit	Category	Default	Min	Max	Description	Tags
Hrat	10.0	K	Fixed	10.0	0.0	500.0	Minimum approach temperature	[]
Max.Time	60.0	second	Fixed	60.0	0.0	10000.0	Maximum allowable time for heat integration	[]
Net.Power	null	MW	Fixed	0.0	0.0	1000.0	Net power output without CCS	[]

Name	Value	Unit	Description	Tags
Cooling_Water.Consumption	null	GJ/hr	Cooling water (20 C) consumption (Cost: \$0.21/GJ)	[]
FH.Heat.Addition	null	GJ/hr	Heat addition to feed water heaters	[]
HP_Steam.Consumption	null	GJ/hr	High-pressure steam (230 C) consumption (Cost: \$8.04/GJ)	[]
MP_Steam.Consumption	null	GJ/hr	Medium-pressure steam (164 C) consumption (Cost: \$6.25/GJ)	[]
Min.No.HX	null	None	Minimum number of heat exchangers	[]
Utility.Cost	null	\$/hr	Total utility cost	[]

Case Study



Case Study Results

Objective Function: Maximizing Net Efficiency

Constraint: CO₂ 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)

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