

Applications in Optimizing Dynamic Systems Under Uncertainty



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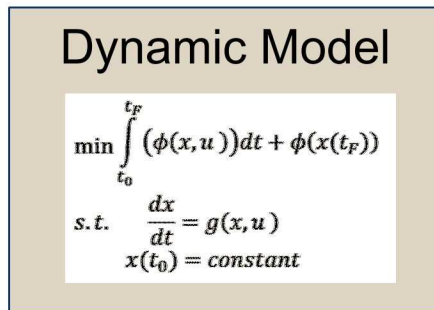
Center for Computing Research
Sandia National Laboratories
Albuquerque, NM

INFORMS Annual Meeting October 20-23, 2019

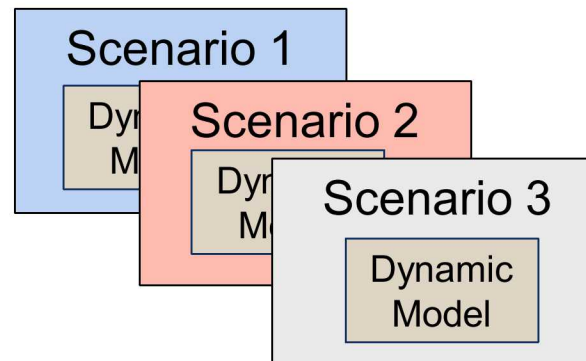
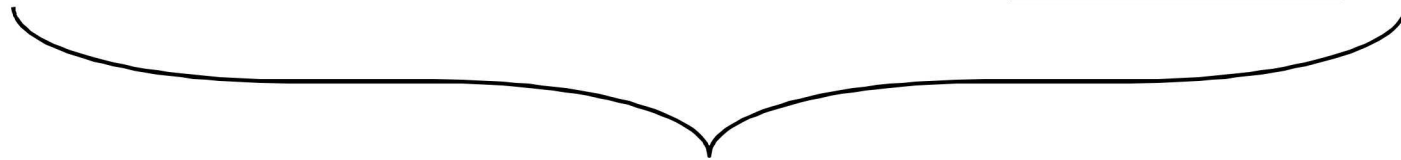
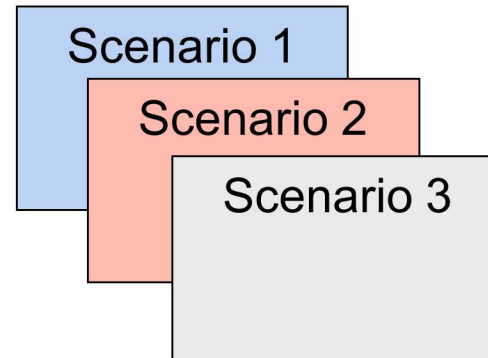


“Dynamic system under uncertainty”

Dynamic Optimization



Stochastic Programming



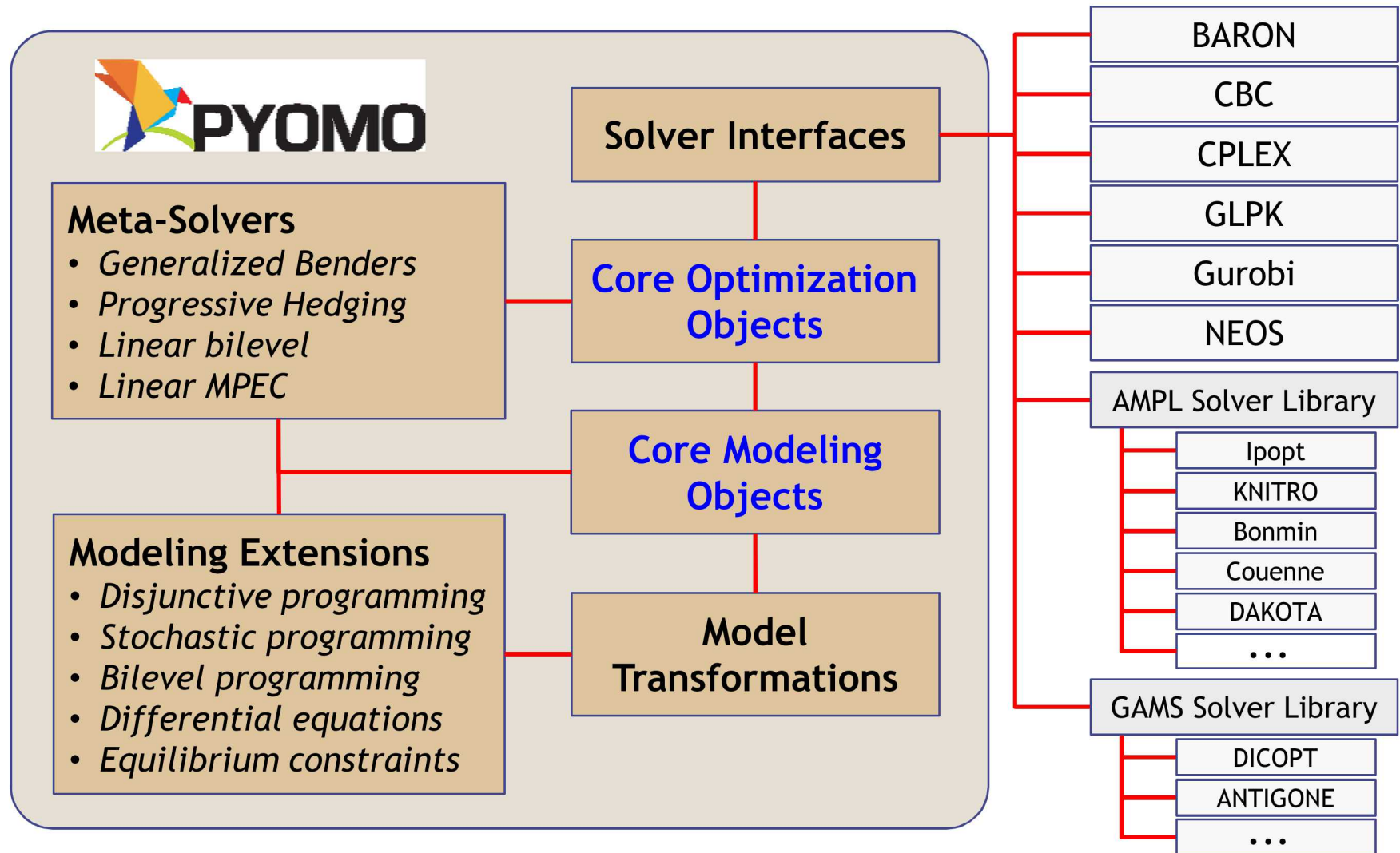
- Pyomo: Python Optimization Modeling Objects
- Formulate optimization models within Python



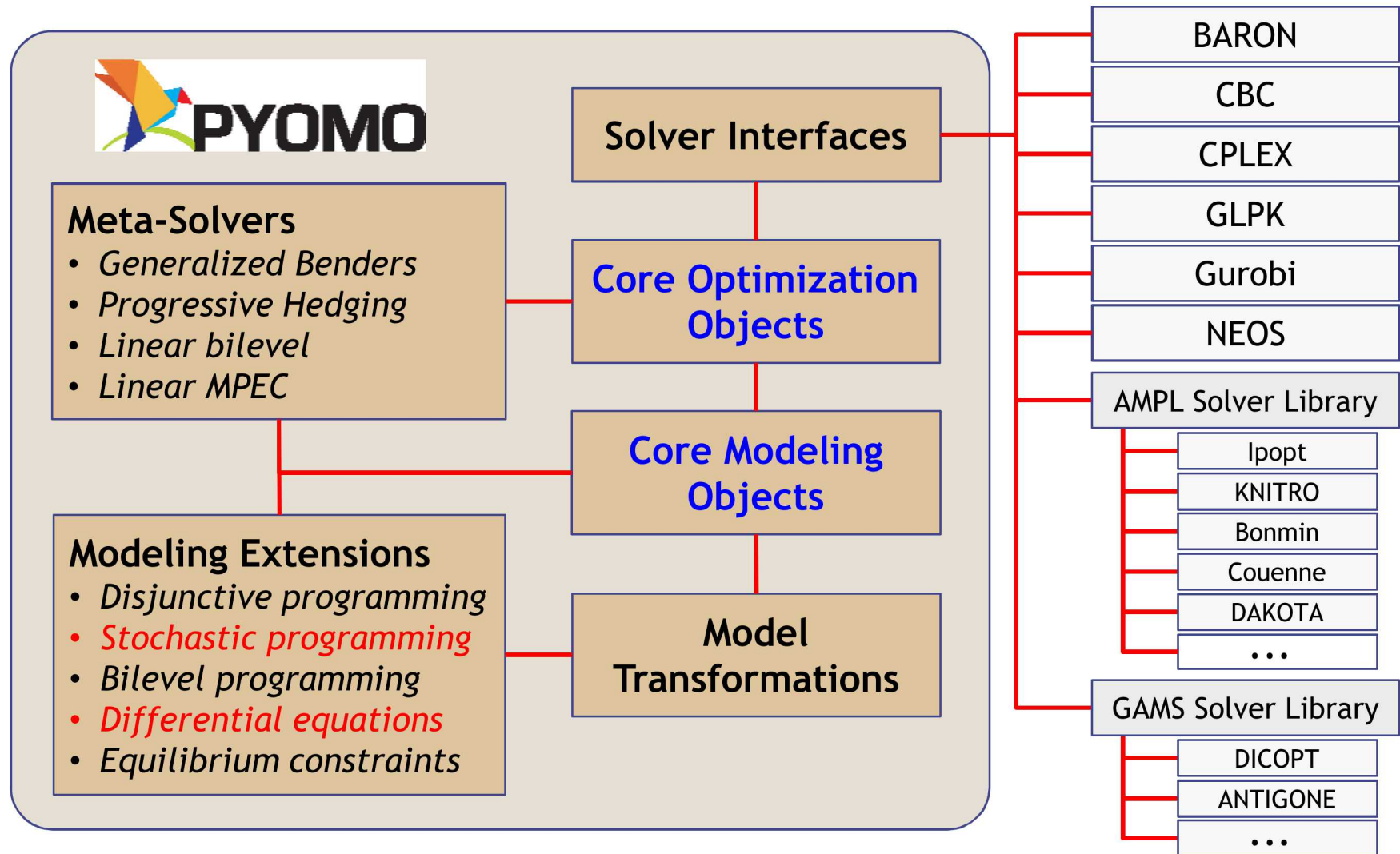
```
from pyomo.environ import *  
m = ConcreteModel()  
m.x1 = Var()  
m.x2 = Var(bounds=(-1,1))  
m.x3 = Var(bounds=(1,2))  
m.obj = Objective(sense = minimize,  
    expr = m.x1**2 + (m.x2*m.x3)**4 + m.x1*m.x3  
    + m.x2 + m.x2*sin(m.x1+m.x3) )
```

- Utilize high-level programming language to write scripts and manipulate model objects
- Leverage third-party Python libraries
e.g. SciPy, NumPy, Matplotlib, Pandas

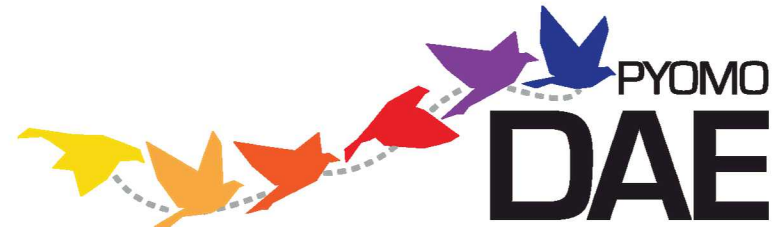
Pyomo at a Glance



Pyomo at a Glance



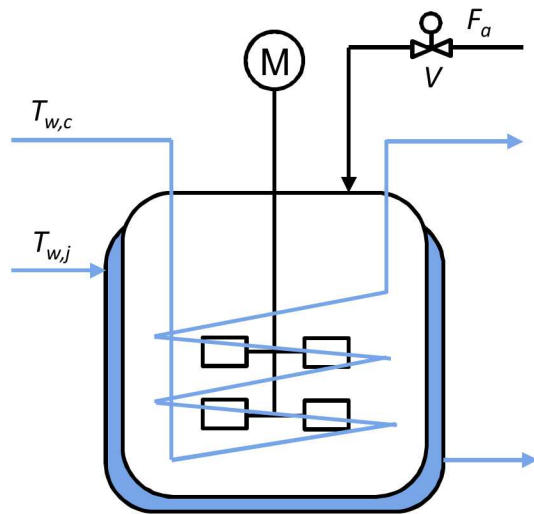
- Extend Pyomo syntax to represent:
 - Continuous domains
 - Ordinary differential equations
 - Partial differential equations
 - Systems of differential algebraic equations
 - Higher order differential equations and mixed partial derivatives
- Available discretization schemes
 - Finite difference methods (Backward/Forward/Central)
 - Collocation (Radau or Legendre roots)
- Extensible framework
 - Write general implementations of custom discretization schemes
 - Build frameworks/meta-algorithms including dynamic optimization
- Interface with numerical simulators
 - Scipy for simulating ODEs
 - CasADi for simulating ODEs and DAEs



- Framework for simplifying implementation of stochastic programming models, only requiring:
 - deterministic base model
 - scenario tree defining the problem stages and uncertain parameters
- PySP provides two primary solution strategies
 - build and solve the deterministic equivalent (extensive form)
 - Progressive Hedging
 - (plus beta implementations of others, including 2-stage Benders and an interface to DDSIP)
- Parallel infrastructure for generating and solving subproblems on parallel (distributed) computing platforms

Dynamic system under uncertainty

■ Semibatch reactor^[2]



Model inputs (control variables)

F_a : Inlet flow rate of A

$T_{w,c}$: Water temperature in cooling coil

$T_{w,j}$: Water temperature in cooling jacket

$$\dot{C}_a = \frac{F_a}{V_r} - k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a$$

$$\dot{C}_b = k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a - k_2 \exp\left(-\frac{E_2}{RT_r}\right) C_b$$

$$\dot{C}_c = k_2 \exp\left(-\frac{E_2}{RT_r}\right) C_b$$

$$\dot{V}_r = \frac{F_a M_{W_a}}{\rho_r}$$

$$(\rho_r c_{p_r}) \dot{T}_r = \frac{F_a M_{W_a} c_{p_r}}{V_r} (T_f - T_r)$$

$$- k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a \Delta H_1 - k_2 \exp\left(-\frac{E_2}{RT_r}\right) C_b \Delta H_2$$

$$+ \alpha_{w,j} \frac{A_j}{V_{r,0}} (T_{w,j} - T_r) + \alpha_{w,c} \frac{A_c}{V_{r,0}} (T_{w,c} - T_r)$$

Dynamic model implementation

```

from pyomo.environ import *
from pyomo.dae import *

def build_semibatch_model(data):

    m = ConcreteModel()

    # Continuous time domain
    m.t = ContinuousSet(bounds=(0,21600), initialize=m.measT)

    # Other variable/parameter/constraint declarations
    ...

    # Differential Variable
    m.Ca = Var(m.t)
    m.dCa = DerivativeVar(m.Ca)

    # Differential equation
    def _dCacon(m,t):
        if t == 0:
            return Constraint.Skip
        return m.dCa[t] == m.Fa[t]/m.Vr[t] - \
            m.k1*exp(-m.E1/(m.R*m.Tr[t]))*m.Ca[t]
    m.dCa = Constraint(m.t, rule=_dCacon)

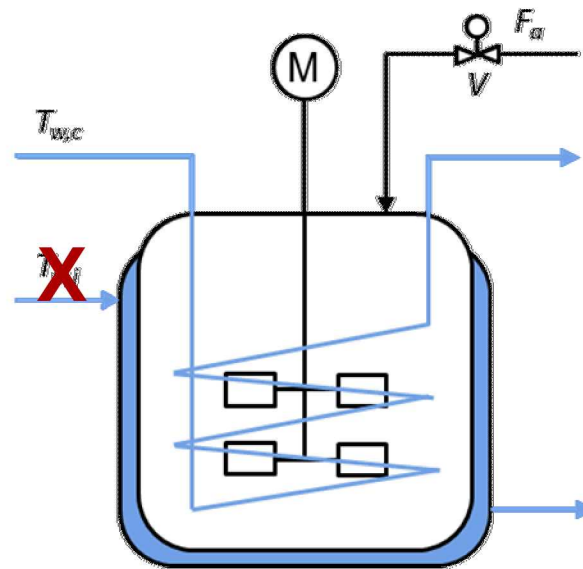
    # Automatically apply collocation over finite elements discretization
    discretizer = TransformationFactory('dae.collocation')
    discretizer.apply_to(m, nfe=20, ncp=4)

    return m

```

$$\dot{C}_a = \frac{F_a}{V_r} - k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a$$


- Find the nominal control profiles such that the batch can be 'saved' given a partial cooling system failure at any point during the batch time^[2]



$$\left. \begin{aligned} T_{w,j}(t) &= T_{w,c}(t) & t &\leq t_{fail} \\ (\rho_w C_{p_w} V_j) \dot{T}_{w,j} &= \alpha_{w,j} A_j \frac{V_r}{V_{r,0}} (T_{w,j} - T_r) & t &> t_{fail} \end{aligned} \right\}$$

Optimal control scenarios

Nonanticipativity Constraints

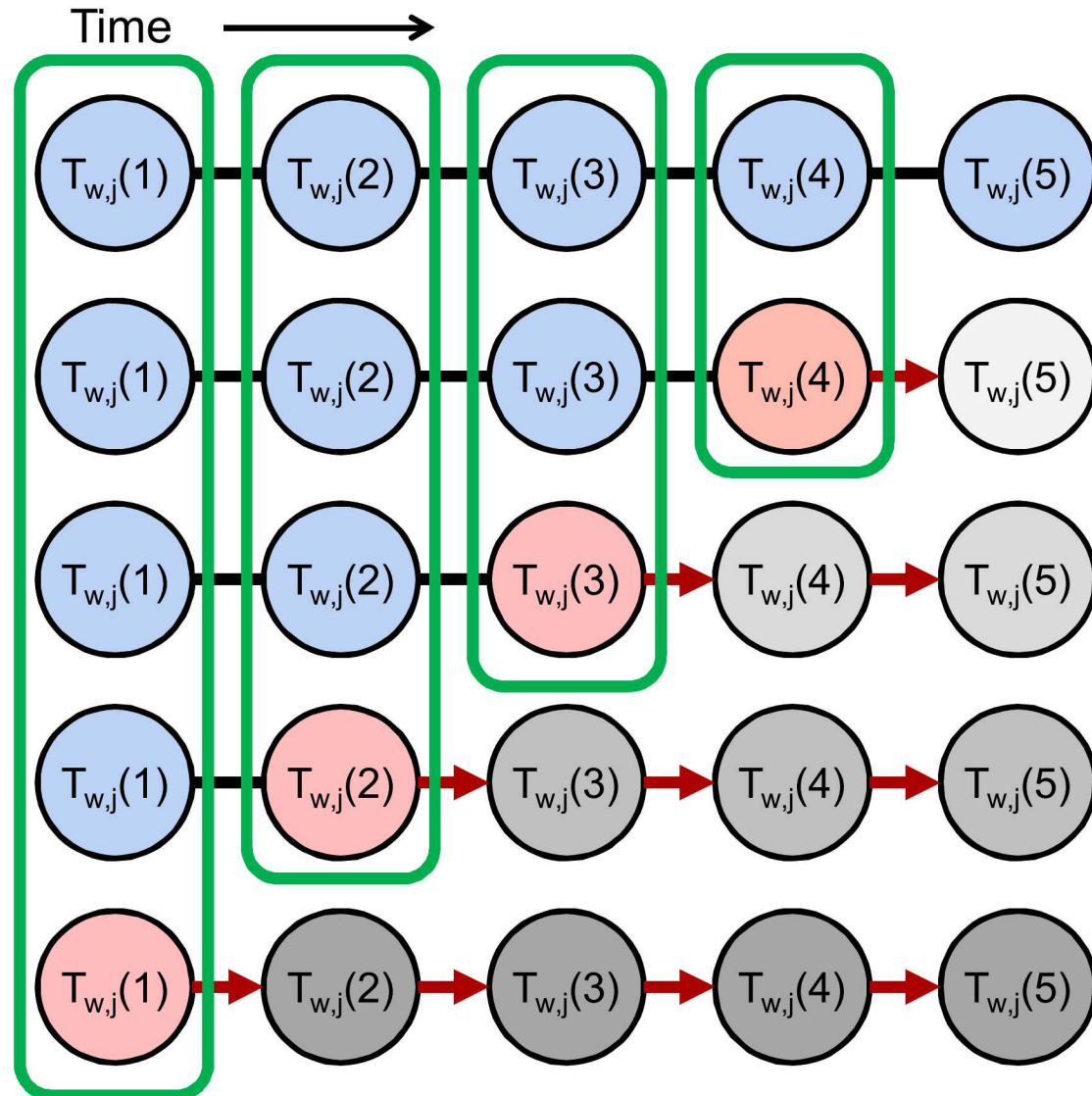
Nominal

$t_{\text{fail}} = 4$

$t_{\text{fail}} = 3$

$t_{\text{fail}} = 2$

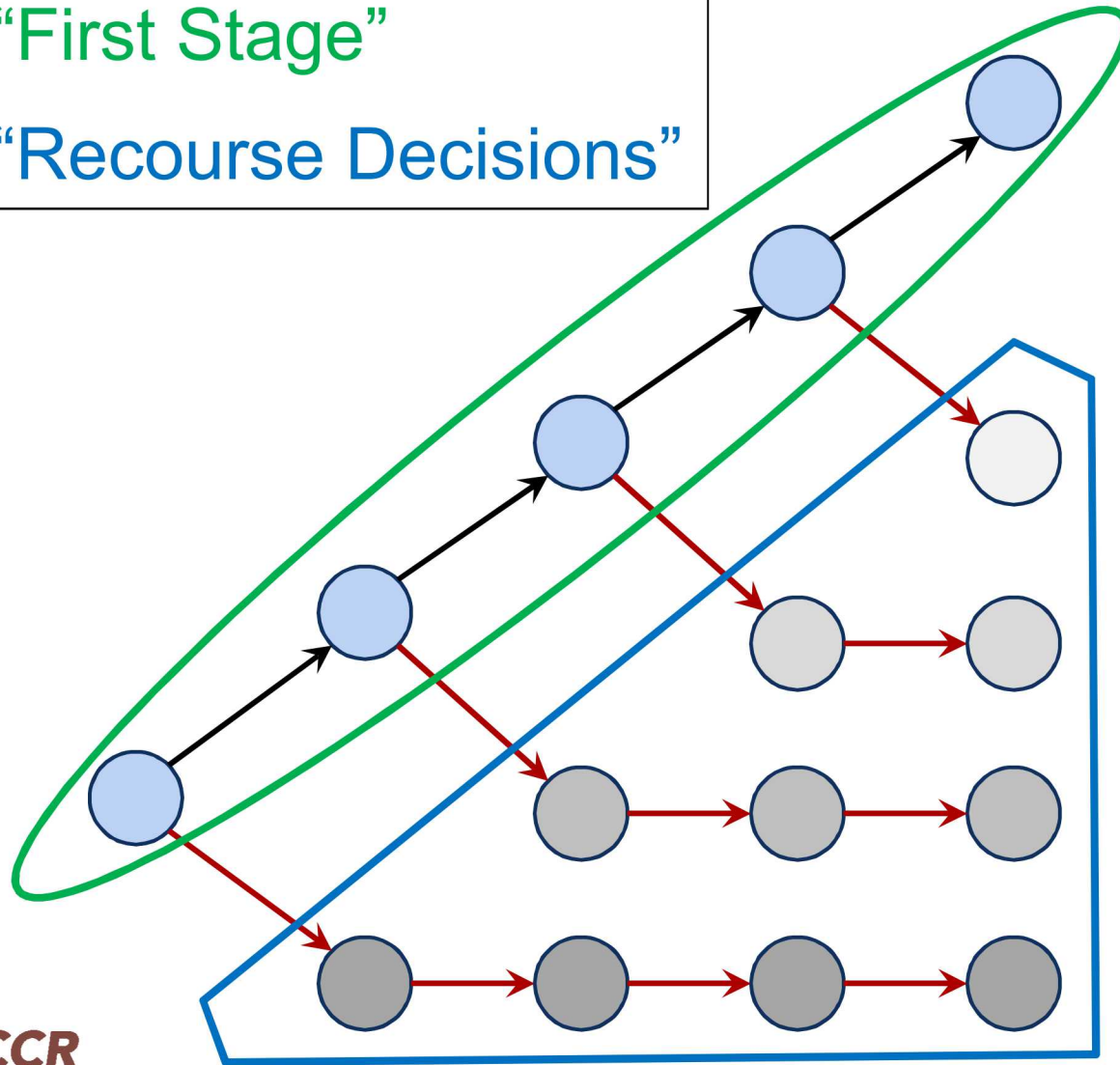
$t_{\text{fail}} = 1$



n-Stage SP as a 2-stage problem

“First Stage”

“Recourse Decisions”



Nominal Scenario

Failure
scenarios

Stochastic structure implementation

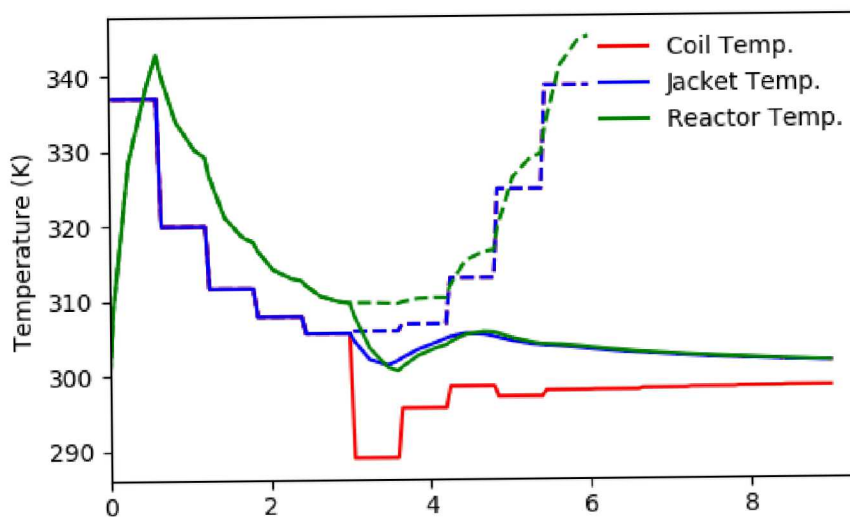
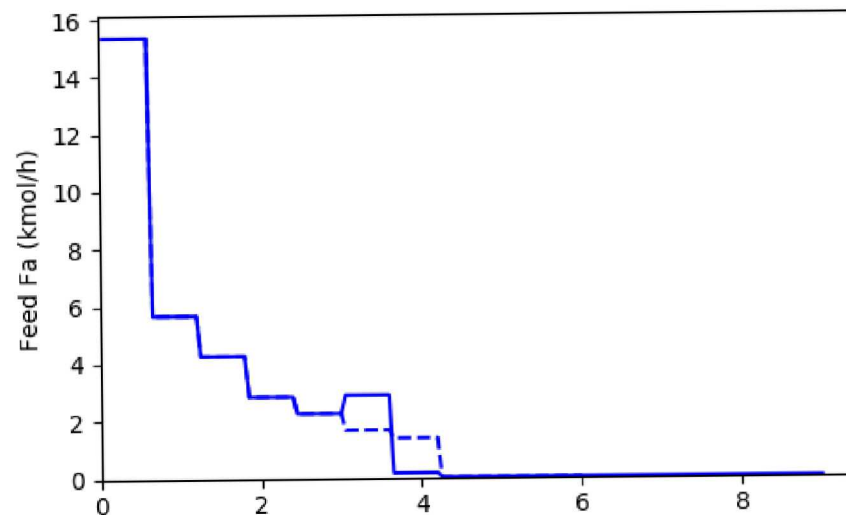
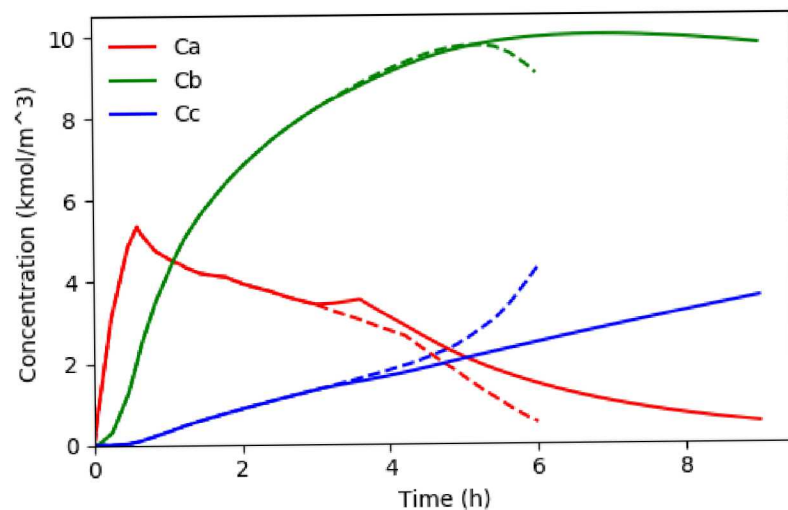
- Implement callback functions to:
 - Define the scenario tree structure
 - Build a model for each scenario
- Create and solve extensive form

```
runef --solve --solver ipopt --output-solver-log -m semibatch.py
```

- Solve using progressive hedging

```
runph --solver ipopt --output-solver-log -m semibatch.py --default-rho=.25
```

Optimal control: $t_{\text{fail}} = 3 \text{ h}$



- 

```
# Extra components so that PySP can be used to enforce the nonanticipativity constraints
n.Tc_nonant = Var(n.all_fail_times, initialize=310.0, bounds=(288, 432))
n.Fa_nonant = Var(n.all_fail_times, initialize=0.0, bounds=(0.0, 0.05))
```

```
# Bound on cumulative Fa
n.cuFaInit = Constraint(expr==n.cuFa[n.time.last()]== 20)

# Bound on final Ca
n.CaFinal = Constraint(expr==n.Ca[n.time.last()] <= 0.5)
```

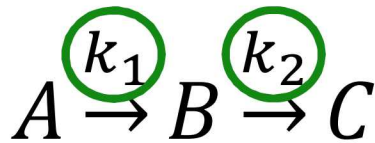
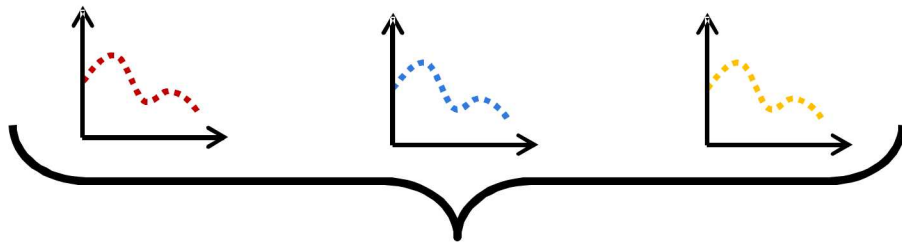
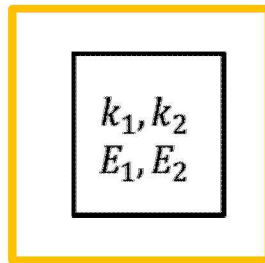
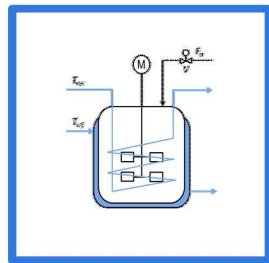
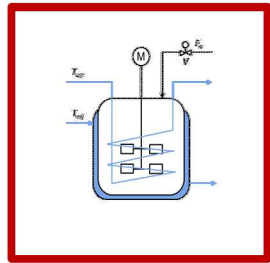
```
def pysp_instance_creation_callback(scenario_name, node_names):
    failtimestep = int(scenario_name.replace('Scenario', ''))
    instance = generate_sembatch_model(failtimestep-1)

    return instance
```

```
plt.plot(time,[value(n.Tr[t]) for t in n.time],label='Reactor Temp.',color=grey3)
plt.legend(loc='best')
plt.ylabel('Temperature (K)')
plt.xlabel('time')
plt.show()
```

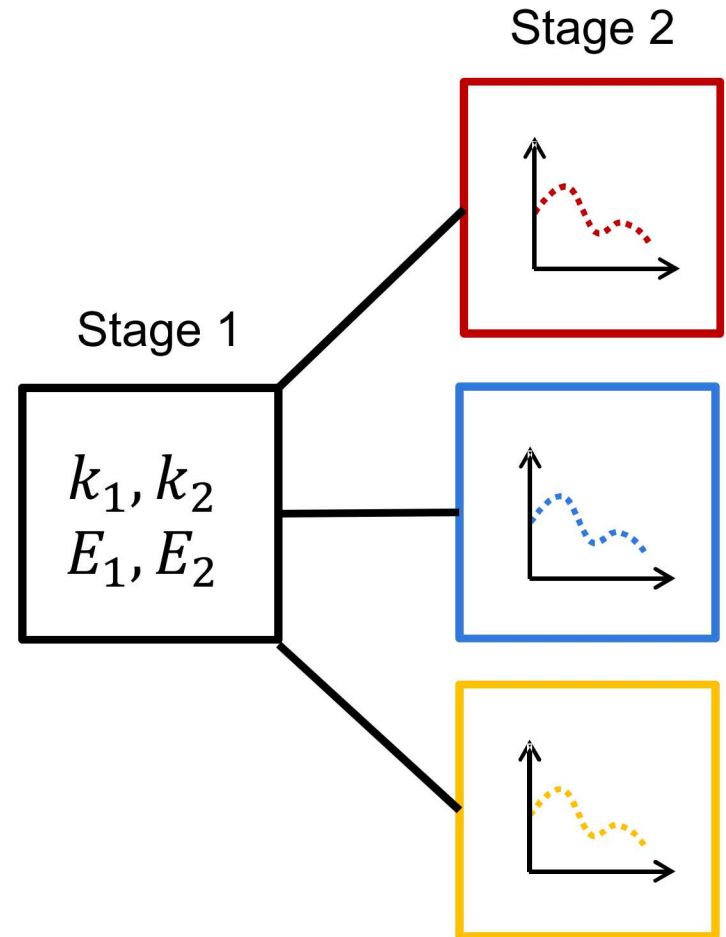
Parameter estimation

Experiment 1 Experiment 2 Experiment 3



$$\min_{\{k_1, k_2, E_1, E_2\}} \sum_{exp.} (error_{meas})^2$$

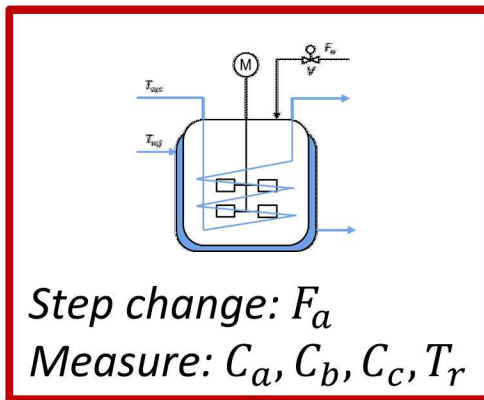
s.t. semibatch model equations



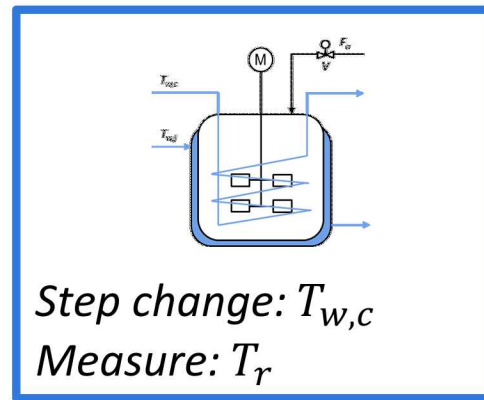
Parameter estimation

- Three ***different*** experiments
 - different manipulated variables, different measured data

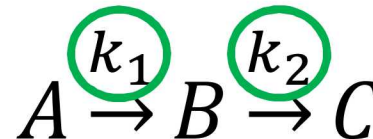
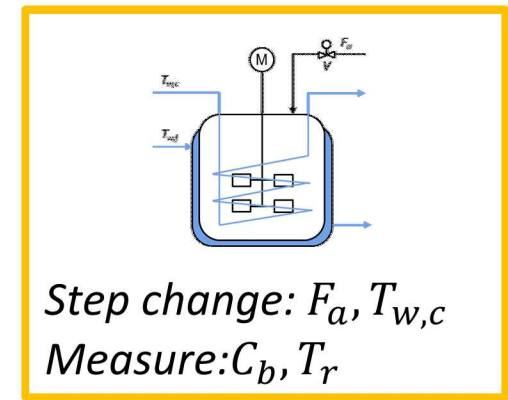
Experiment 1



Experiment 2



Experiment 3



Semibatch parameter estimation results

■ Extensive form results

	k_1 (1/s)	k_2 (1/s)	E_1 (kJ/kmol)	E_2 (kJ/kmol)	Objective
Actual	15.01	85.01	30,000	40,000	-
All Meas.	16.84	81.19	30,322	39,861	2.147
Missing Meas.	20.69	77.42	30,850	39,697	24.976

all: 47 IPOPT iterations, 2674 variables, 2670 constraints, 1.08 s to run

missing: 33 IPOPT iterations, 2674 variables, 2670 constraints, 0.87 s to run

■ Progressive Hedging results*

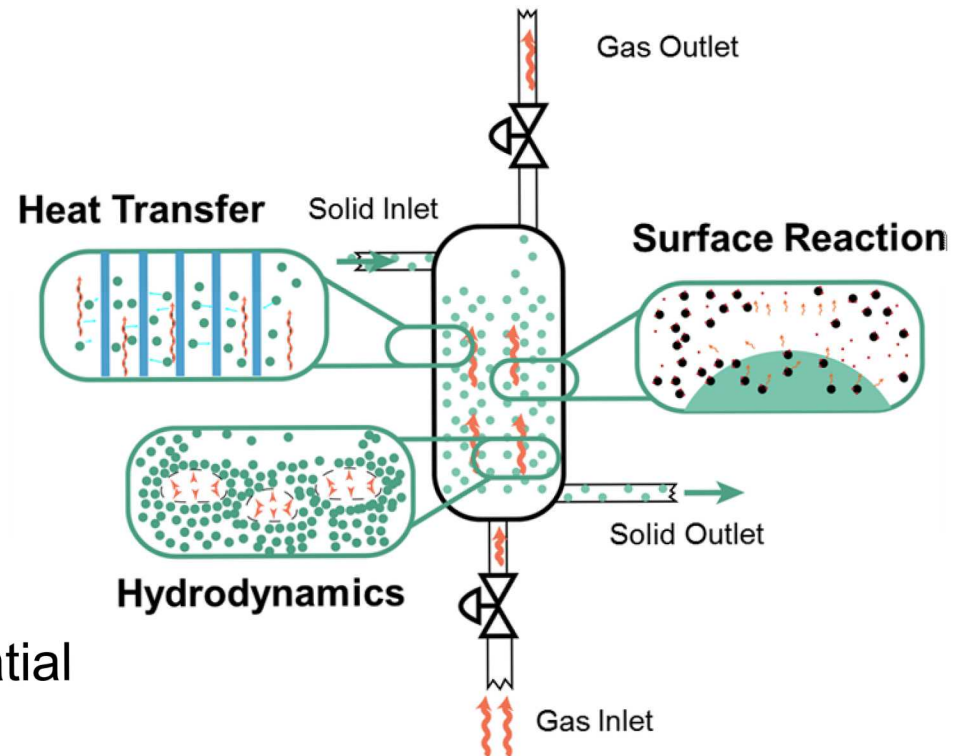
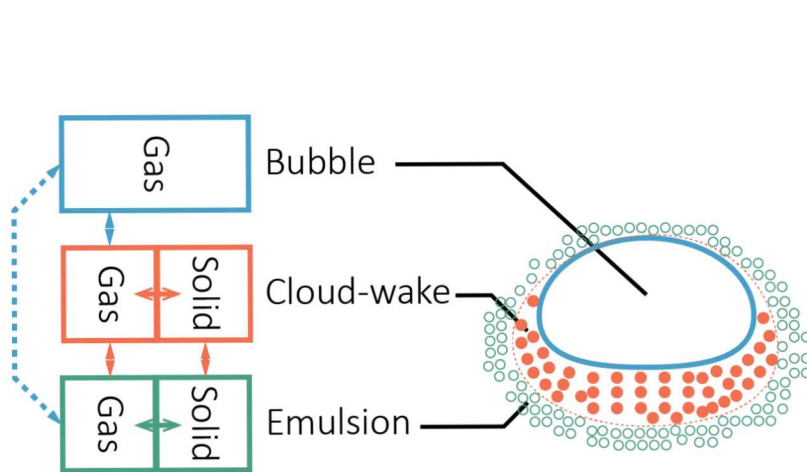
	k_1 (1/s)	k_2 (1/s)	E_1 (kJ/kmol)	E_2 (kJ/kmol)	Objective
Actual	15.01	85.01	30,000	40,000	-
All Meas.	15.72	30.59	30,146	37,017	3.170
Missing Meas.	24.38	69.49	31,302	39,400	25.051

all: 50 PH iterations, 15.08 s to run missing: 35 PH iterations, 11.05 s to run

IPOPT subproblem size: 890 variables, 886 constraints, ~7 iterations

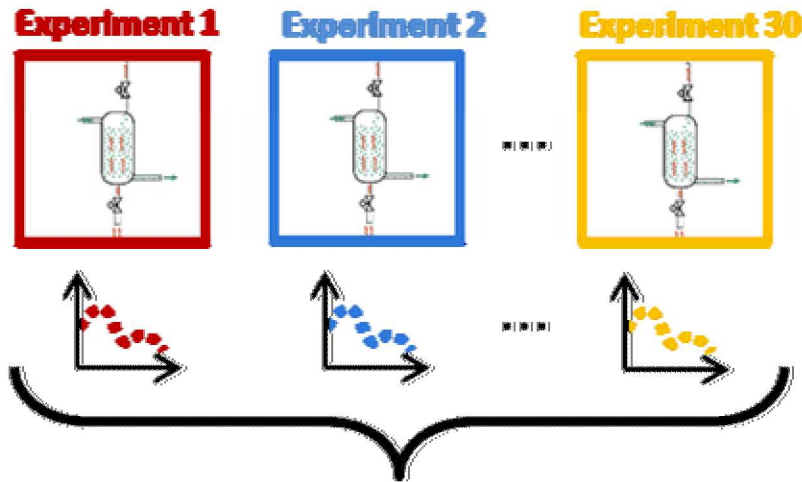
Bubbling Fluidized Bed (BFB) Model

- Gas-solid, 3 region model
(Lee and Miller, 2013, Ind. Eng. Chem. Res.)



- Steady state model with 1-D spatial variation

BFB Parameter Estimation (1/2)

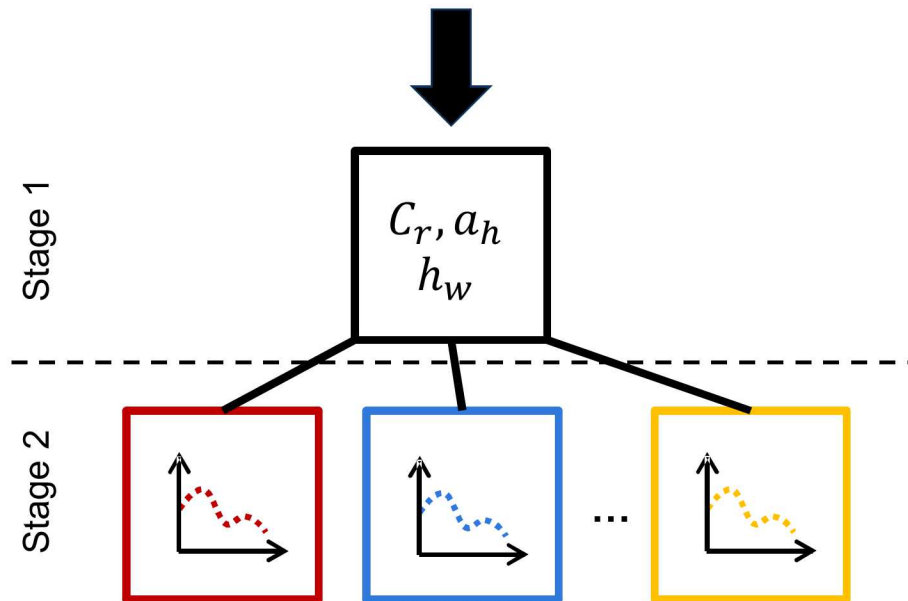


Heat Exchanger Model Parameters

C_r	Average correction factor for tube model
a_h	Empirical factor for tube model
h_w	Heat transfer coefficient of tube walls

$$\min_{\{C_r, a_h, h_w\}} \sum_{exp.} (error_{meas})^2$$

s.t. BFB model equations



BFB Parameter Estimation (2/2)

- Solve using progressive hedging in parallel

```
mpirun -np 1 pyomo_ns : -np 1 dispatch_srvr : -np 30 phsolverserver : \  
-np 1 runph --solver-manager=phpyro --shutdown-pyro \  
-m bfb_paramest.py --solver=ipopt --default-rho=0.25
```

	C_r	a_h	h_w	Solve Time (s)
Actual	1.0	0.8	1500.0	-
Extensive Form	1.016	0.51	1450.35	604.45
Progressive Hedging (15 processors)	0.9824	0.7850	1501.74	610.98
Progressive Hedging (30 processors)	0.9824	0.7850	1501.74	459.10

Extensive form problem size ~400,000 variables and constraints
PH subproblem size ~13,000 variables and constraints

Summary

- Explicitly capturing both uncertainty and system dynamics can be important for many real-world applications
- Pyomo provides high-level modeling constructs that can be easily combined to solve complex, structured optimization problems. (www.pyomo.org)

New application areas

- Dynamics-informed optimization for resilient energy
- Trajectory planning under uncertainty

Thursday morning sessions

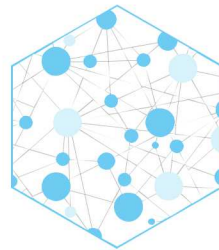
TA33. Pyomo I

TB33. Pyomo II

Questions?

■ Acknowledgements

- John Siirola, Carl Laird, Jean-Paul Watson, Pyomo team
- This work was conducted as part of the Institute for the Design of Advanced Energy Systems (IDAES) with funding from the Office of Fossil Energy, Cross-Cutting Research, U.S. Department of Energy



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Why capture model structure?

- Challenges with a flat representation
 - manual reformulation is required to write a ‘solvable’ model
 - difficult to reverse engineer the intent or goal of the original problem
 - tedious to experiment with alternative model reformulations

- Benefits to explicitly capturing structure
 - models are formulated in a more natural, intuitive form
 - fewer coding mistakes
 - separates model specification from the solution approach
 - easy to experiment with different model reformulations
 - encourages general implementations of common solution approaches

Stochastic structure implementation (1/2)

```
def pysp_scenario_tree_model_callback():
    from pyomo.pysp.scenariotree.tree_structure_model \
        import CreateConcreteTwoStageScenarioTreeModel

    st_model = CreateConcreteTwoStageScenarioTreeModel(scenarios)

    first_stage = st_model.Stages.first()
    second_stage = st_model.Stages.last()

    # First Stage
    st_model.StageCost[first_stage] = 'FirstStageCost'
    st_model.StageVariables[first_stage].add('k1')
    st_model.StageVariables[first_stage].add('k2')
    st_model.StageVariables[first_stage].add('E1')
    st_model.StageVariables[first_stage].add('E2')

    # Second Stage
    st_model.StageCost[second_stage] = 'SecondStageCost'

    return st_model
```