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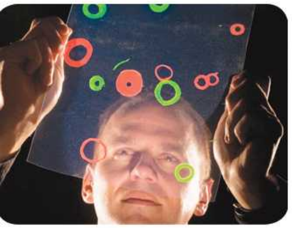

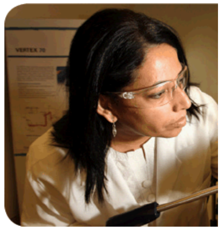

# A Framework for Modeling and Optimizing Dynamic Systems Under Uncertainty


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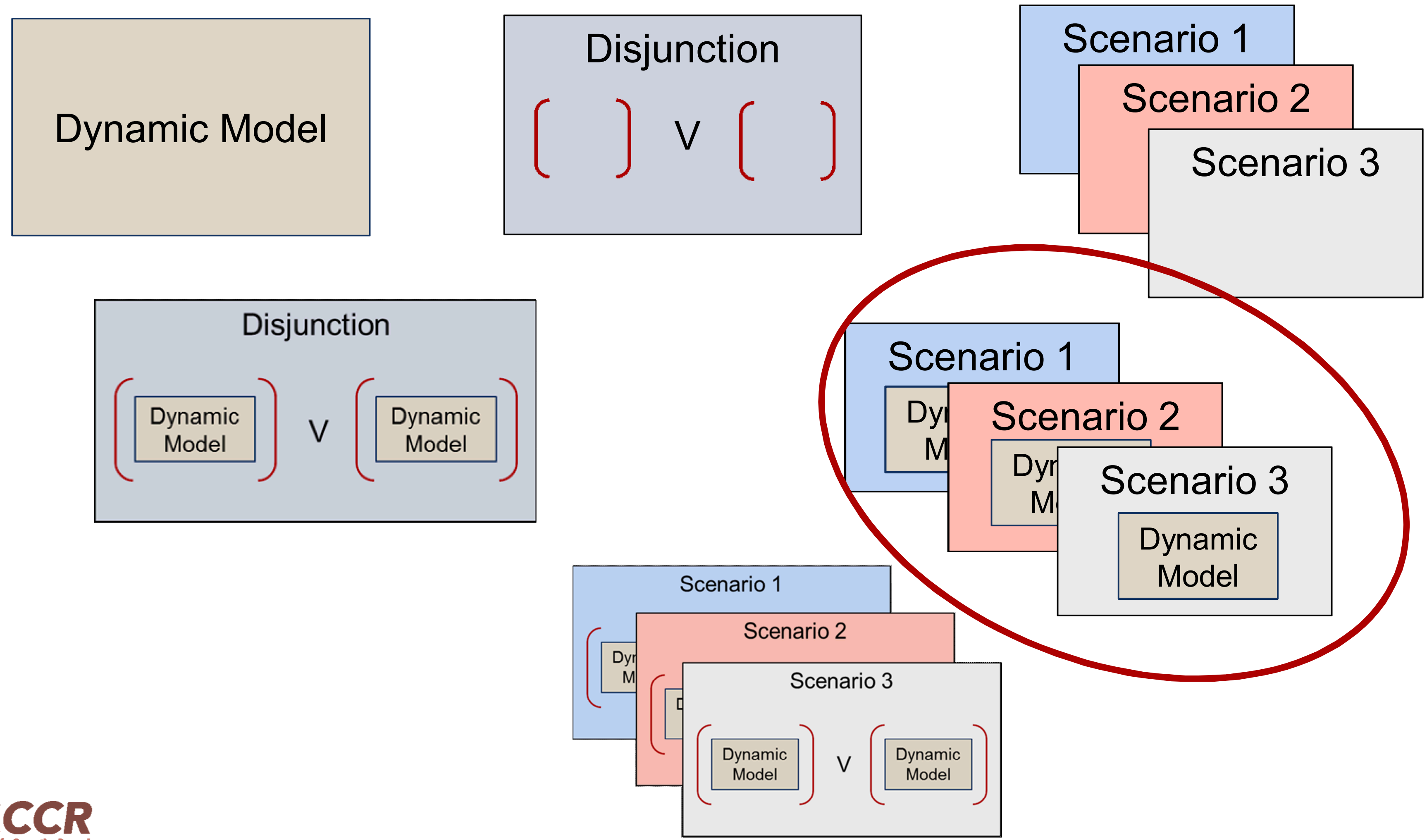
# Implement this…

Dynamic Optimization

Generalized Disjuntive Programming

Stochastic Programming



# 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

# Software platform

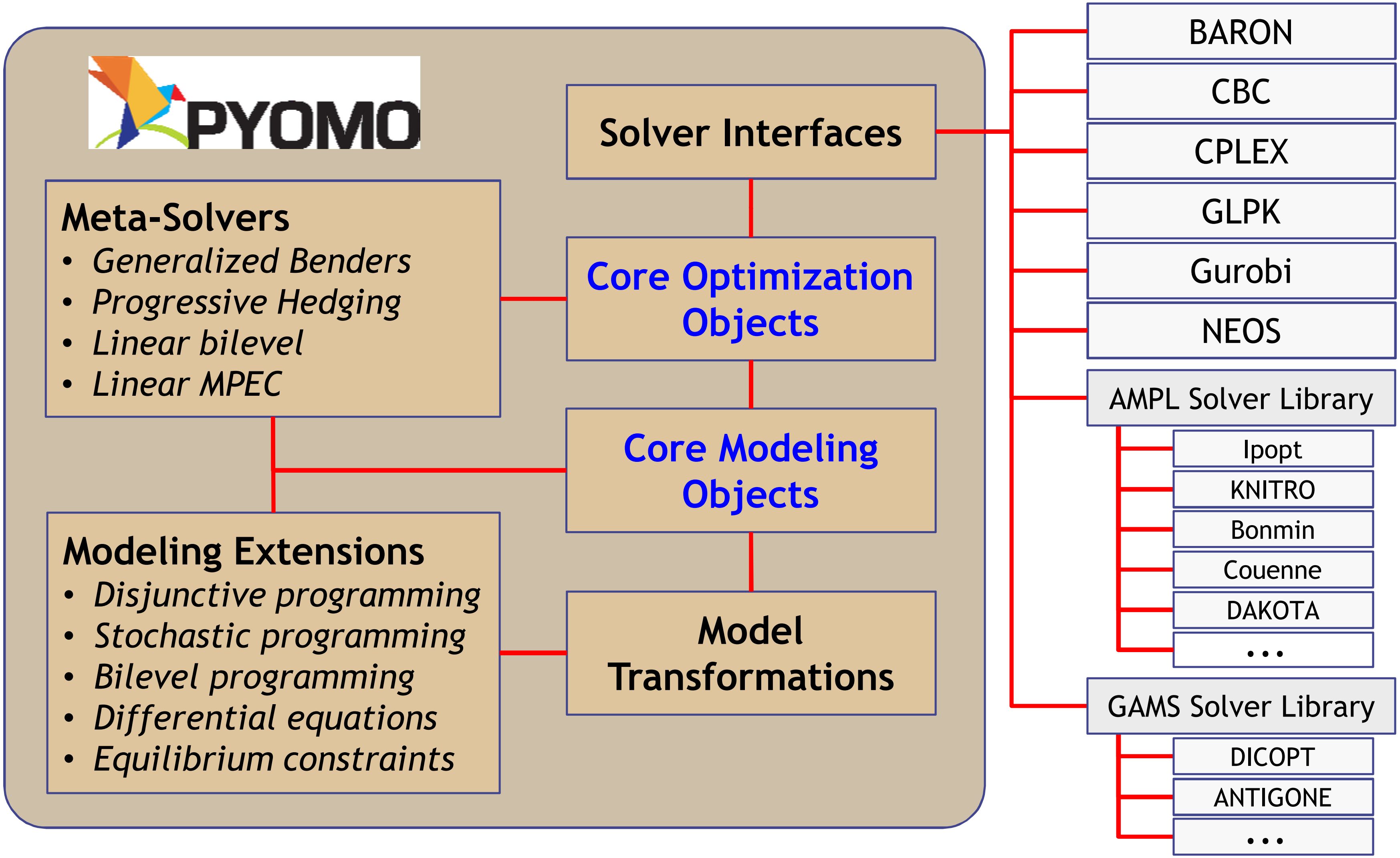
- Pyomo: Python Optimization Modeling Objects
- Formulate optimization models within Python

```
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



# Solving dynamic optimization problems

$$\min \int_{t_0}^{t_F} \left(\phi(x,u)\right)dt + \phi(x(t_F))$$

$$s.t. \quad \frac{dx}{dt} = g(x,u)$$

$$x(t_0) = constant$$

*x: State variables*

*u: Control variables*

Discretize Model

$$\min \sum_{k=1}^{N-1} \left(\phi(x_k,u_k)\right) + \phi(x_N)$$

$$s.t. \quad x_{i+1} = f(x_i,u_i), i = 1,\dots,N-1$$

$$x_1 = constant$$

*Approximate dynamics using algebraic equations*

$$z^K(t) = \sum_{j=0}^{K} z_{ij}\ell_j(\tau), \qquad \ell_j(\tau) = \prod_{\substack{k=0\\k\neq j}}^{K} \frac{(\tau-\tau_k)}{(\tau_j-\tau_k)}, \qquad t_{ij} = t_{i-1} + \tau_j h_i$$

$$\sum_{j=0}^{K} z_{ij}\,\dot{\ell}_j(\tau_k) = h_i f(z_{ik}, y_{ik}, u_{ik}, t_{ik}), \qquad z_{i+1,0} = \sum_{j=0}^{K} \ell_j(1)\, z_{ij}, \qquad z_f = \sum_{j=0}^{K} \ell_j(1)\, z_{Nj}, z_{1,0} = 0$$

# Solving dynamic optimization problems

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$$\min \int_{t_0}^{t_F} (\phi(x,u))dt + \phi(x(t_F))$$

$$s.t. \quad \frac{dx}{dt} = g(x,u)$$

$$x(t_0) = constant$$

*x: State variables*

*u: Control variables*

Discretize Model

$$\min \sum_{k=1}^{N-1} (\phi(x_k,u_k)) + \phi(x_N)$$

$$s.t. \quad x_{i+1} = f(x_i,u_i), i = 1, \dots, N-1$$

$$x_1 = constant$$

*Approximate dynamics using algebraic equations*

**Automated with Pyomo.DAE**

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# Pyomo.dae

- 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

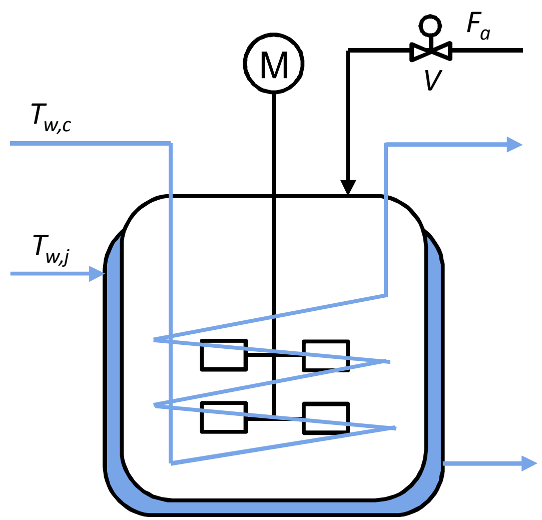
# PySP

- 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]

$$A \rightarrow B \rightarrow C$$




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

$$\begin{aligned}
\dot{C}_a &= \frac{F_a}{V_r} - k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a \\
\dot{C}_b &= k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a - k_2 \exp\left(-\frac{E_2}{RT_r}\right) C_b \\
\dot{C}_c &= k_2 \exp\left(-\frac{E_2}{RT_r}\right) C_b \\
\dot{V}_r &= \frac{F_a M_{W_a}}{\rho_r} \\
(\rho_r c_{p_r})\dot{T}_r &= \frac{F_a M_{W_a} c_{p_r}}{V_r}(T_f - T_r) \\
&\quad - k_1 \exp\left(-\frac{E_1}{RT_r}\right) C_a \Delta H_1 - k_2 \exp\left(-\frac{E_2}{RT_r}\right) C_b \Delta H_2 \\
&\quad + \alpha_{w,j} \frac{A_j}{V_{r,0}}(T_{w,j} - T_r) + \alpha_{w,c} \frac{A_c}{V_{r,0}}(T_{w,c} - T_r)
\end{aligned}$$

- Two case studies
  - parameter estimation
  - optimal control under partial system failure[2]

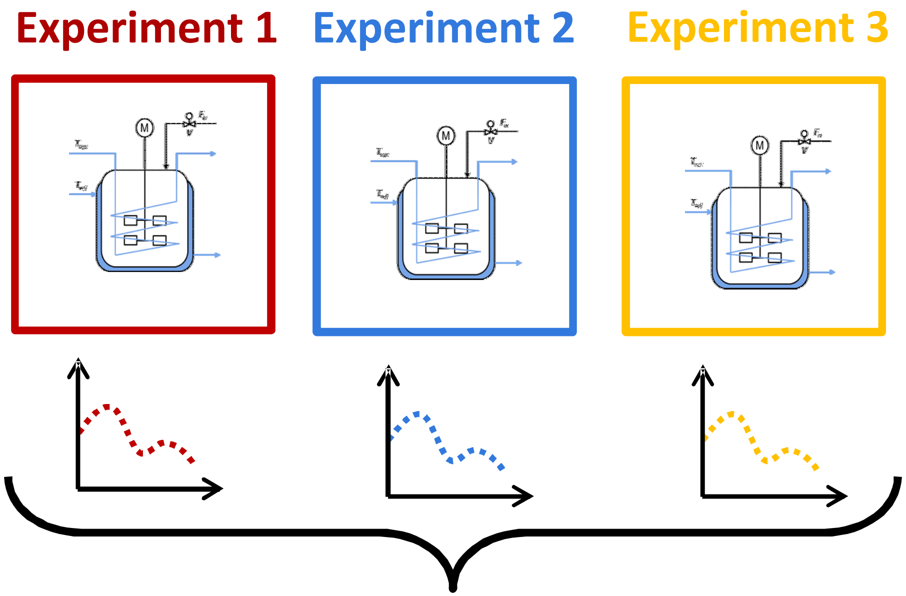
[2] Abel and Marquardt, AIChE Journal (2000)

# 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
```

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

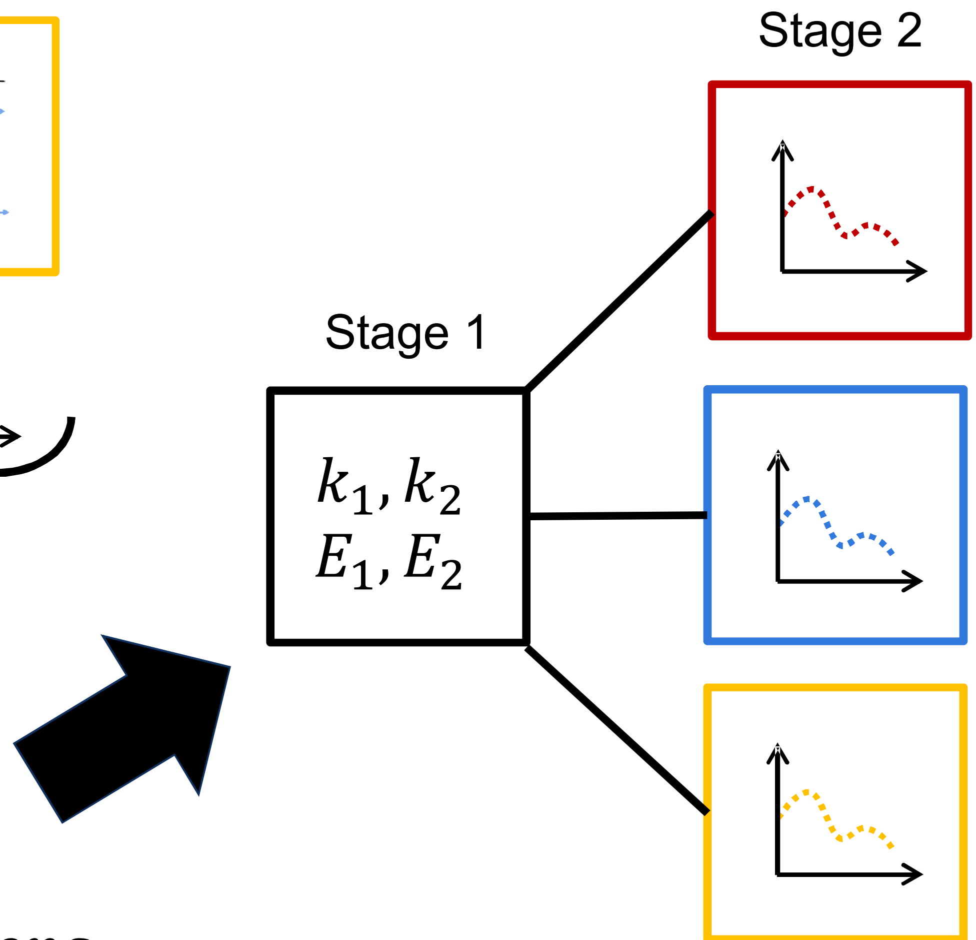
# Parameter estimation




$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

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

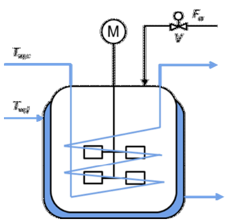
$$s.t. \quad semibatch\ model\ equations$$



# Parameter estimation

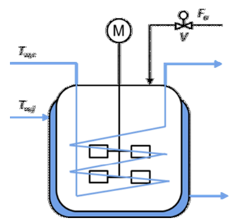
- Three ***different*** experiments
  - different manipulated variables, different measured data

**Experiment 1**



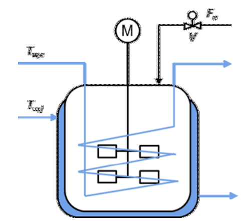

*Step change:* $F_a$
*Measure:* $C_a, C_b, C_c, T_r$

**Experiment 2**




*Step change:* $T_{w,c}$
*Measure:* $T_r$

**Experiment 3**




*Step change:* $F_a, T_{w,c}$
*Measure:* $C_b, T_r$

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

# 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
```

# Stochastic structure implementation (2/2)

```python
def pysp_instance_creation_callback(scenario_name, node_names):
    experiment = int(scenario_name.replace('Scenario',''))

    # Experiments with measurement noise
    explist = [1,2,3] # Different step changes in control inputs

    experiment = explist[experiment-1]
    instance = generate_semibatch_model_paramest(experiment)

    return instance
```

- 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
```

# 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*

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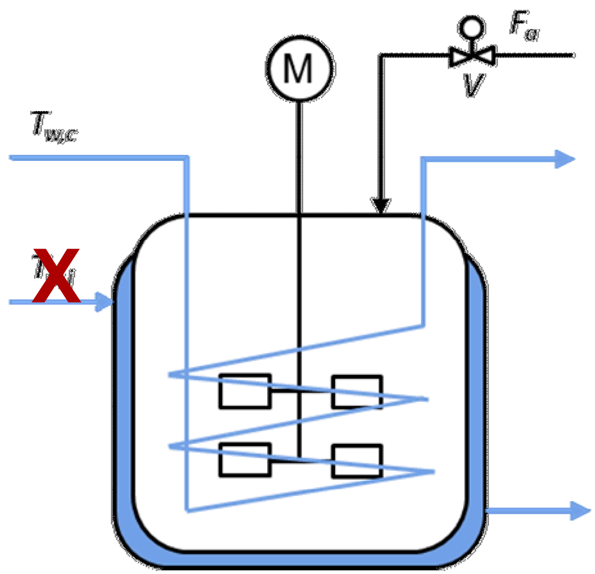
** PH is not guaranteed to converge on nonconvex problems*

# Optimal control

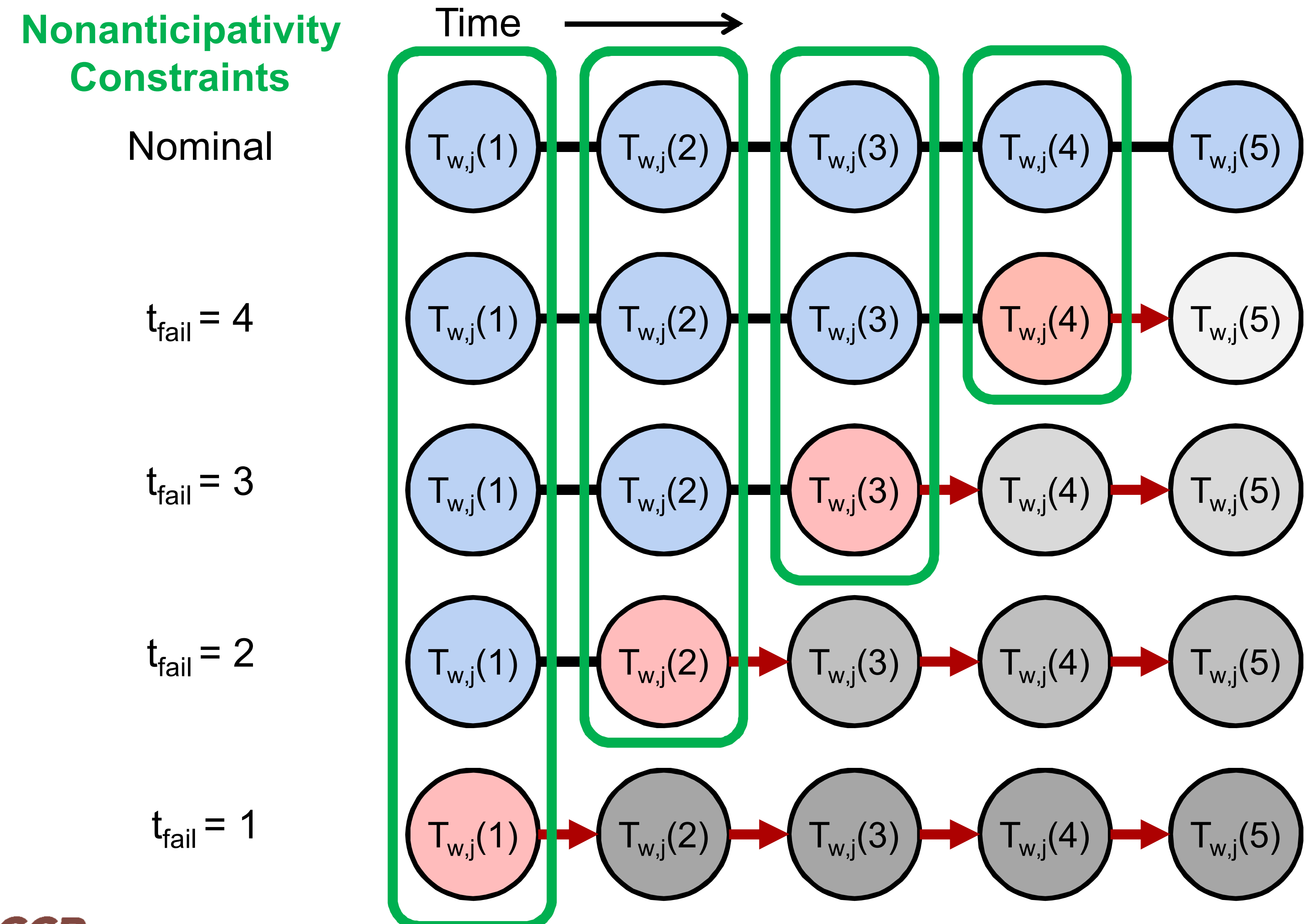
- Find the nominal control profiles such that the batch can be ‘saved’ given a partial cooling system failure at any point during the batch time[2]



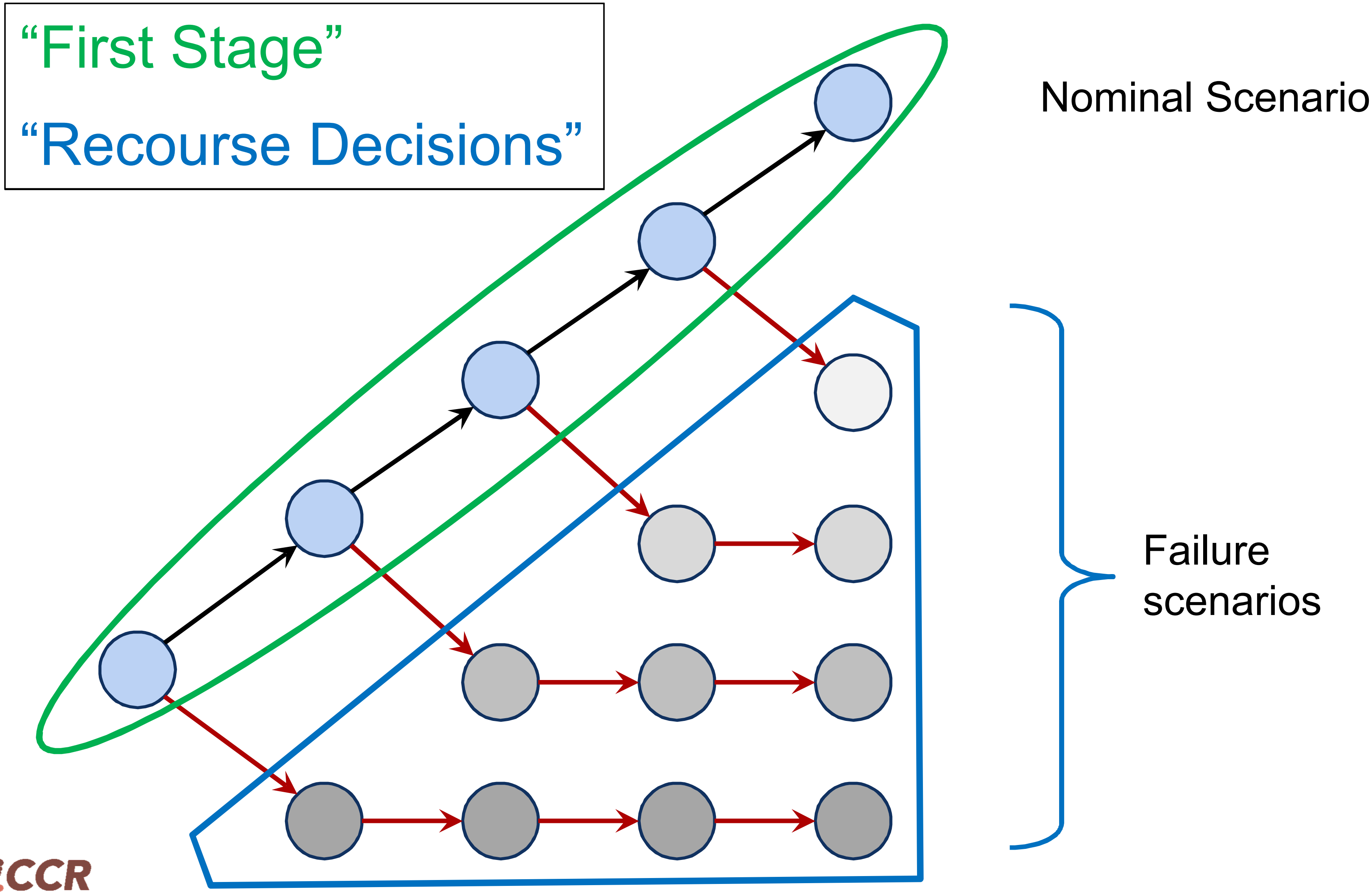

$$
\left.
\begin{array}{ll}
T_{w,j}(t) = T_{w,c}(t) & t \le t_{fail} \\
(\rho_w C_{p_w} V_j)\dot{T}_{w,j} = \alpha_{w,js} A_j \dfrac{V_r}{V_{r,0}} (T_{w,j} - T_r) & t > t_{fail}
\end{array}
\right\}
$$

[2] Abel and Marquardt, AIChE Journal (2000)

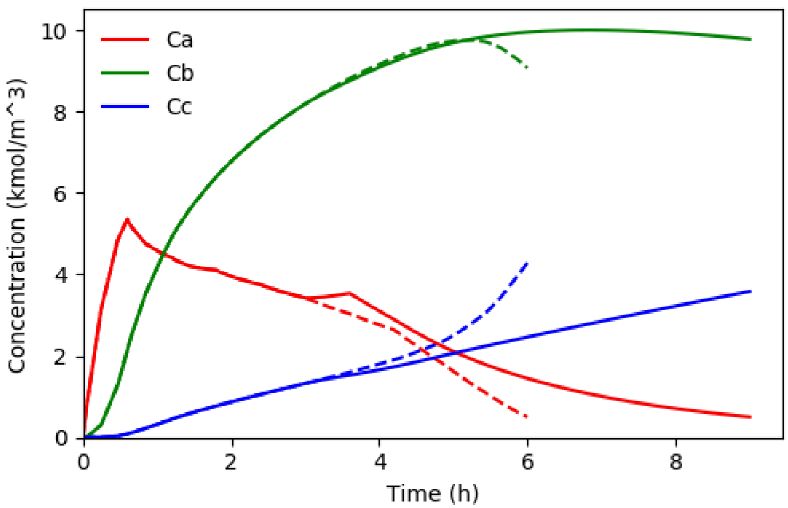
# Optimal control scenarios

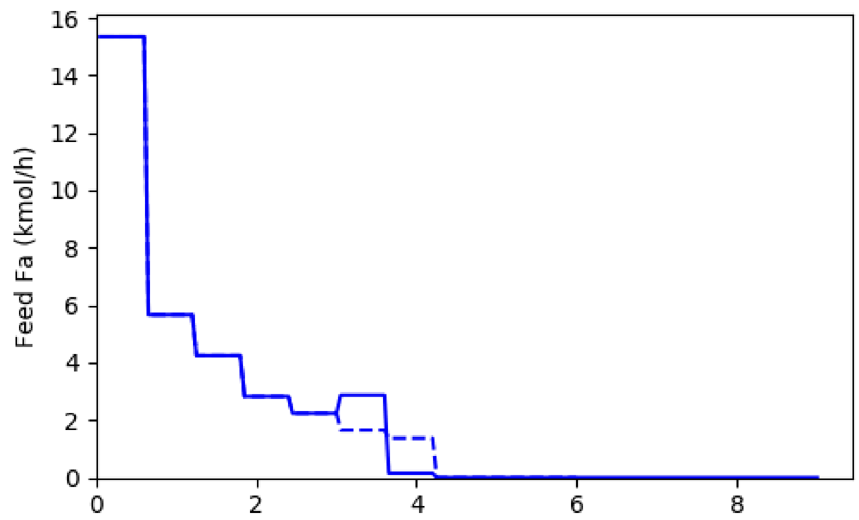


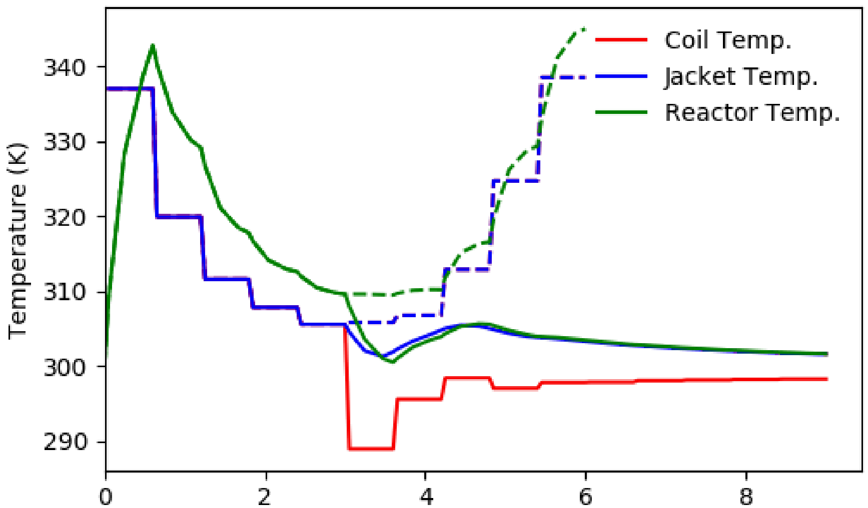
# n-Stage SP as a 2-stage problem



# Optimal control: $t_{fail}$ = 3 h

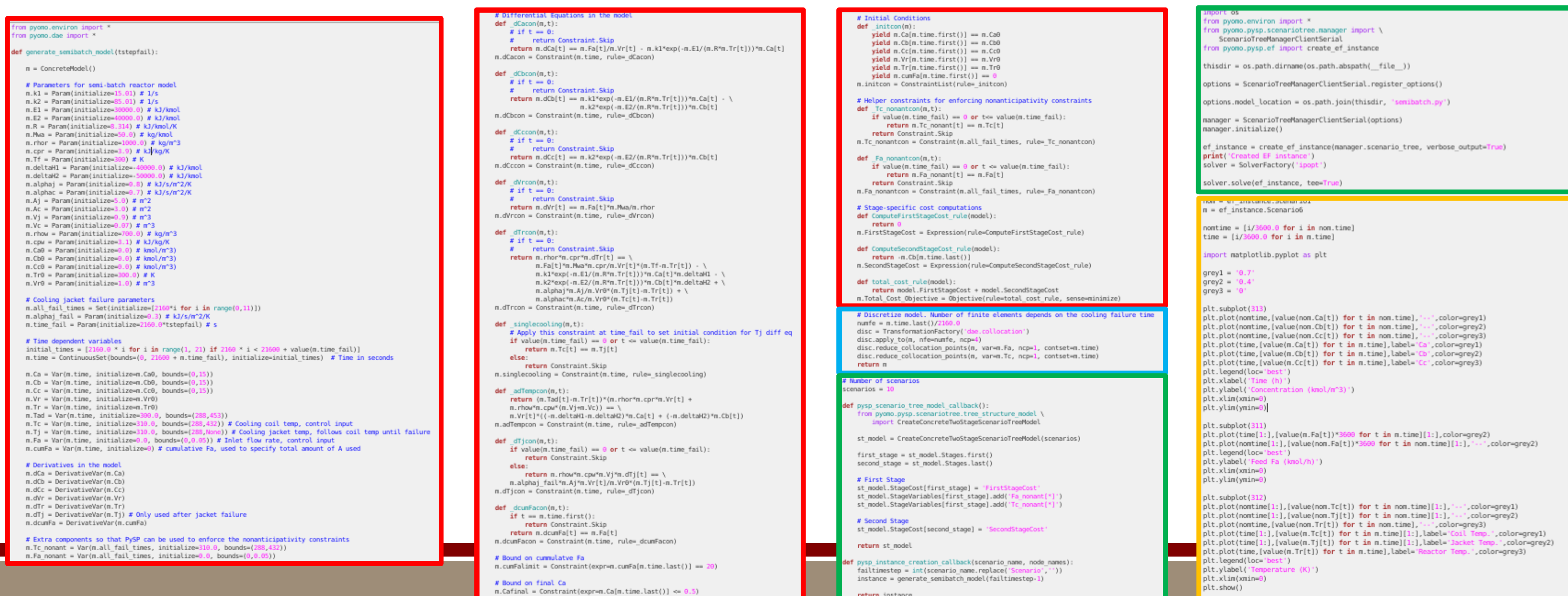


# Optimal control implementation

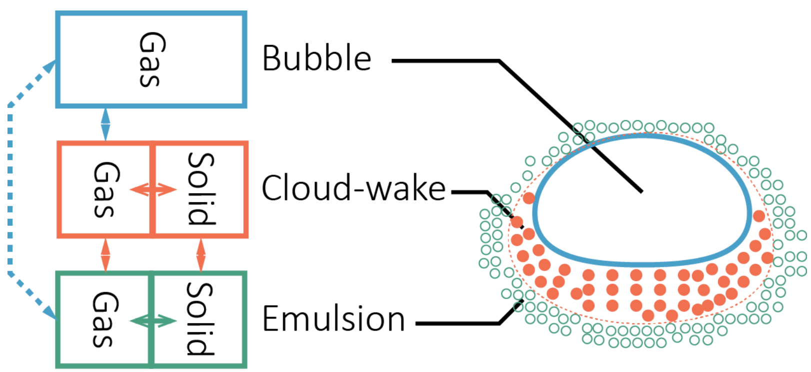
- 15 hours (including debugging)
- 300 lines of code
  - (60%)Deterministic dynamic model specification
  - (2%) Discretization
  - (18%) Stochastic problem formulation
  - (20%) Result plotting

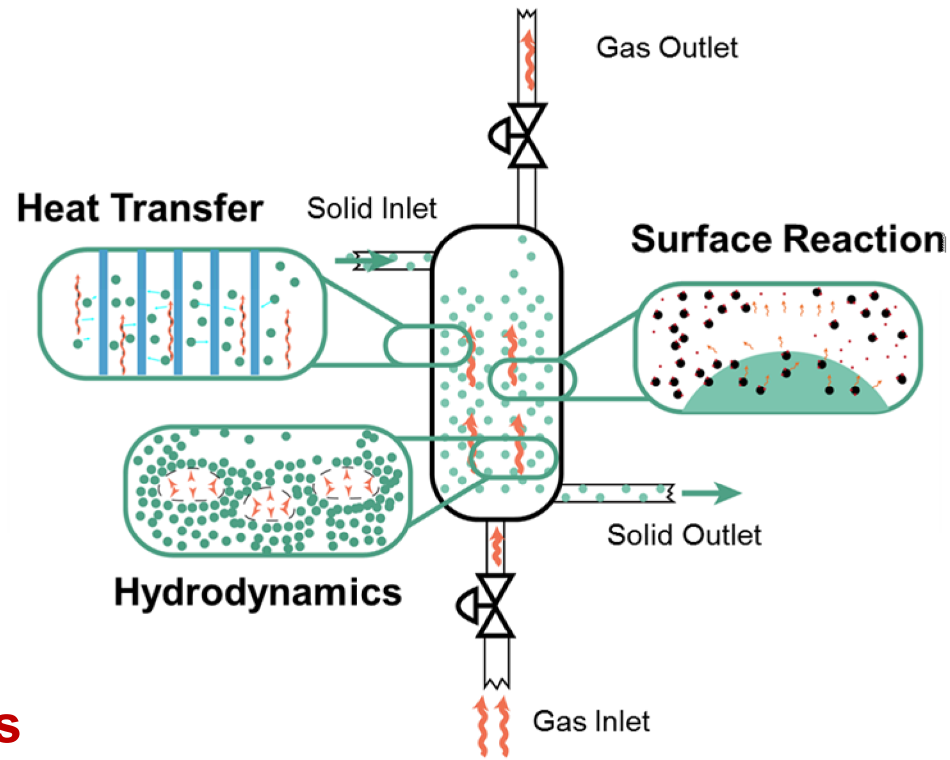


# Bubbling Fluidized Bed (BFB) Model

- Gas-solid, 3 region model

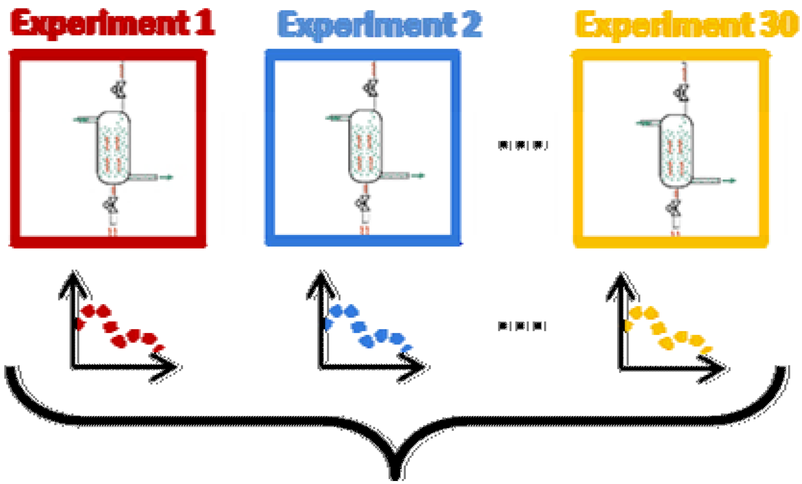
(Lee and Miller, 2013, Ind. Eng. Chem. Res.)




- Modeled using system of **partial differential algebraic equations** (PDAEs)

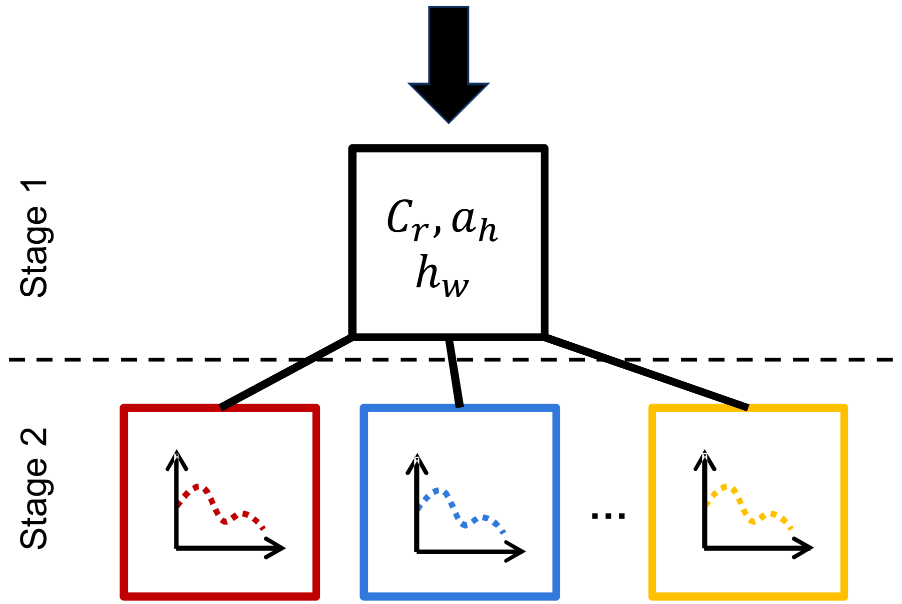
# BFB Parameter Estimation (1/2)




| Heat Exchanger Model Parameters | |
|---|---|
| [redacted] | |
| $a_h$ | Empirical factor for tube model |
| [redacted] | |

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

$$s.t. \quad BFB\ model\ equations$$



# 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 proc) | 0.9824 | 0.7850 | 1501.74 | 610.98 |
| Progressive Hedging (30 proc) | 0.9824 | 0.7850 | 1501.74 | 459.10 |

# Summary

- Explicitly capturing high-level structure leads to significantly easier, faster, and more flexible implementations
- Pyomo provides high-level modeling constructs that can be easily combined to solve complex, structured optimization problems. (www.pyomo.org)

On-going pyomo.dae work

- Interface to DAE simulators
- Shooting methods for dynamic optimization

New challenges and open questions

- general implementations of meta-solvers to exploit layered/nested structure
- scalability of these techniques

# Questions?

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- Acknowledgements

  - 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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