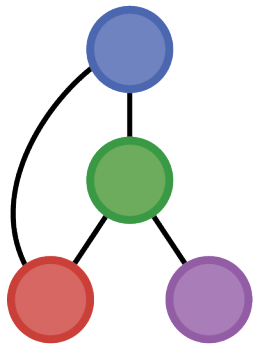
UCONN
UNIVERSITY OF CONNECTICUT

# Optimization Abstraction Layer for Acausal/Equation-Oriented Models in Julia

**Dimitri Alston,** Joseph Choi, Pengfei Xu
Matthew Stuber, P&W Associate Professor in Advanced Systems Engineering

November 5th, 2025

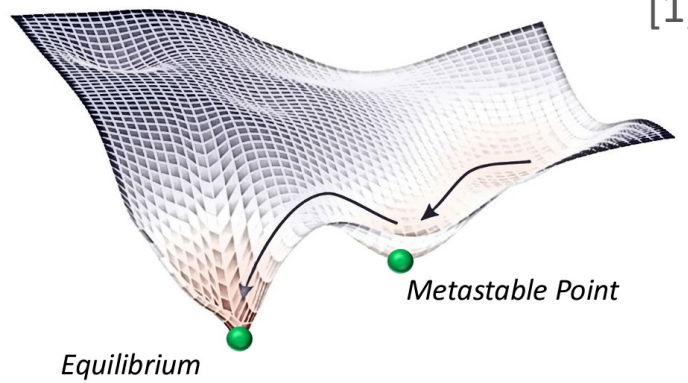
2025 AIChE ANNUAL MEETING



Process Systems and Operations Research Laboratory

# Global Optimization

- Nonconvex problems arise in many applications
  - Thermodynamic stability
  - Kinetic parameter estimation
  - Design under uncertainty



[1]

[1] Grajcarova, L. Simulations of structural phase transitions in crystals using ab initio metadynamics. INIS-IAEA. (2013).

# Global Optimization

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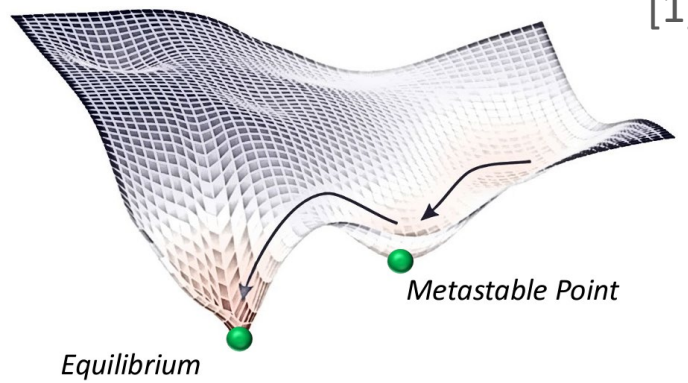
  - Thermodynamic stability
  - Kinetic parameter estimation
  - Design under uncertainty
- Dynamic optimization problems



[1]

$$\min_{\mathbf{p}\in P} \phi(\mathbf{x}(\mathbf{p},t_f),\mathbf{p})$$

$$\text{s.t.} \quad \dot{\mathbf{x}}(\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{p},t),\mathbf{p},t) = \mathbf{0} \quad \forall t \in I = [t_0,t_f]$$

$$\mathbf{x}(\mathbf{p},t_0) = \mathbf{x_0}(\mathbf{p})$$

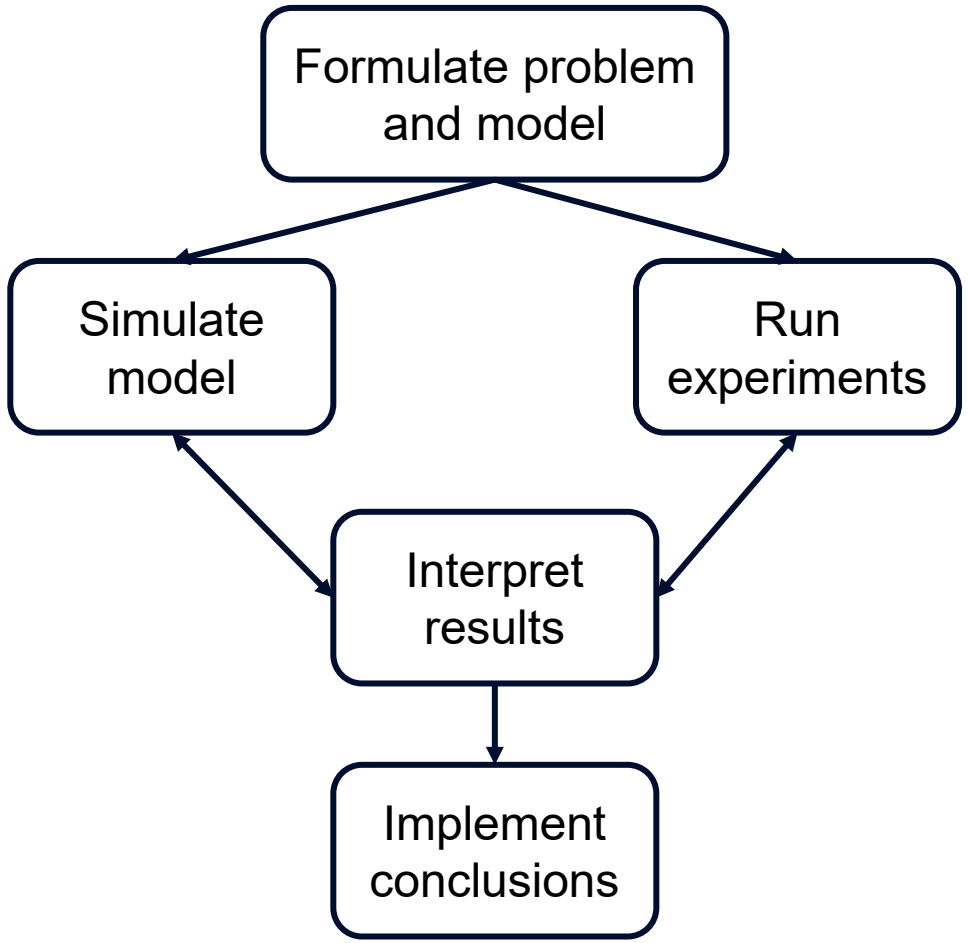
$$\mathbf{g}(\mathbf{x}(\mathbf{p},t),\mathbf{p}) \le \mathbf{0}$$

$$P = \{\mathbf{p} \in \mathbb{R}^m : \mathbf{p}^L \le \mathbf{p} \le \mathbf{p}^U\}$$

[1] Grajcarova, L. Simulations of structural phase transitions in crystals using ab initio metadynamics. INIS-IAEA. (2013).

# Modeling and Simulation

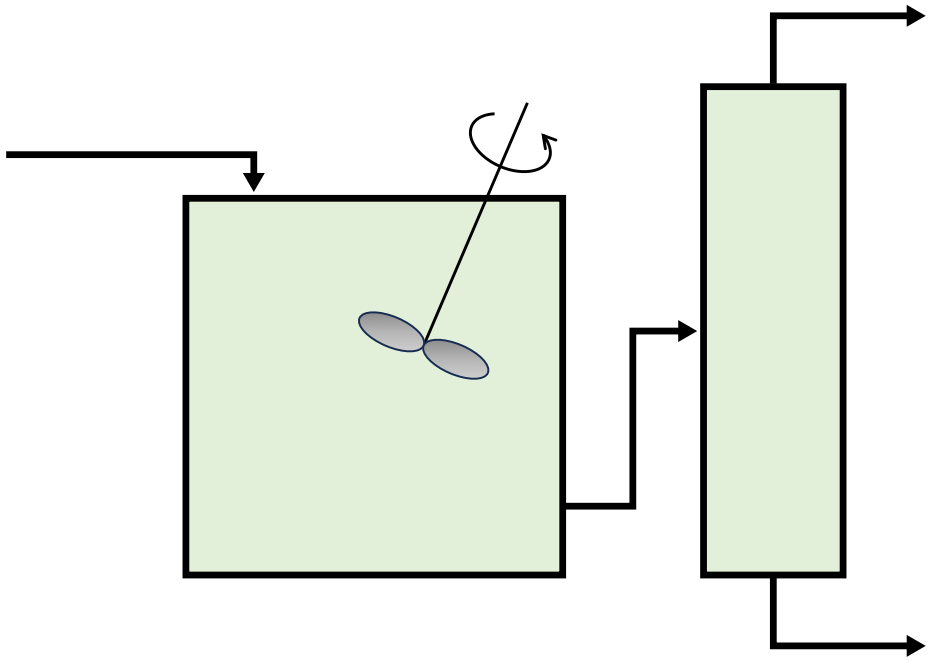
- Applicable in various contexts
  - Proof-of-concept
  - Modification
  - Comparison
  - Optimization
- Eliminate costs of real-world experiments
- Provide support at all stages of design




[2] Menner, W.A. Introduction to Modeling and Simulation. *Johns Hopkins APL Technical Digest.* 16:1 (1995).

# Modeling and Simulation Approaches

## Causal/Sequential-Modular



## Acausal/Equation-Oriented

$$y_{2,\mathrm{A}} + y_{2,\mathrm{B}} + y_{2,\mathrm{C}} = 1$$

$$y_{2,\mathrm{B}} F = y_{1,\mathrm{B}} + Vr_{\mathrm{B}}$$

$$y_{2,\mathrm{C}} F = y_{1,\mathrm{C}} + Vr_{\mathrm{C}}$$

$$y_{3,\mathrm{A}} = y_{1,\mathrm{A}} - Vr_{\mathrm{A}}$$

$$y_{4,\mathrm{B}} + y_{4,\mathrm{C}} = y_{2,\mathrm{B}} + y_{2,\mathrm{C}}$$

[3] Schweiger, G. et al. Modeling and simulation of large-scale systems: A systematic comparison of modeling paradigms. *Applied Mathematics and Computation.* 365, 124713 (2020).

# Modeling and Simulation Approaches

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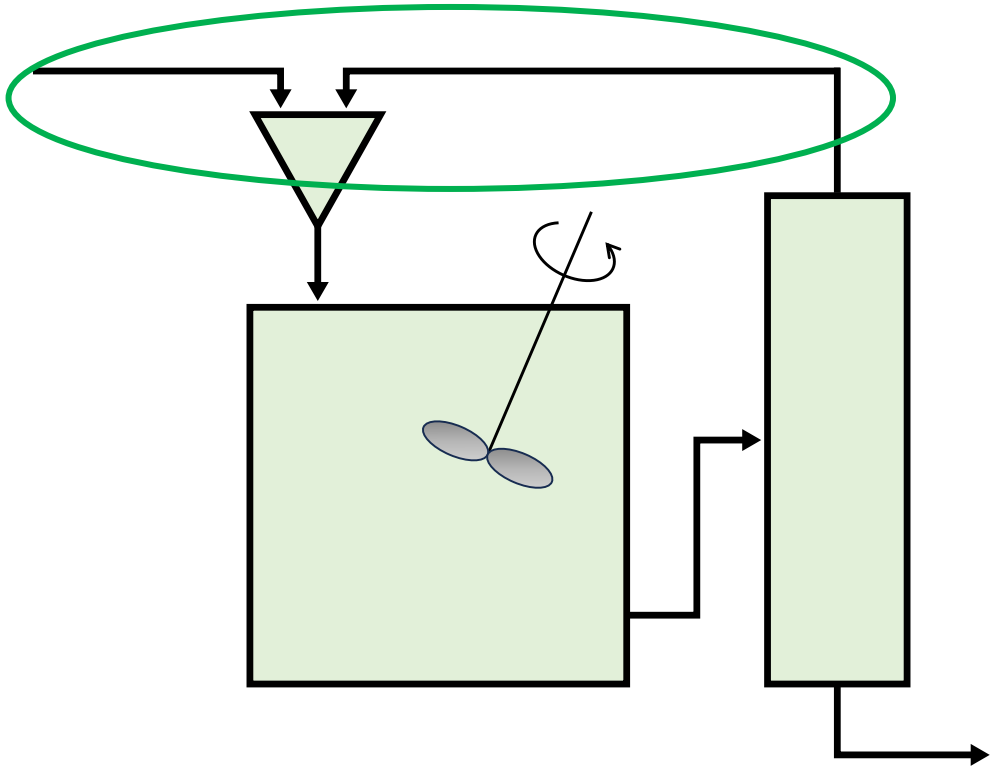

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$$y_{3,\mathrm{B}} F = y_{2,\mathrm{B}} + Vr_{\mathrm{B}}$$

$$y_{3,\mathrm{C}} F = y_{2,\mathrm{C}} + Vr_{\mathrm{C}}$$

$$y_{4,\mathrm{A}} = y_{2,\mathrm{A}} - Vr_{\mathrm{A}}$$

$$y_{5,\mathrm{B}} + y_{5,\mathrm{C}} = y_{3,\mathrm{B}} + y_{3,\mathrm{C}}$$

$$y_{2,\mathrm{A}} = y_{1,\mathrm{A}} + y_{4,\mathrm{A}}$$

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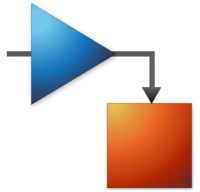
# Available Software*

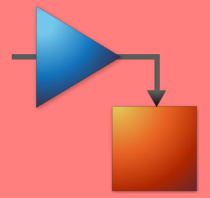





*Non-exhaustive list

# Available Software*

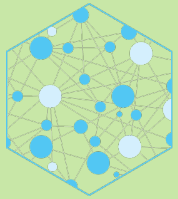
**Commercial**



gPROMS

**Open-source**

Modelica Language



IDAES®
Institute for the Design of Advanced Energy Systems

*Non-exhaustive list

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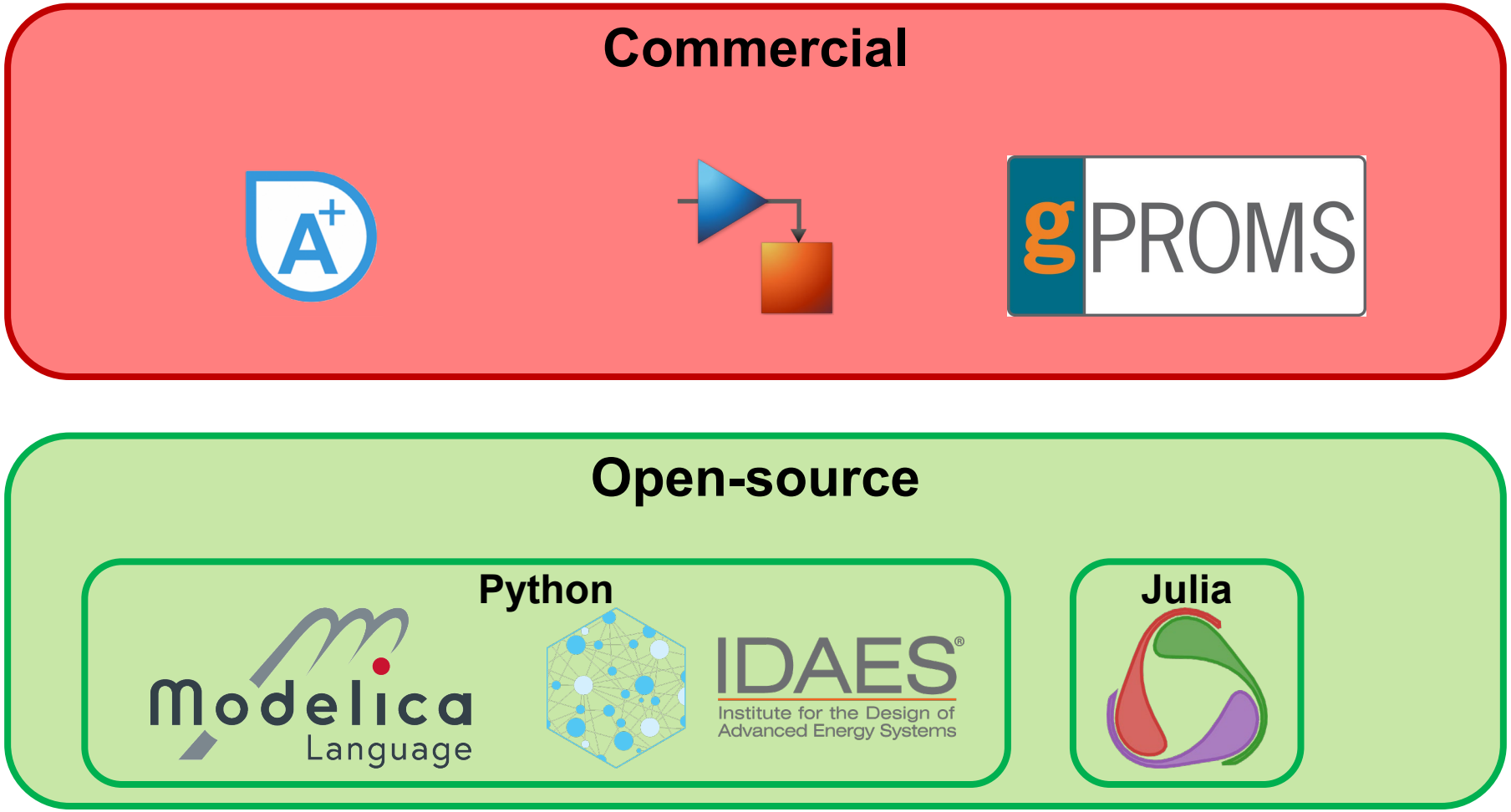


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# Why Julia?

[4]

- Speed of C/Fortran
- Easy to use
- Strong scientific computing community

[5]

JuMP

[6]

SciML


[4] Bezanson, J. et al. Julia: A Fresh Approach to Numerical Computing. *SIAM Review.* 59: 65 -98 (2017).
[5] Lubin, M., Dowson, O., Garcia, J.D. et al. JuMP 1.0: recent improvements to a modeling language for mathematical optimization. *Math. Prog. Comp*. 15, 581–589 (2023).
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- High-performance deterministic global solver
  - Dynamic optimization
  - User-defined functions
  - Semi-infinite programs
- Open-source


[4] Bezanson, J. et al. Julia: A Fresh Approach to Numerical Computing. *SIAM Review.* 59: 65 -98 (2017).
[5] Lubin, M., Dowson, O., Garcia, J.D. et al. JuMP 1.0: recent improvements to a modeling language for mathematical optimization. *Math. Prog. Comp*. 15, 581–589 (2023).
[6] Dixit, V.K. and Rackauckas C. Optimization.jl: A Unified Optimization Package. (2023).
[7] Wilhelm, M.E. and Stuber, M.D. EAGO.jl: easy advanced global optimization in Julia. *Optimization Methods and Software.* 37:2, 425-450 (2022).

# ModelingToolkit.jl

- Open-source, acausal modeling framework in Julia
- Supports a broad range of system types
  - ODEs, SDEs, PDEs
  - Nonlinear systems
  - Optimization problems
- Automatically composes, transforms, and reduces models
  - Dimensionality reduction through algebraic simplification

[8] Ma, Y. et al. Modelingtoolkit: A composable graph transformation system for equation-based modeling. arXiv preprint arXiv:2103.05244 (2021).

# Optimization in Julia

**SciML** [6]

- 25+ libraries, 100+ solvers
- No deterministic global optimization support

**JuMP** [5]

- Algebraic modeling language designed for mathematical optimization

[5] Lubin, M., Dowson, O., Garcia, J.D. et al. JuMP 1.0: recent improvements to a modeling language for mathematical optimization. *Math. Prog. Comp.* 15, 581–589 (2023).
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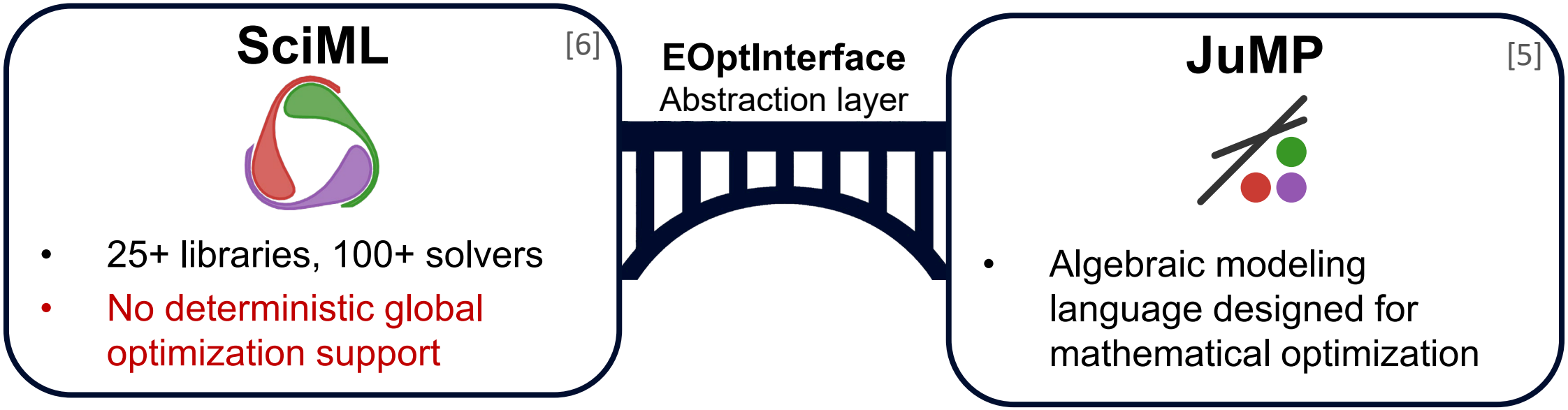


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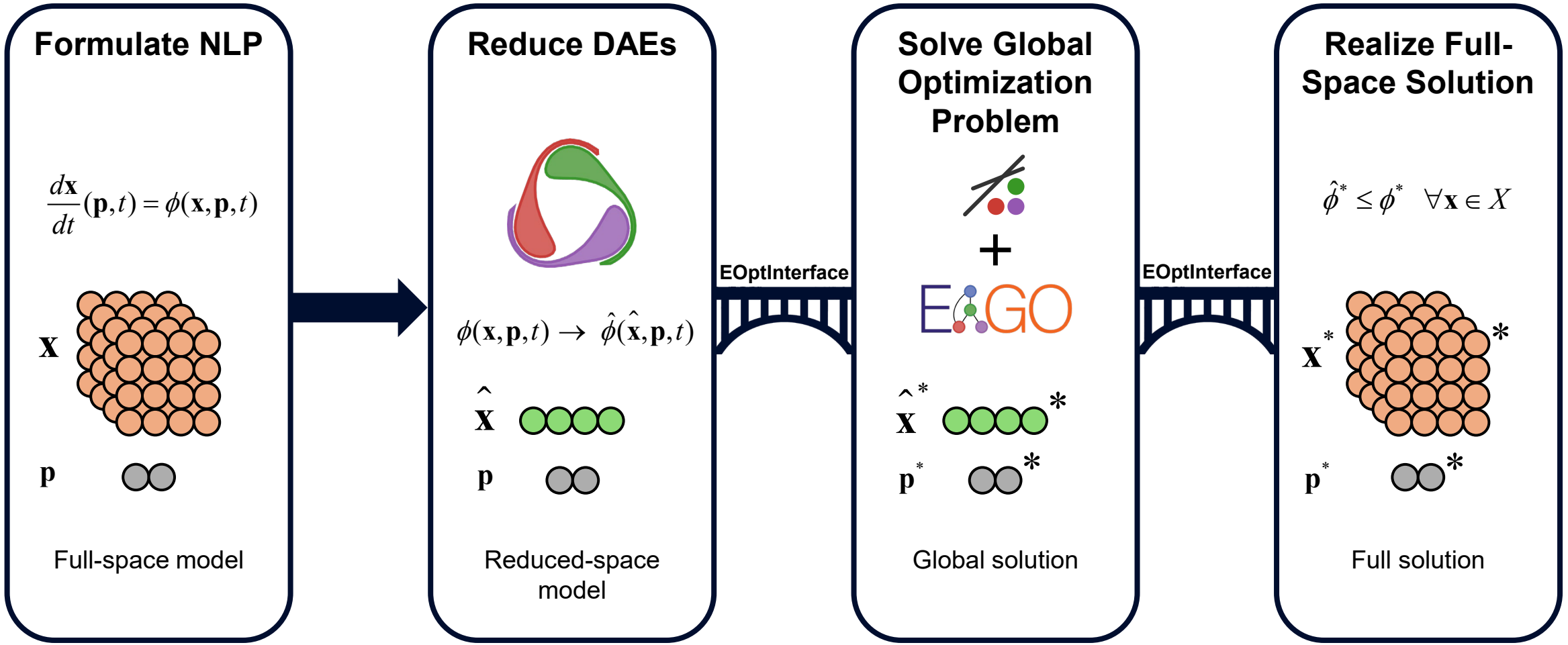
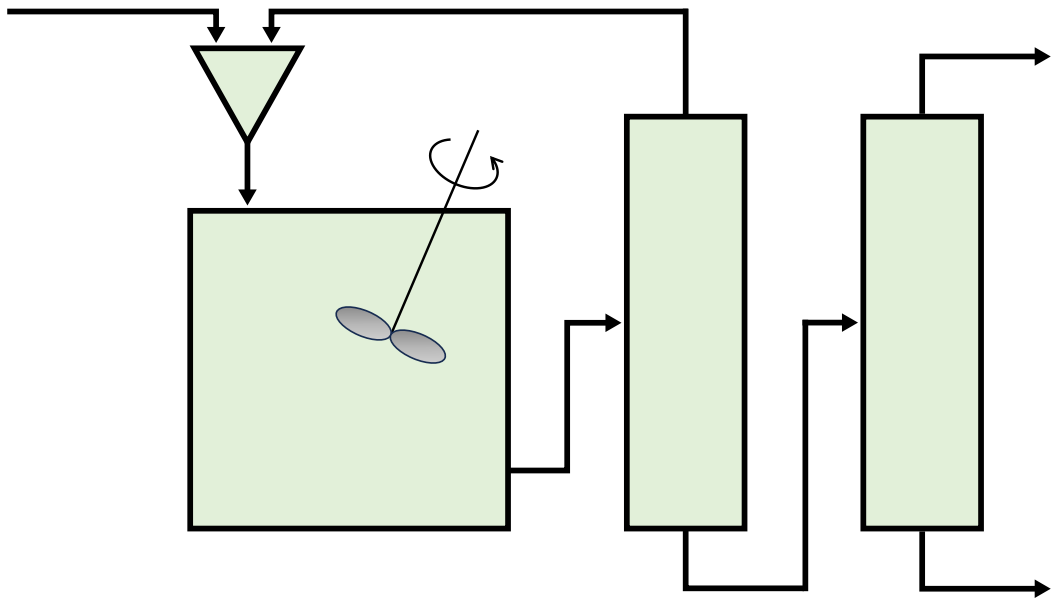
# EOptInterface.jl



# Steady-State Reactor Design Example

- Minimize total annualized costs
- Design variables:
  - Feed flowrate
  - Reactor volume

$$C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl$$
$$C_6H_5Cl + Cl_2 \rightarrow C_6H_4Cl_2 + HCl$$



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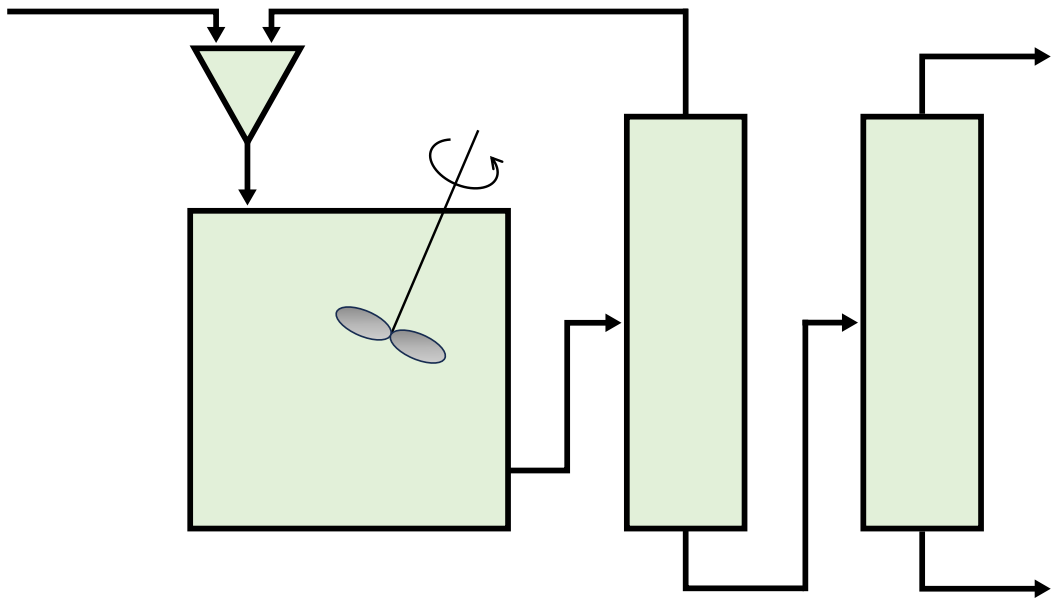
| Model | Number of variables | Solve Time (s) |
|---|---|---|
| Full-space | 50 | 202.0 |
| Reduced-space | 6 | 3.441 |



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# Kinetic Parameter Estimation Example

- Oxidation of cyclohexadienyl

$$\min_{\mathbf{p}} \phi(\mathbf{p},t) = \sum_{i=0}^{N} (I_i^{calc} - I_i^{exp})^2$$

$$\text{s.t. } \mathbf{p} \in [\mathbf{p}^L, \mathbf{p}^U]$$

$$I_i^{calc} = x_{A,i} + \frac{2}{21} x_{B,i} + \frac{2}{21} x_{D,i}$$

$$\frac{dx_A}{dt} = k_1 x_Z x_Y - c_{O_2}(k_{2f} + k_{3f}) x_A + \frac{k_{2f}}{K_2} x_D + \frac{k_{3f}}{K_3} x_B - k_5 x_A^2$$

$$\frac{dx_B}{dt} = c_{O_2} k_{3f} x_A - \left( \frac{k_{3f}}{K_3} + k_4 \right) x_B$$

$$\frac{dx_D}{dt} = c_{O_2} k_{2f} x_A - \frac{k_{2f}}{K_2} x_D$$

$$\frac{dx_Y}{dt} = -k_{1s} x_Z x_Y$$

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[10] Mitsos, A., Chachuat, B., and Barton, P.I. McCormick-based relaxations of algorithms. *SIAM Journal on Optimization, SIAM.* 20:2, 573-601 (2009).

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$$\frac{dx_Y}{dt} = -k_{1s} x_Z x_Y$$

$$\frac{dx_Z}{dt} = -k_1 x_Z x_Y$$

```
@mtkmodel KineticParameterEstimation begin
    @parameters begin
        T = 273
        K_2 = 46*exp(6500/T-18)
        K_3 = 2*K_2
        k_1 = 53
        k_1s = k_1*1e-6
        k_5 = 1.2e-3
        c_O2 = 2e-3

        k_2f
        k_3f
        k_4
    end
    @variables begin
        x_A(t) = 0.0
        x_B(t) = 0.0
        x_D(t) = 0.0
        x_Y(t) = 0.4
        x_Z(t) = 140.0
        I(t)
    end
    @equations begin
        D(x_A) ~ k_1*x_Z*x_Y - c_O2*(k_2f + k_3f)*x_A + k_2f/K_2*x_D + k_3f/K_3*x_B - k_5*x_A^2
        D(x_B) ~ c_O2*k_3f*x_A - (k_3f/K_3 + k_4)*x_B
        D(x_D) ~ c_O2*k_2f*x_A - k_2f/K_2*x_D
        D(x_Y) ~ -k_1s*x_Z*x_Y
        D(x_Z) ~ -k_1*x_Z*x_Y
        I ~ x_A + 2/21*x_B + 2/21*x_D
    end
end
```

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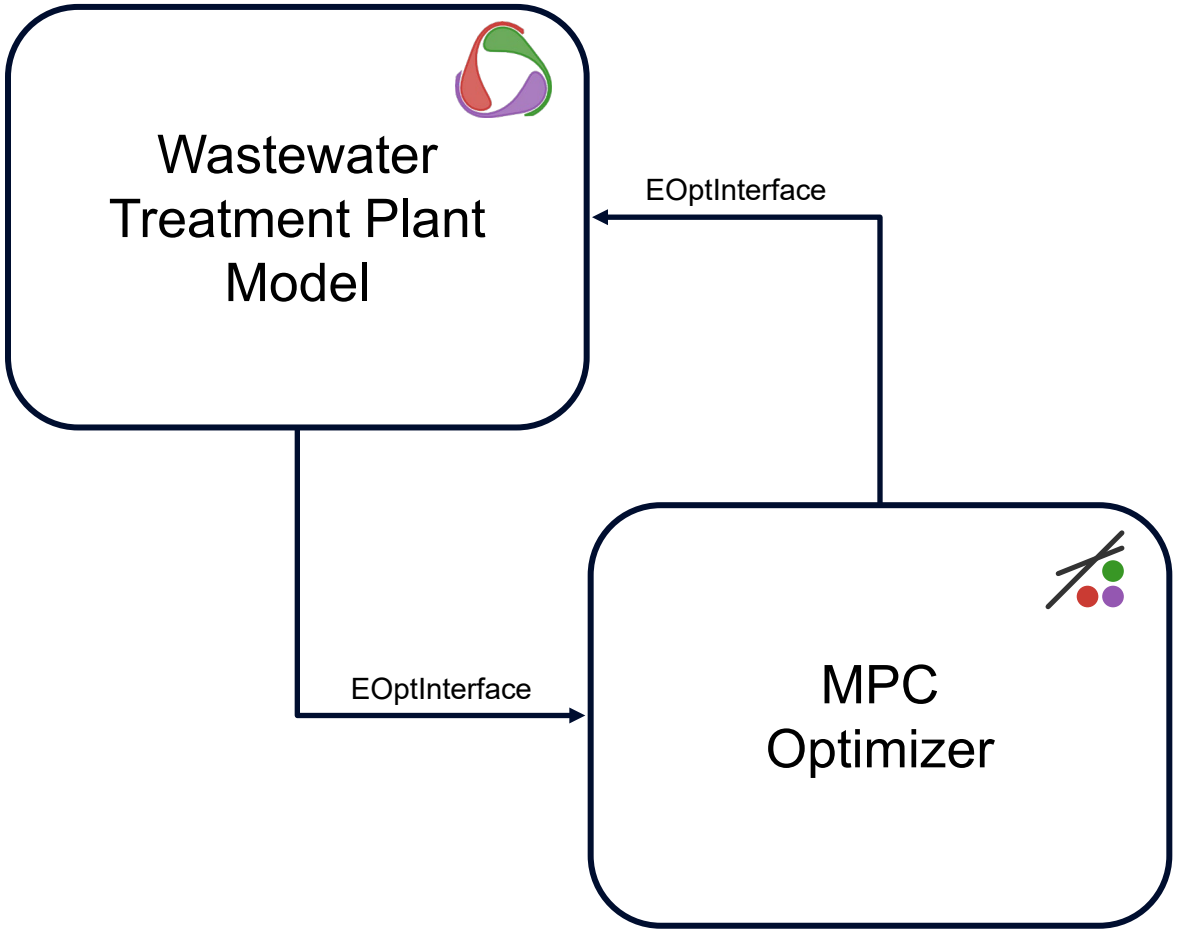
# Kinetic Parameter Estimation Example

- Oxidation of cyclohexadienyl

| Integration Method | Objective Value | Solve Time (s) |
|---|---|---|
| Explicit | 9622.8 | 0.1072 |
| Implicit | 16796.0 | 0.1006 |

[10] Mitsos, A., Chachuat, B., and Barton, P.I. McCormick-based relaxations of algorithms. *SIAM Journal on Optimization, SIAM.* 20:2, 573-601 (2009).

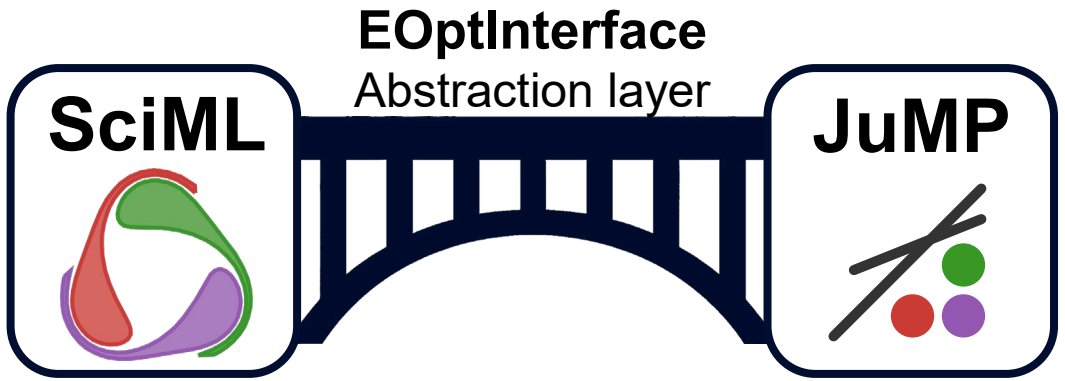
# Nonlinear Model Predictive Control




124e Improving Operations of Wastewater Treatment Plants Using Economic MPC

# Conclusion

- Deterministic global optimization tools are necessary for complex engineering models
- EOptInterface.jl
  - Seamlessly integrates modeling and simulation with formal optimization
  - Contains multiple discretization techniques for ODEs
  - You can use your favorite solver



# Acknowledgements

Members of the Process Systems and Operations Research Laboratory at the University of Connecticut (https://www.psor.uconn.edu)

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Process Systems and Operations Research Laboratory

Pratt & Whitney Institute for Advanced Systems Engineering UNIVERSITY OF CONNECTICUT

2025 AIChE ANNUAL MEETING

**Funding:**

**Department of Energy, Award No.: DE-EE0010991**

**National Science Foundation, Award No.: 2051084**

**Pratt & Whitney Endowed Professorship**

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation or the United States Government.

# Questions?

## Process Systems and Operations Research Laboratory

The PSOR Laboratory at UConn develops numerical analysis methods and software for process systems engineering applications.

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https://psor.uconn.edu

https://github.com/PSORLab