IDAES – Where Now?

Revisiting The Original Vision: Foundational & Mathematical Needs – Planning For The Future

Marriott City Center, Pittsburgh

September 18, 2024

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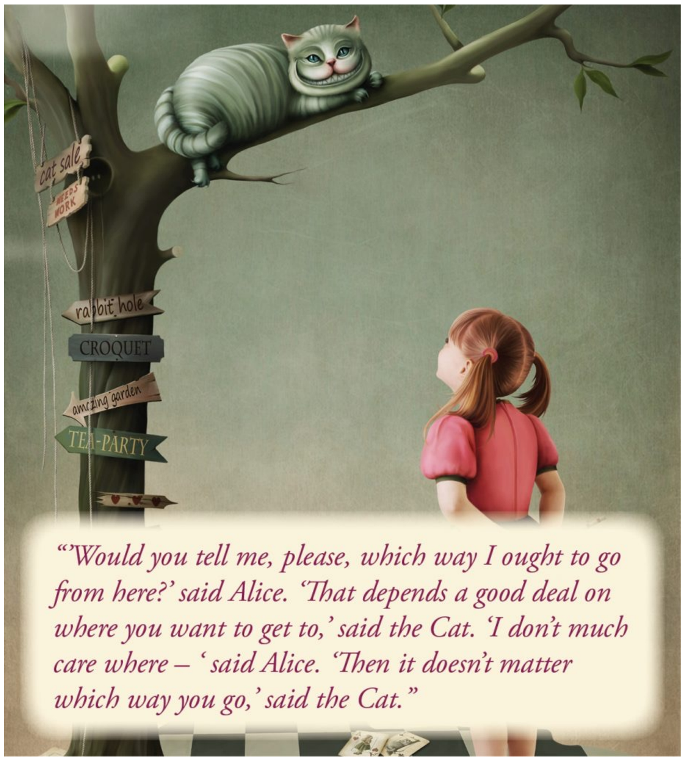
Why Are We Here?



IDAES has choices to make – where to invest and what drivers to pay attention to that can be influenced by mathematics – modeling for sure but optimization and real time control

Computational mathematics for real-time, *in situ* optimization and decision-making applied to large-scale, complex systems

You've got to be very careful if you don't know where you are going, because you might not get there.

[Yogi Berra]

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Key Points

- IDAES – applications ***and*** technology ***have been really instrumental in moving things forward for PSE*** – this has been a great program from 2017-today
- Applications are now the current focus – ***there is a broad footprint which is great***
- Having said this - ***we are now greedily eating our seed corn***
- ***What this means is that underlying technology – "math" – is a necessary investment*** (and does not come overnight or for free) and has diminished from the IDAES (read: DOE) portfolio

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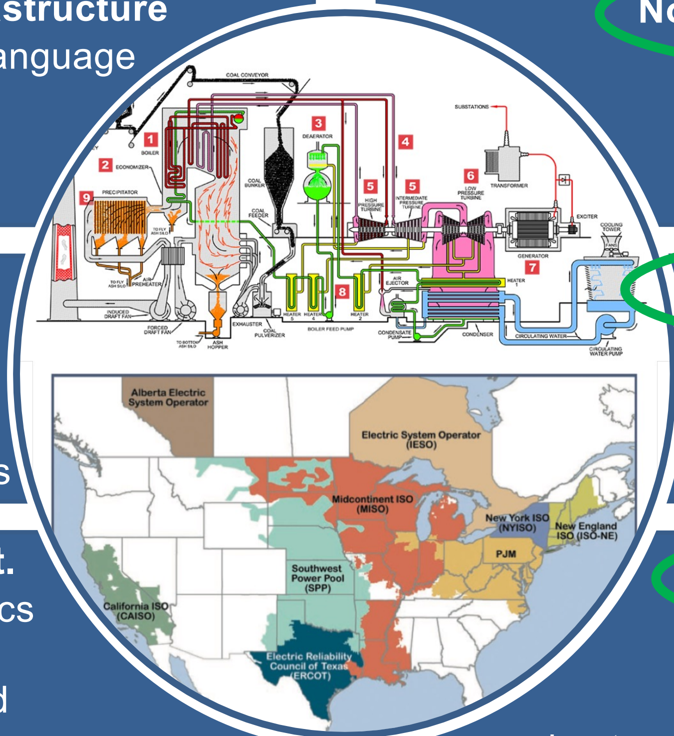
2017 Vision

Core Enabling Technologies for IDAES

Software and Computational Infrastructure
- open-source, algebraic modeling language with rich programming capabilities
- advanced solvers / architectures
- full data provenance (DMF)

Modeling Framework & Library
- library of process unit operations
- rigorous thermo, properties multiphase physics
- grid operation and planning models

Machine Learning / Parameter Est.
- physical properties, thermodynamics reaction kinetics
- multi-scale surrogate modeling and optimization



Nonlinear Simulation & Optimization
- design, operations, estimation
- optimal control and dynamics, trajectory, state estimation
- rigorous embedded black-box

Discrete Optimization (MILP/NLP)
- design, integration, intensification
- materials optimization
- grid integration, market analysis, grid operations and planning

Uncertainty Quant. / Optimization
- comprehensive, end-to-end UQ
- efficient sensitivity analysis
- two-stage stochastic programming
- robust optimization, adaptive robust optimization

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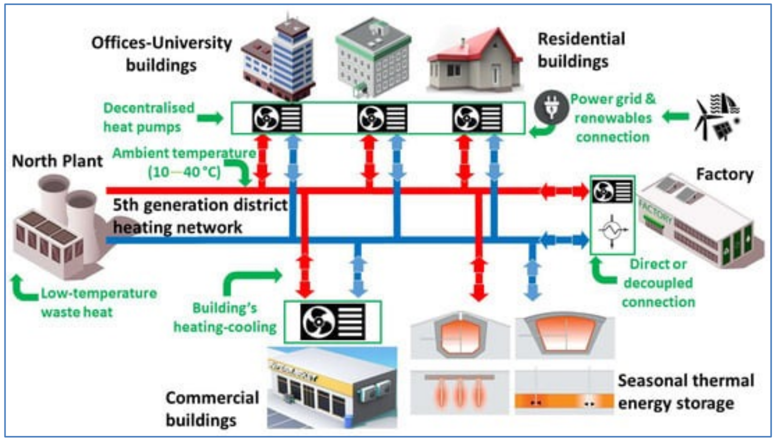
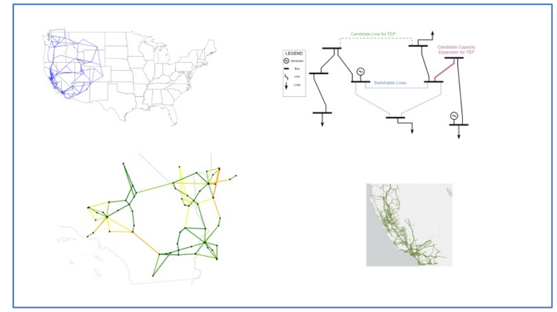
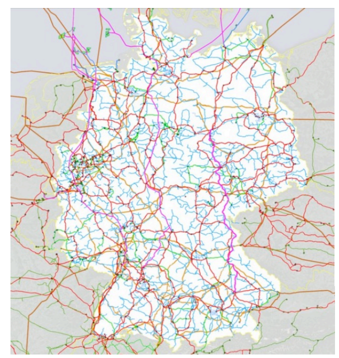
Things Are Changing…

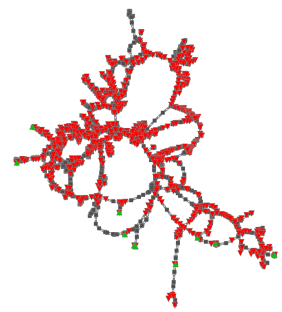


District Energy

Electric grids







Gas piplines
metric networks

Abstraction: all of these are "dynamic architectures" – dynamics (resource allocation on a network) and "changing the network" (robust, resilient)

Mathematical Needs and Future Research
IDAES Is Not Done…(End Of The Beginning…)

- **Decomposition – reduce complexity**
  - This is no longer hierarchical
  - Spatial, temporal, uncertainty all matter
- **Overall problem: MINLP – continue to find ways to solve higher fidelity**
  - Decompose by: space, time, uncertainty
  - We need an optimization strategy that decomposes the problem into linked components with explicit coupling information
    - We need fast, scalable algorithms for each component
    - We need robust iterative approaches to resolve coupling equations\
    - We need to use ML/AI methods
- **Parallelized Dynamic Optimization Algorithms – much (!) better NLP**
- **Extensible modeling approaches to support capturing and exploiting higher levels of abstractions**

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The Engines for Nonlinear Optimization

1980s: Flowsheet optimization - > 100 variables and constraints

1990s: Static real-time optimization (RTO) > 100 000 variables and constraints

2000s: Simultaneous dynamic optimization > 1 000 000 variables and constraints

2010s: Dynamic real-time optimization - on-line solves for large NLPs: ~ 1 CPUs

SQP → **rSQP** → **IPOPT** → **sIPOPT**

- ***Don't Search! - Solve Optimality conditions directly***
- Newton-based, optimization solvers
- Large-scale: fast, global convergence properties
- Exact 1st & 2nd derivatives
- Exploit structure, parallelism at linear algebra level
- Interface with external objects
- Efficient NLP solvers allow

$>10^6$ variables, constraints.

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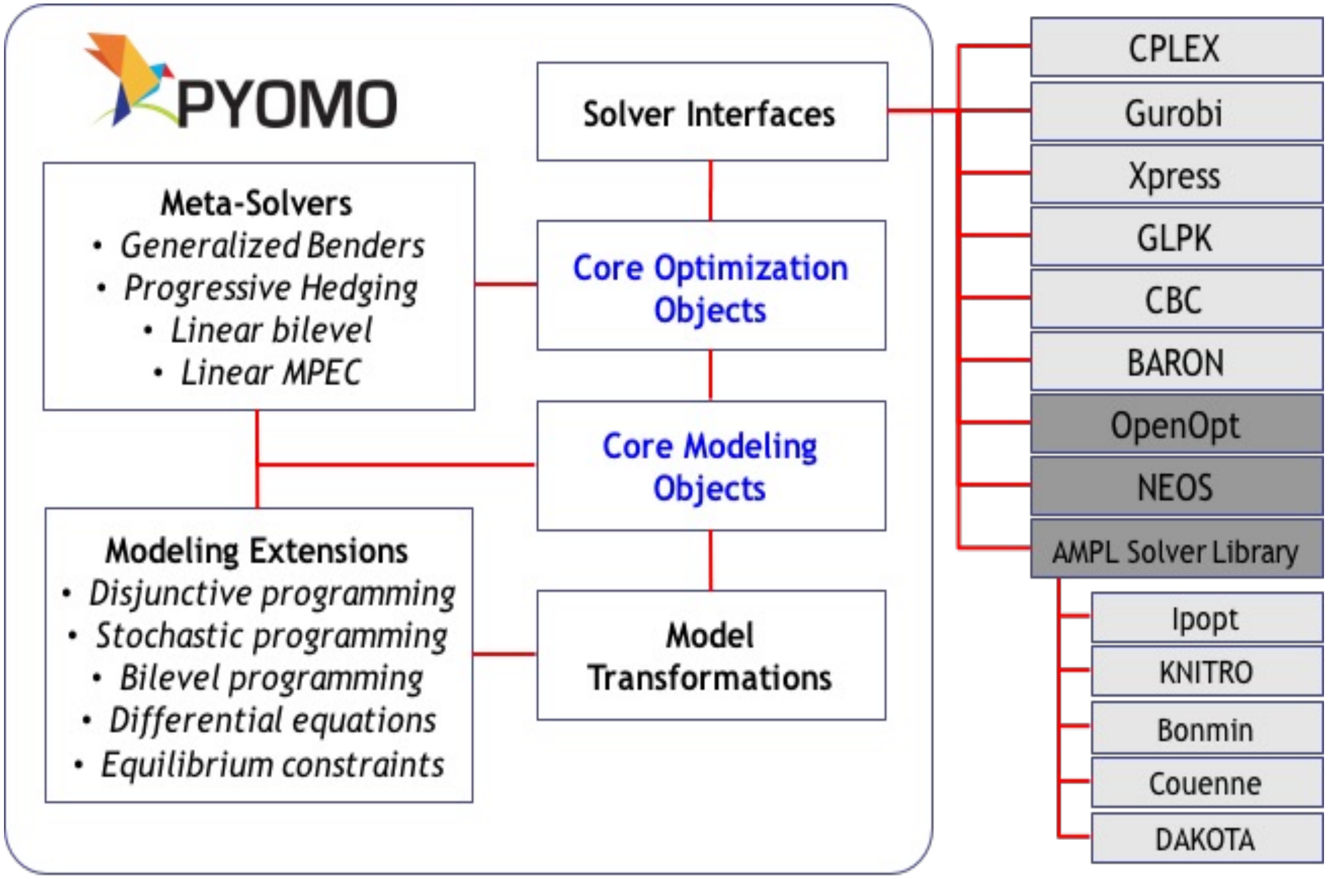
State of Art Optimization Modeling Platform



Extended Models: Continuous Optimization for (Some) Discrete Decisions

Min Overall Objective
s.t. Conservation Laws
Performance Equations
Constitutive Equations
Process/Product Specifications

Minimize Gibbs Free Energy
(Phase/Chem. Equilibrium)

Minimize Utilities
(Heat Integration)

→ Consider MPCCs derived from Bi-level Optimization

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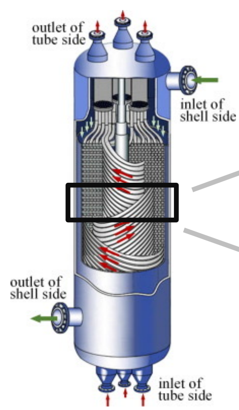
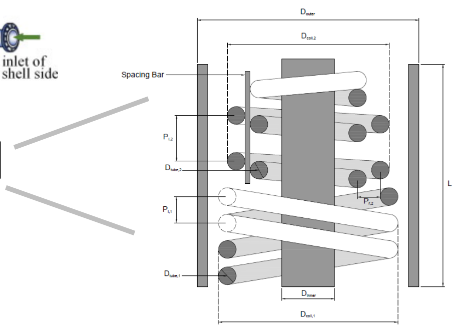
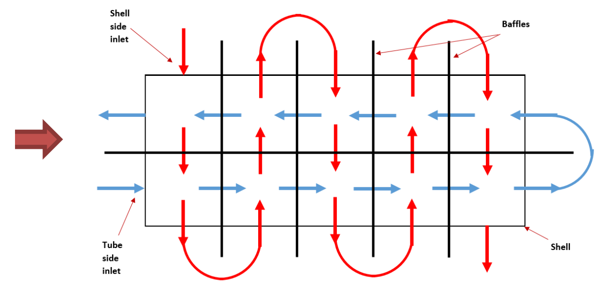
LNG Spiral Wound Heat Exchangers



Ding et al. (2017)



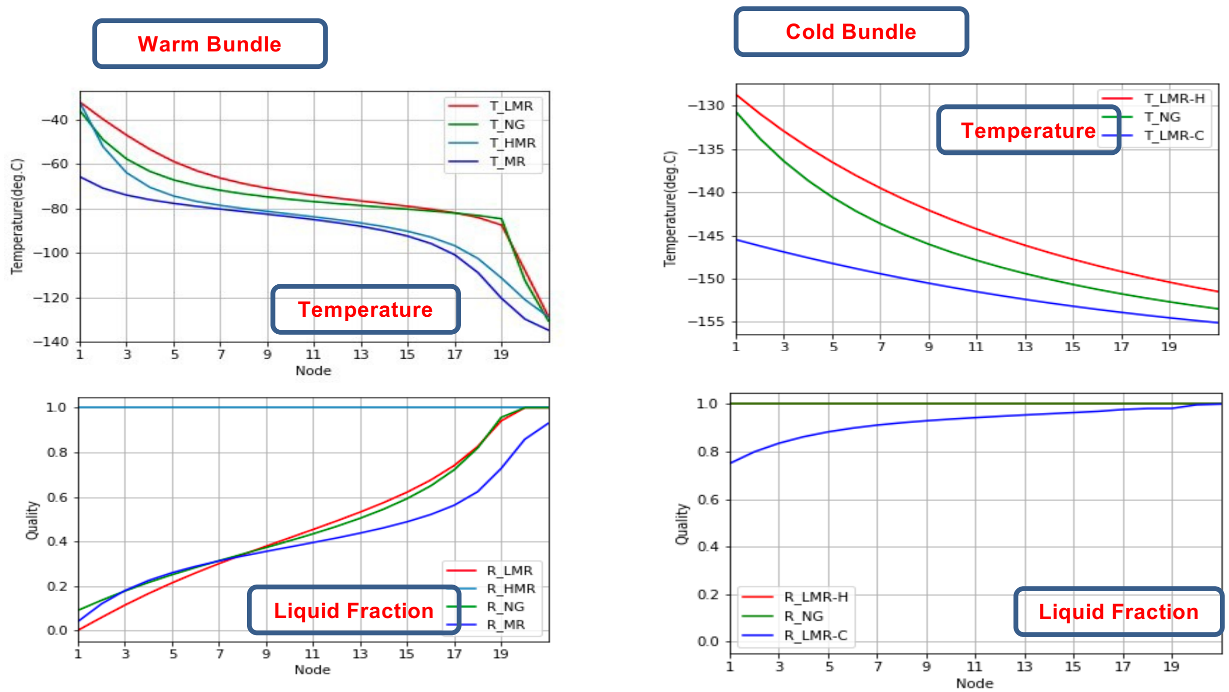


- Spiral wound heat exchanger (SWHX): tubes coiled around central rod with shell fluid flowing over tubes
- SWHX streams discretized to finite elements to solve heat equation

Optimal MR Composition

Variable	Value
Nitrogen	0.046
Methane	0.404
Ethane	0.5
Propane	0.05

Optimum Multi-Phase LNG SWHX



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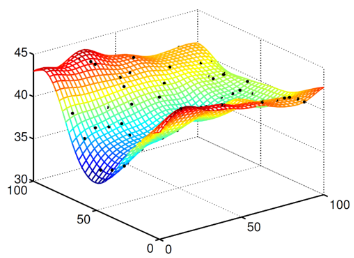
Data-Driven Surrogate Models: Main Ingredients

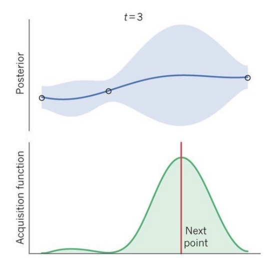
Experimental Design
- Factorial
- Central Composite
- Box-Behnken
- D-Optimal
- G-Optimal
- Orthogonal Array
- Plackett-Burman
- Hexagon
- Hybrid
- **Latin Hypercube**
- Random Selection
- **Quasi-Random**

Model Selection
- **Polynomial**
- Splines
- Realization of a Stochastic Process
- Kernel Smoothing
- **Radial Basis Functions**
- **(Kriging)**
- **Gaussian processes**
- **Neural Networks**
- Rule-based or Decision Trees

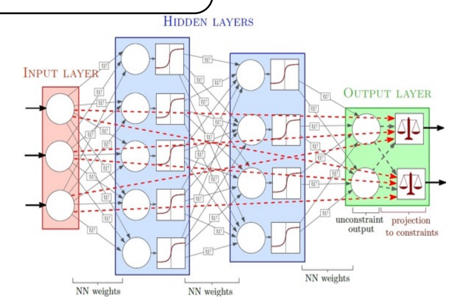
Model Fitting
- Least Squares Regression
- **Weighted Least Squares Regression**
- Best Linear Unbiased Predictor
- **Best Linear Predictor**
- Log-likelihood
- Back-propagation
- Entropy
- **Stochastic Gradient Descent (SGD)**



Kriging



Gaussian Processes



Machine learning
Neural Networks

Do surrogate models extend to optimization?
- Accurate fit?
- Well-poised models?
- Preserve the physics?

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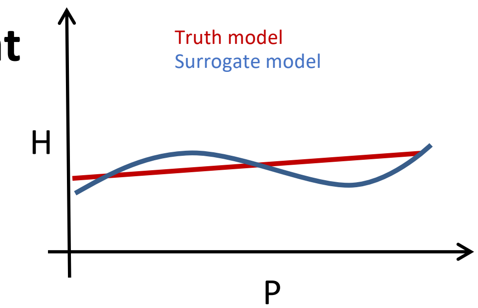
... Even good surrogate models may not lead to accurate optima!

- Optimizer can exploit small errors **and cheat**
- <u>Example:</u> Enthalpy of vapor stream



Propose surrogate $r(T,P) \approx H(T,P)$

$\frac{\partial H}{\partial P} \approx 0$ at high T and low P (equality holds for ideal gas)

However, supposed $\frac{\partial r}{\partial P} = -\epsilon$ at some T, P

This means that an arbitrarily accurate surrogate can give us **compressors that create work!**

- <u>Need to add some 'Reality' to control the errors!</u>

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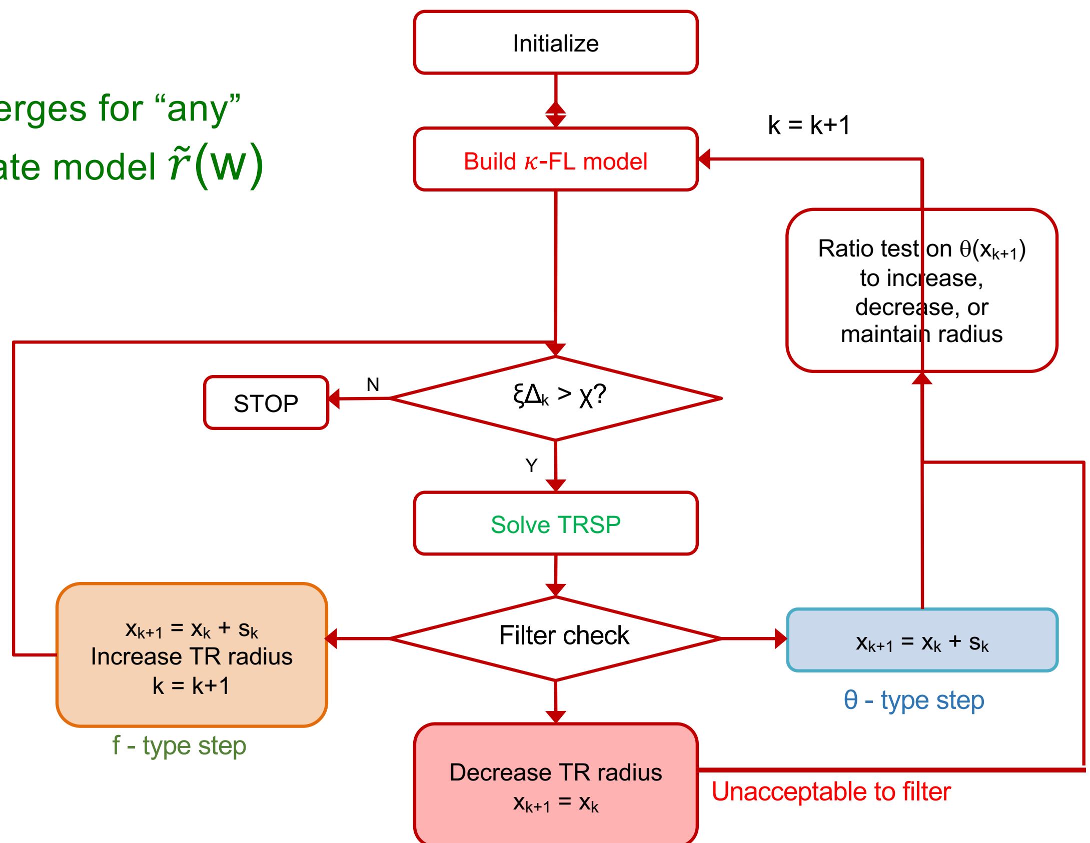
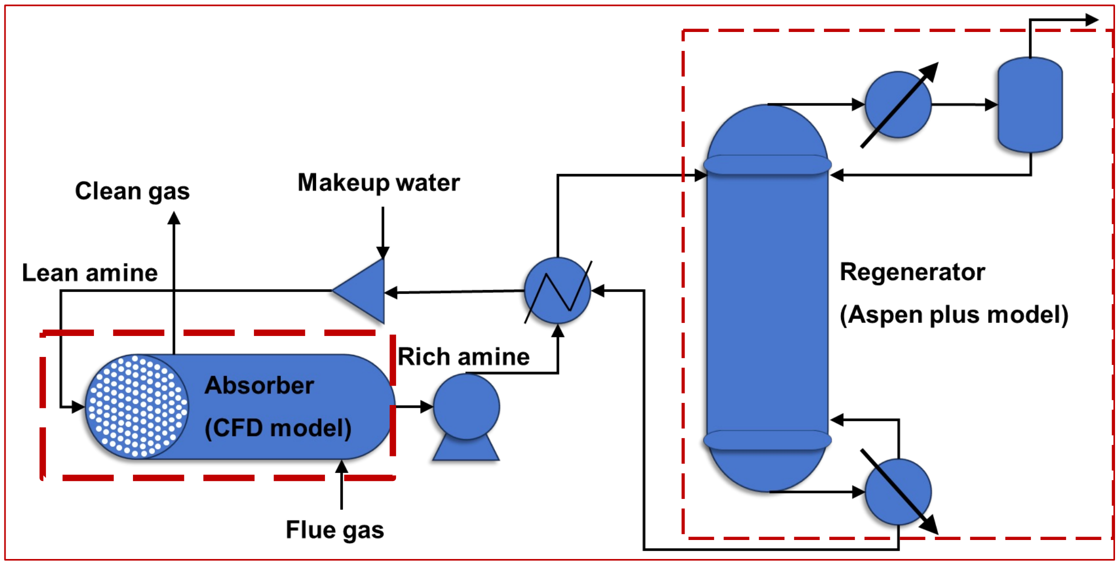
Trust Region Filter (TRF) Algorithm (*w/TM gradients*)

$$y = r_k(w) = \tilde{r}(w) + (t(w_k) - \tilde{r}(w_k)) + (\nabla t(w_k) - \nabla \tilde{r}(w_k))^T (w - w_k)$$

Converges for "any" surrogate model $\tilde{r}(w)$

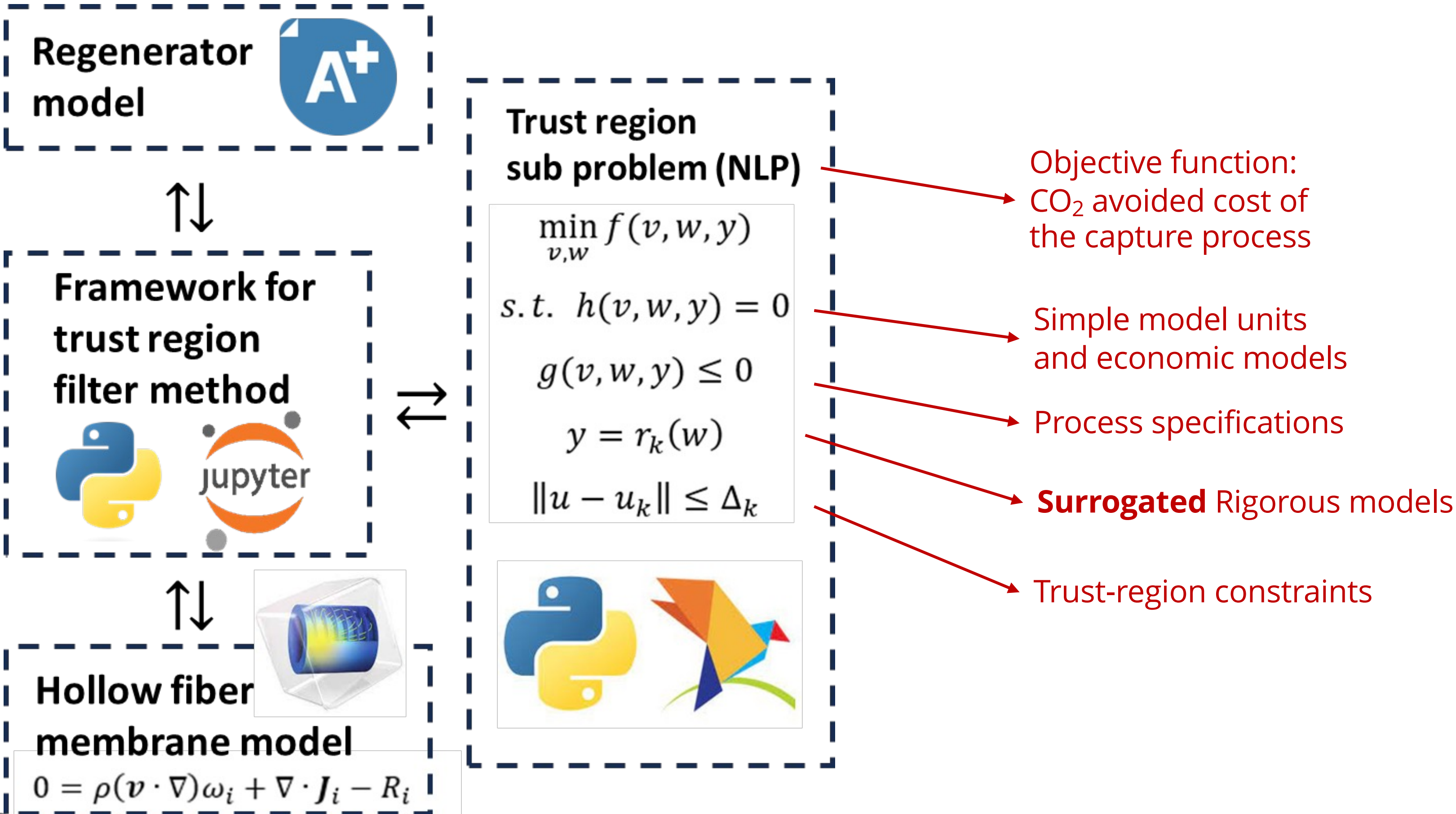


Carbon Capture with Membrane Contactors (Pedrozo et al.,2024)



Models for simple units (heat exchangers and pumps) are implemented in Pyomo directly

Integrated Multi-Model Solution strategy



Optimal Results: Performance Metrics

	Base Case	Optimal Design	
CO_2 avoided cost (\$/t-CO_2)	118.01	**54.16**	-54%
Capital cost (MM\$)	105.80	**39.74**	-62%
Operating cost (MM\$/y)	12.52	**9.52**	-24%
Total annual cost (MM\$/y)	35.23	**17.87**	-49%
Reboiler demand (GJ/t-CO_2)	4.68	**3.52**	-25%
Capture cost (\$/t-CO_2)	76.19	**39.71**	-48%
CO_2 recovery (%)	92.43	**90.00**	-3%

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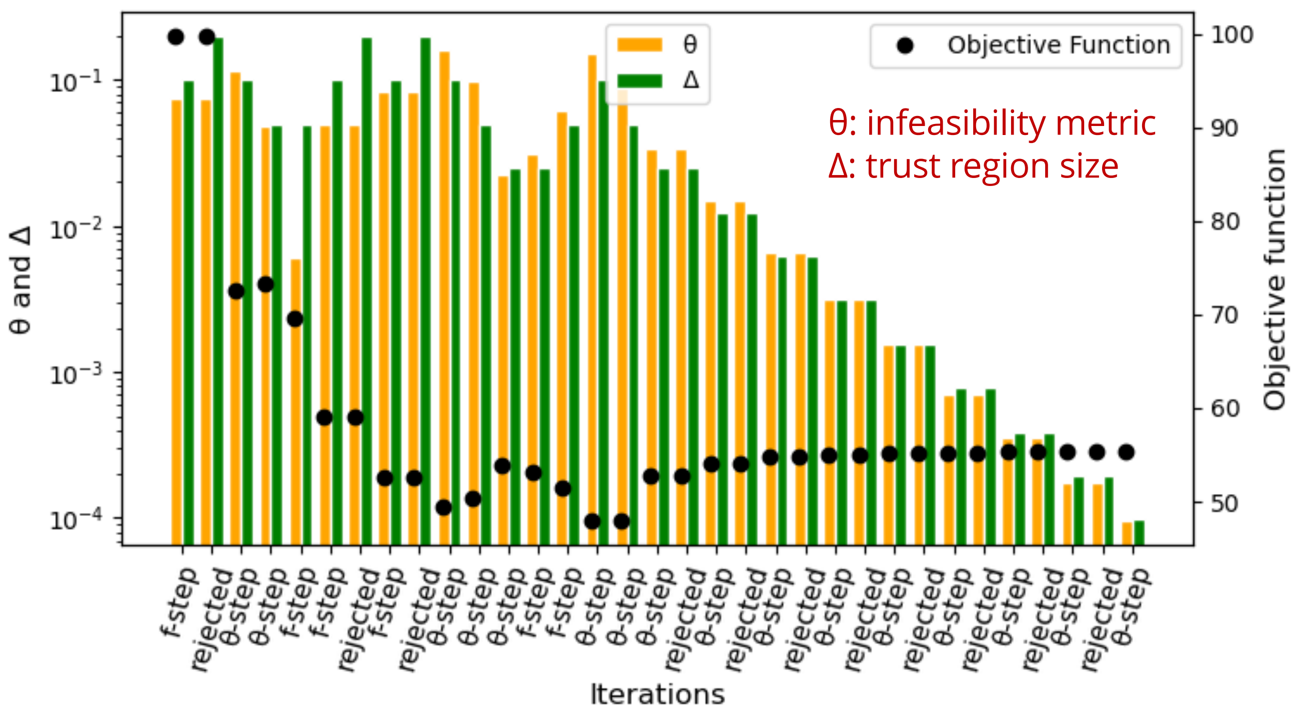
Performance of TRF algorithm



33 Iterations (1080 CPUs) of the trust-region filter method

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Summary and Conclusions

Fast Equation-Oriented Optimization is a reality

- Fast NLP tools, parallelized, with sensitivity
- Powerful modeling tools, esp. for structured large-scale models
- Optimization extensions to dynamic systems and under uncertainty

NLP → MPCC

- Switching models as NLPs with Complementarities
- Multi-phase Phase Transitions for VLE Models
- Well-posed EO reformulation → fast solutions

Multi-scale Optimization

- Heterogeneous models (PDAE/DAE/AE)
- Wealth of reduced/surrogate models
- Convergent TR-based optimization strategies

Huge Potential for Process Optimization Applications

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