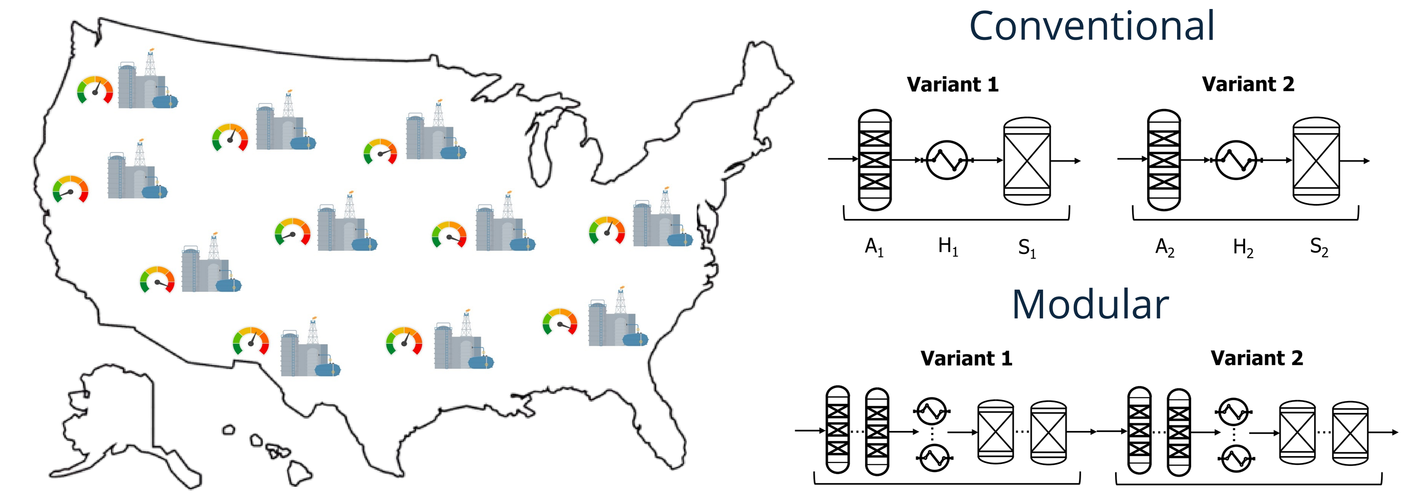
Efficient Global Optimization for Design of Chemical Process Families

Ali Asger[a], Georgia Stinchfield[a], Miguel Zamarripa[b,c], Carl D. Laird[a]

[a] Carnegie Mellon University, Pittsburgh, PA 15213; [b] National Energy and Technology Laboratory (NETL), Pittsburgh, PA 15236; [c] NETL Support Contractor, Pittsburgh, PA 15236

Motivation[1]

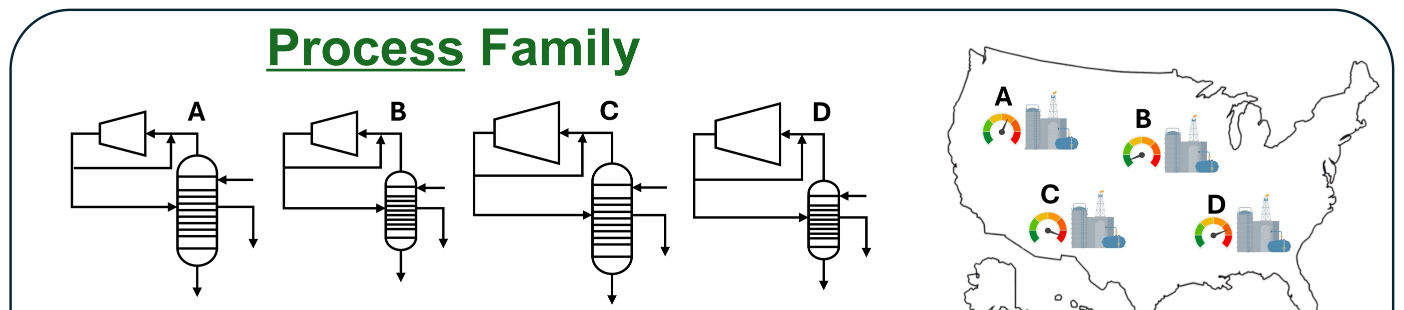
Rapid deployment of a **process system** across **decentralized sites** with **different** geographical, environmental and operating requirements.



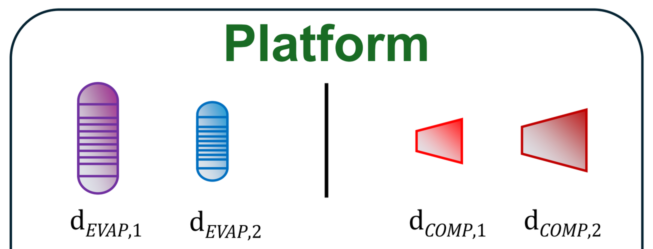
Process Family Design enables **reduced manufacturing costs, shared engineering effort** and **design flexibility**.

Process Family Design[2]

Simultaneous design of a **family of variants** with different design requirements, while **optimizing a platform** of **common shared components** and **their distribution** across the family.



Process *variants* assembled from units in the platform



Optimal balance between:
Uniqueness
Commonality

Optimization Formulation

$$\min \sum_{v \in V} \boldsymbol{w}_v \boldsymbol{p}_v \quad (1.1)$$ Minimize weighted sum of cost of every variant in family

s.t.

$$p_v = f_v^p(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}, \mathbf{o}_v) \quad \forall v \in V \quad (1.2)$$ Cost

$$\mathbf{i}_v = f_v^i(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}, \mathbf{o}_v) \quad \forall v \in V \quad (1.3)$$ Performance

$$0 = h(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}, \mathbf{o}_v) \quad \forall v \in V \quad (1.4)$$ Process physics

Model equations

$$\bigvee_{l \in L_c} \begin{bmatrix} Y_{v,c,l} \\ \mathbf{d}_{v,c} = \hat{\mathbf{d}}_{c,l} \end{bmatrix} \quad \forall v \in V, c \in C \quad (1.5)$$ → Distribution of common modules across variants

$$\hat{\mathbf{d}}_{c,l-1} \le \hat{\mathbf{d}}_{c,l} \quad \forall c \in C, l \in L_c \quad (1.6)$$ → Ordering platform designs by size

$$\hat{\mathbf{d}}_c^{LB} \le \hat{\mathbf{d}}_{c,l} \le \hat{\mathbf{d}}_c^{UB} \quad \forall c \in C, l \in L_c \quad (1.7)$$

$$\mathbf{o}_v^{LB} \le \mathbf{o}_v \le \mathbf{o}_v^{UB} \quad \forall v \in V \quad (1.8)$$

$$\mathbf{i}_v^{LB} \le \mathbf{i}_v \le \mathbf{i}_v^{UB} \quad \forall v \in V \quad (1.9)$$

Design and operating limits

$$Y_{v,c,l} \in \{\text{True}, \text{False}\} \quad \forall v \in V, c \in C, l \in L_c \quad (1.10)$$

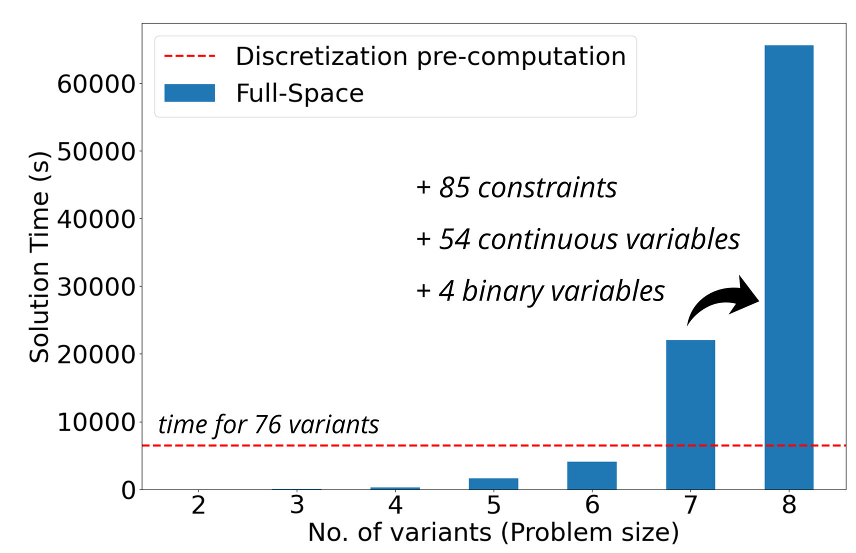
Full-Space Approach

Challenge (1.5) : Decisions within Disjunction

1) which design $l \in L_c$ for common modules $c \in C$ is assigned to each variant $v \in V$? → $Y_{v,c,l}$

2) what are the designs $l \in L_c$ for common modules $c \in C$ on the platform? → $\hat{\mathbf{d}}_{c,l}$

Scalability of problem with increasing problem size

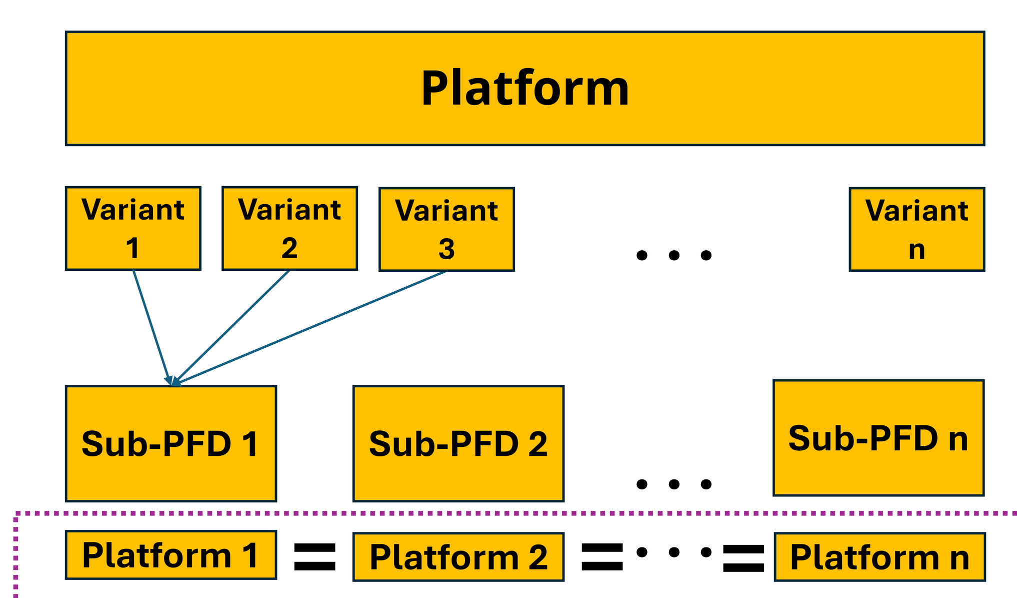


Solved using **BARON** (Off-the-shelf global optimization solver)

Need to improve scalability!

Decomposition Approach[3]

Block angular structure like a **two-stage stochastic program.**



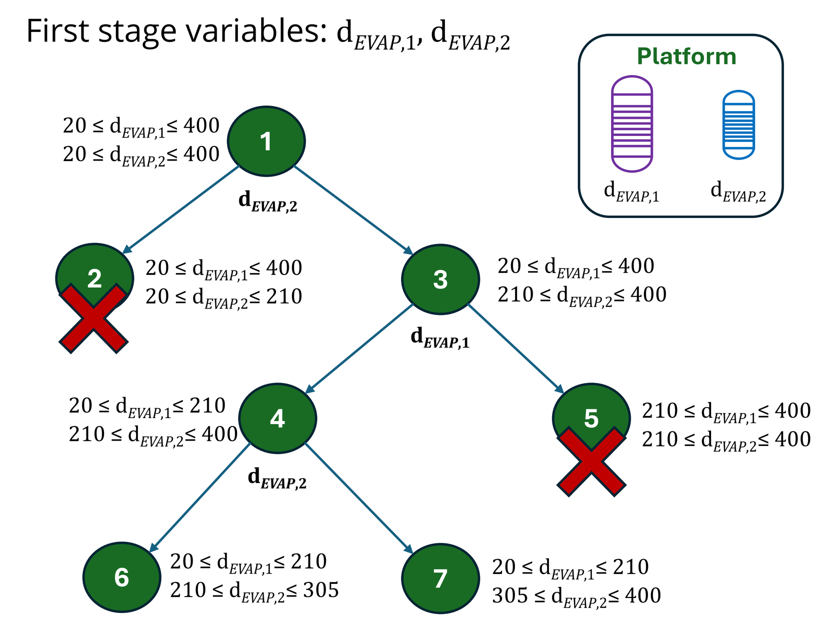
Shared among family of variants

Family of variants

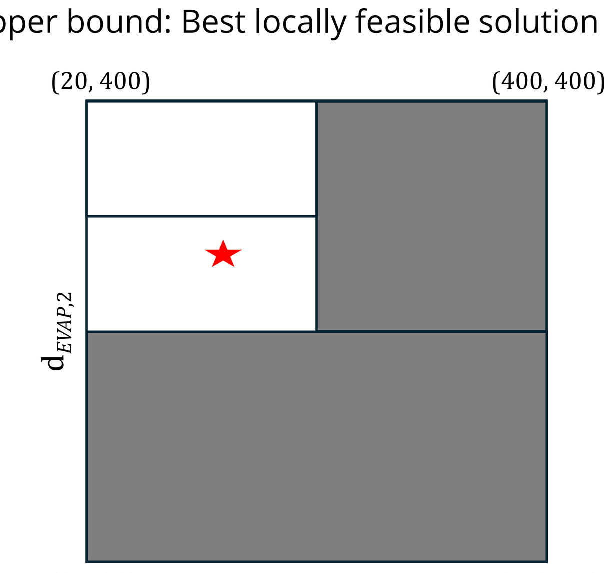
Smaller families with their own platforms

Solved the decomposed problem using a **reduced space branch and bound (B&B) algorithm** for global optimization of nonlinear stochastic programs.

First stage variables: $d_{EVAP,1}$, $d_{EVAP,2}$



Lower bound: Relax non-anticipativity constraint
Upper bound: Best locally feasible solution



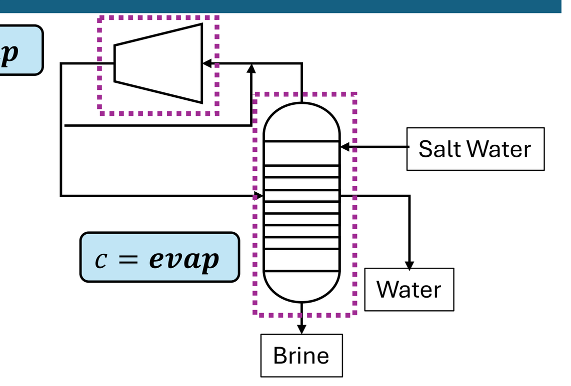
Case Study[4]

Water Desalination

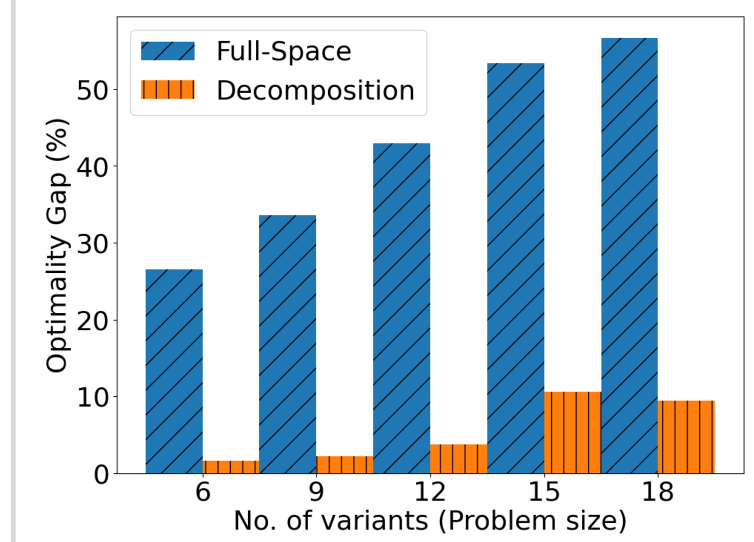
Variant design requirements
1) Salt water flow rate
2) Salt water concentration

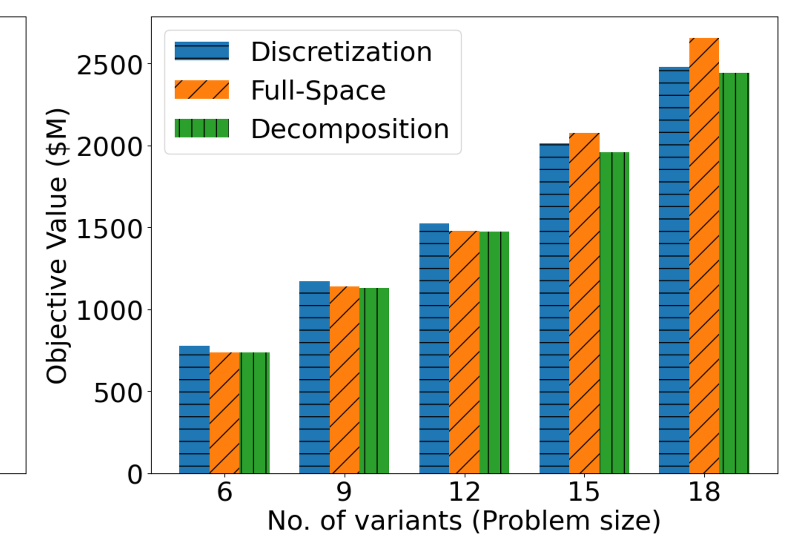
Common Units
1) Evaporator area
2) Compressor design flow

$C = [evap, comp]$



Results





- For the largest case of 18 variants, the **decomposition approach** achieves a **10% optimality gap**, while **the full-space approach** results in **an optimality gap > 50%.**
- For a solution time of **1 hour**, **up to 5% improvement in objective** compared to the **discretization approach,** and **up to 8% improvement in objective** compared to the **full-space approach**.

Conclusions

✓ Reduced manufacturing costs.
✓ Decomposition approach gives improved performance.
  - Scalability
  - Smaller optimality gaps
  - Increased annual cost savings
✓ Avoids large number of upfront simulations.

Future Work

- ❑ Investigate extensions of algorithm to decarbonization case studies.
- ❑ Application to more complex rigorous equation-oriented models.
- ❑ Incorporate quadratic approximations of nonlinear system models.

References

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Contact: Ali Asger, aasger@andrew.cmu.edu

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