IDAES

Institute for the Design of Advanced Energy Systems

David C. Miller NETL), Christopher Hanselman (CMU), Zachary Wilson (CMU), Cristiana Lara (CMU)

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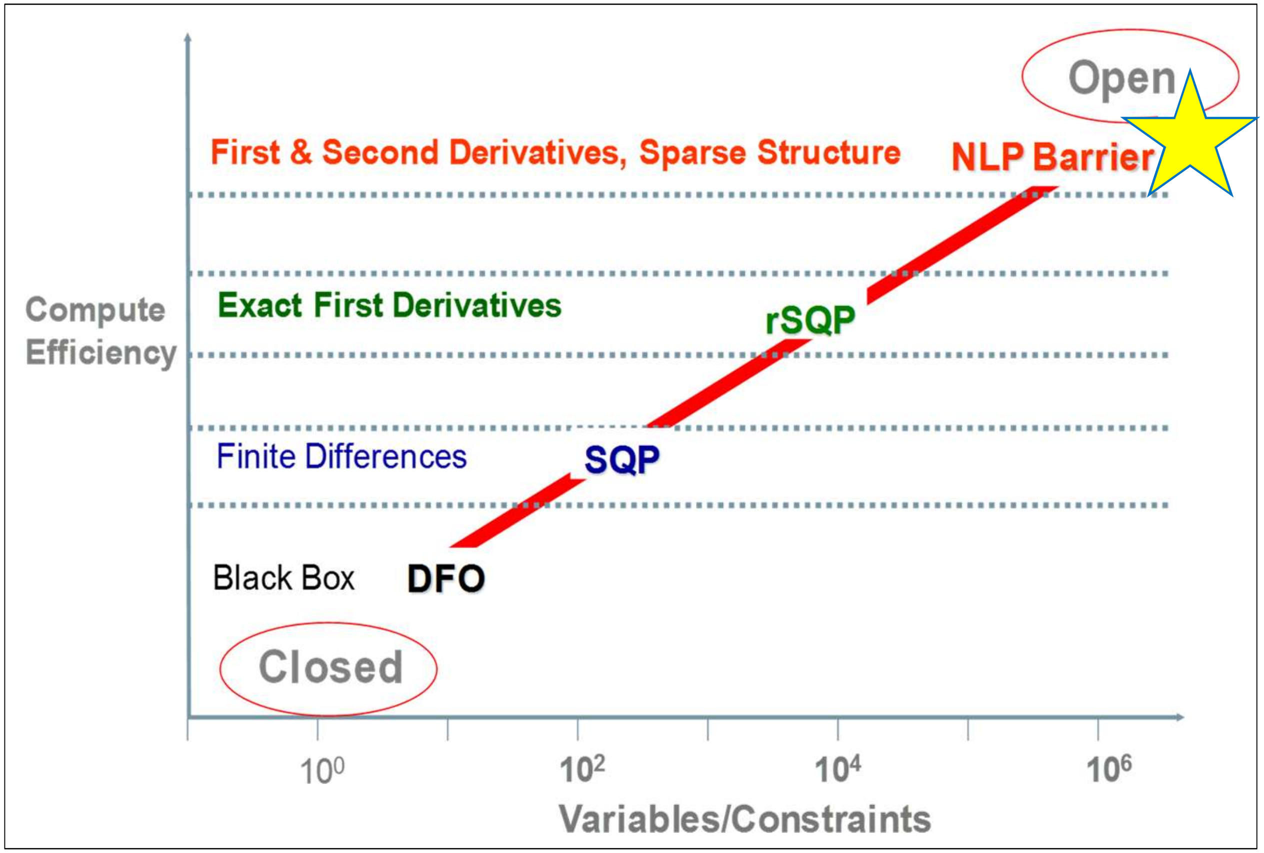
Overview

- **What is IDAES?**
  - Next Generation Multi-Scale Modeling & Optimization Framework
    - Bridges the gap between process simulators and algebraic modeling languages
  - Improving the efficiency and reliability of the existing fleet
  - Accelerating the development of advanced fossil energy systems
- **Why should you care?**
  - Enables optimization of innovative steady-state and dynamic processes
    - Flexible design approaches, which enable optimization over broad range of conditions
  - Extensible, equation-oriented process model library
  - Enables rigorous large-scale mathematical optimization
- **How can you be involved?**
  - Stakeholder Advisory Board
  - Open Source Release

The IDAES Modeling and Optimization Motivation & Approach



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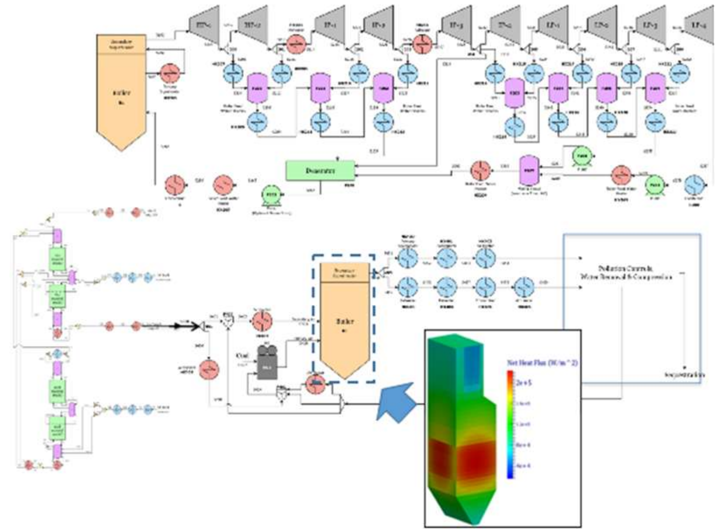
Development Of Innovative Advanced Energy Systems Through Advanced Process Systems Engineering

- **Challenge:** *Develop and utilize multi-scale, simulation-based. computational tools and models to support the design, analysis, optimization, scale-up, operation and troubleshooting of innovative, advanced fossil energy systems*
- **Next generation modeling and optimization platform**
  - Current tools insufficient to address demands of integrated systems
  - Need a more flexible and open modeling environment
- **Key capabilities**
  - Process Synthesis, Integration, and Intensification
  - Process Design and Optimization
  - Process Control and Dynamics
  - Supports advanced solvers and computer architecture
  - Multi-scale modeling capabilities
  - Comprehensive, end-to-end uncertainty quantification
  - Complete provenance information
  - Couple with energy market models
  - Open source



Improve efficiency and reliability of existing plants

Accelerate innovation

- *Identify technology solutions in the context of the full energy portfolio*

Focus and prioritize R&D at low TRLs

- *Assess new concepts using optimization tools to enable prioritization of research areas*
- *Chemical Looping, DPE, sCO_2*

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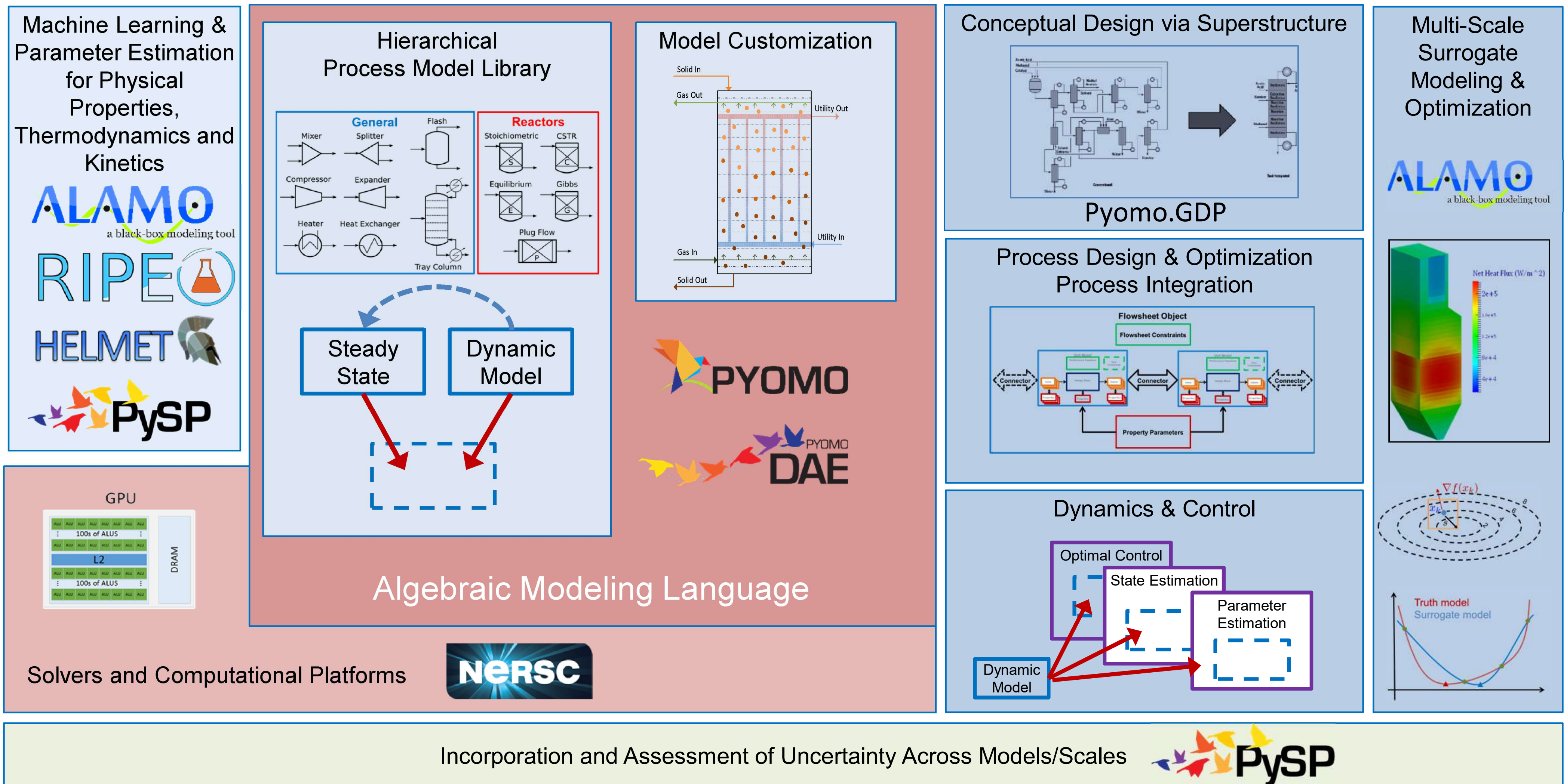

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IDAES Approach to Modeling & Optimization

Data	Submodels	Problem Formulation
Experimental Data	Thermo-physical properties Reaction kinetics & equilibrium Heat and mass transfer	Unit Models Flowsheets

Zachary Wilson
Data driven model selection and optimization

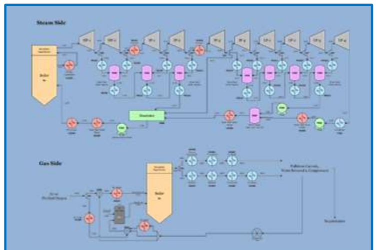
Data	Submodels	Problem Formulation
Computational Chemistry Experimental Data	Molecular Descriptors	Mathematical Model Motifs & Structure

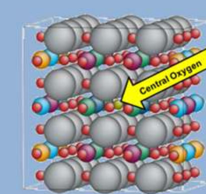
Christopher Hanselman
Designing optimal doped perovskite oxygen carriers

Data	Submodels	Problem Formulation
Grid Data from ISO Generator Cost/Performance Data Transmission Data Load/Demand Curves	Representative Dispatch Days Supply/Demand Models	Multi-scale Infrastructure Planning Model

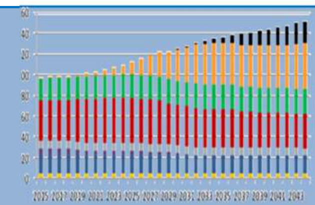
Cristiana Lara
Expanding the scope of electric power infrastructure planning

Transformations
Initialization
Solvers


Process Systems



Materials Optimization


Energy Market Model

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2018 Calendar Summary

- March 31, 2018: CCSI Toolset Open Source Release
- May 23-24 @ Washington, DC.
  - First major stakeholder meeting.
- June 30: Major (limited) release of IDAES software (1.0)
- July 1-5 @ San Diego, PSE2018 conference.
  - 10+ papers and plenary talk
- Nov. 1-2 with AIChE Mtg (Pittsburgh).
  - 2^{nd} major stakeholder meeting
- Dec. 31: Minor release (1.1) – Initial publicly available release

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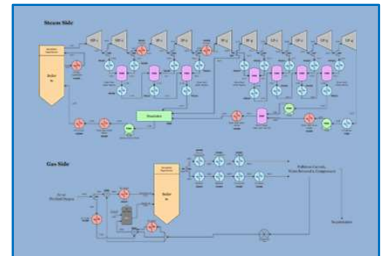
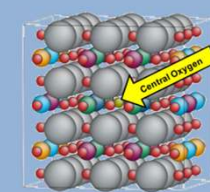
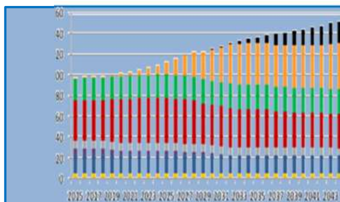


Process Systems



Materials Optimization



Energy Market Model

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ALAMO Python Module

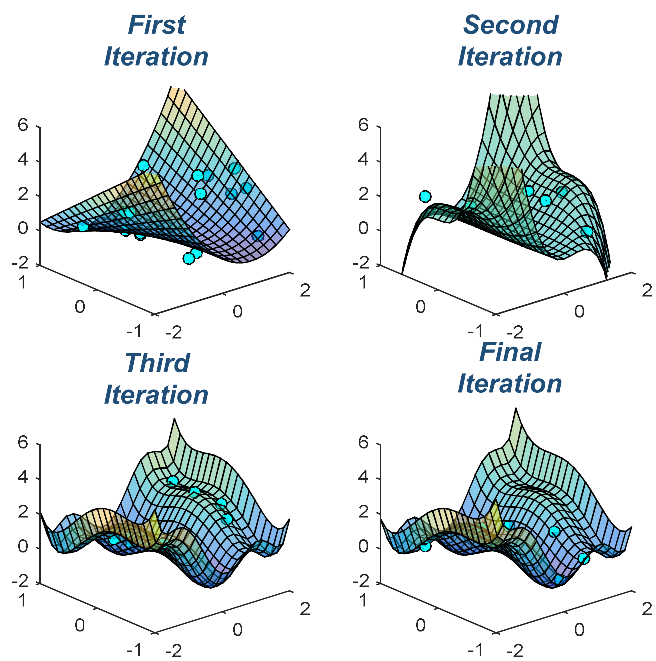
Simulator

Corrupted Six-Hump Camel Function

$$f(x) = \left(4 - 2.1x_1^2 + \frac{x_1^4}{3}\right)x_1^2$$
$$+x_1x_2 + x_2^2\left(4x_2^2 - 4\right) + \epsilon$$

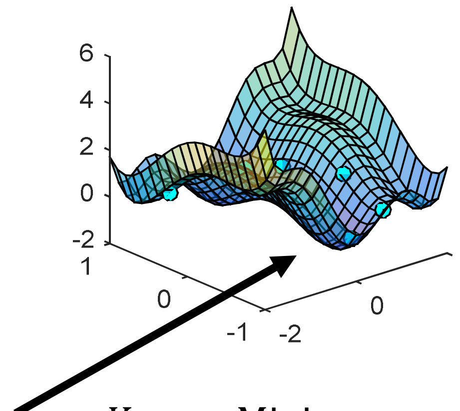
Iteration	N	R^2_{val}	$\lVert\beta\rVert_0$
1	17	0.56	2
2	23	0.61	3
3	31	0.92	11
4	37	0.98	6

Model Building - Alamo



Solvers

PYOMO



Known Minimum

$f(0.0898, -0.7126) = -1.0316$

Surrogate Minimum

$f(0.0881, -0.7114) = -1.0291$

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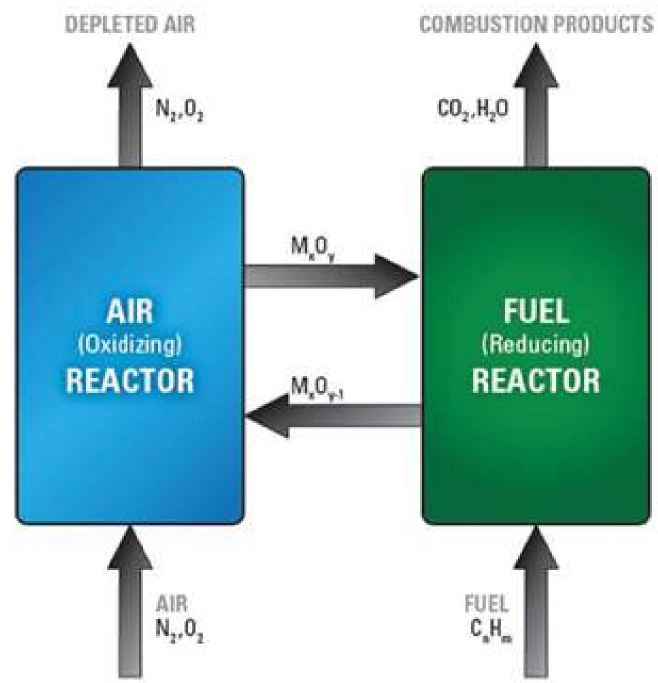
Tools for Kinetic Property Model

RIPE

Reaction Identification and Parameter Estimation

Elucidate unknown kinetics of chemical reactions occurring in a given reactor

Refine existing models through simultaneous consideration of existing and alternative forms



https://www.netl.doe.gov/research/coal/energy-systems/advanced-combustion/clc

Illustrative Example

Reaction network
(11 species and 6 reactions)

$$A \overset{ads}{\longleftrightarrow} B \overset{E}{\rightarrow} F + \frac{1}{2}J$$
$$B \rightarrow 2G + 2I$$

$$C \leftrightarrow D + E$$
$$B + C \rightarrow K + E + F + I + 2H$$
$$B + 2D \overset{E}{\rightarrow} 2F + 2\mathrm{H}$$

Rate laws
(1- through 4-body interactions)

$$r_1 = k_1(T)\phi_A \left(c_A - \frac{c_B}{K_1(T)}\right)$$
$$r_2 = k_2(T)\phi_B c_B^2 c_E$$
$$r_3 = k_3(T)\phi_B c_B$$
$$r_4 = k_4(T)\left(c_C - \frac{c_D c_E}{K_2(T)}\right)$$
$$r_5 = k_5(T)\phi_B c_B c_C$$
$$r_6 = k_6(T)\phi_B c_B c_D^2 c_E$$
$$k_j(T) = k_j^0 \exp\left(-\frac{E_j}{RT}\right)$$

- **Easy problem**
  - Given network and laws, calculate species concentrations
- **Our problem**
  - Find network and laws that match measurements

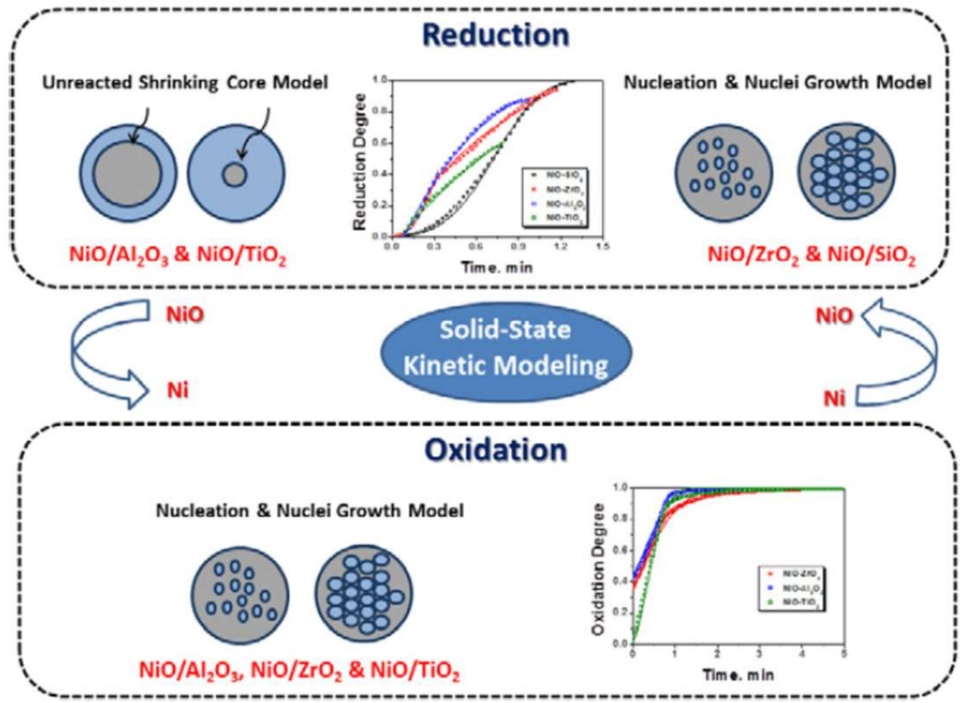
Parameter Estimates

- **33 possible reactions considered**
  - Reversible and irreversible mass action kinetics
  - Homogeneous and heterogeneous catalysis
- **Simultaneous identification and estimation**
  - 100 binary variables, 858 continuous variables, solved in 350 seconds using BARON 17.1.2

	$\hat{r}_1$	$\hat{r}_2$	$\hat{r}_3$	$\hat{r}_4$	$\hat{r}_5$	$\hat{r}_6$
$\hat{k}_j$	12.01 ± 0.2	$9.1 \pm .01$	6.9 ± 0.11	20 ± 2.0	5.1 ± 0.1	0.99 ± 0.01
k_j	**12**	**9**	**7**	**20**	**5**	**1**
$\hat{E}_j$	1001 ± 40	5012 ± 41	6955 ± 43	4010 ± 22	3531 ± 56	1986 ± 31
E_j	**1000**	**5000**	**7000**	**4000**	**3500**	**2000**

Experimental Case Study

- **Goal:** Identify mechanisms and estimate kinetic parameters in both reactors
- **Experimental details**
  - Fuel reactor $(650°C)$ in methane
  - Air reactor $(800°C)$
  - Two catalyst: NiO/Al_2O_3, NiO/TiO_2
- **RIPE methodology**
  - Dynamic problems require Alamo to estimate conversion profile



Ipsakis, Dimitris, et al. "Reduction and oxidation kinetic modeling of NiO-based oxygen transfer materials." *Chemical Engineering Journal* 308 (2017): 840-852.

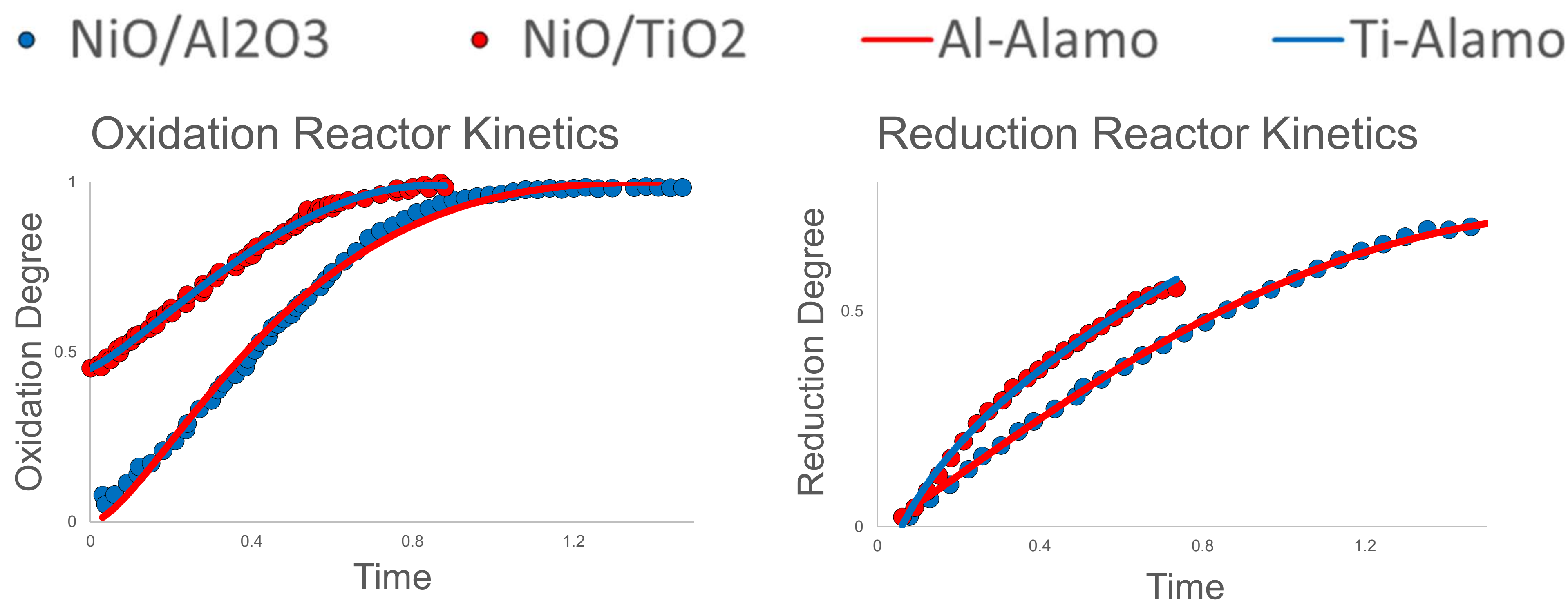
Application of RIPE

$$\frac{dX}{dt} = k(T)f(X)g(y_{gas})$$

- **User supplied functional form for $f(X)$ and $g(y)$**
- **19 possible rate forms included in superset**

- Nucleation and nuclei growth
  - Avrami-Erofeev of $\mathrm{n^{th}}$ order
    - $n(1-X)(-\ln(1-X))^{n-1/n}$
  - Prout-Tompkins
    - $X-(1-X)$
  - Random nucleation
    - $(1-X)$
- Diffusion equations
  - Parabolic law (1D)
    - $1/(2X)$
  - Valensi equation (2D)
    - $1/(-\ln(1-X))$
  - Jander equation (3D)
    - $3(1-X)^{4/3}\left((1-X)^{-1/3}-1\right)^{-1}$
- Reaction-based models
  - Mampel power law
    - $n(X)^{1-1/n}$
  - Power law
    - $n(1-X)^{1-1/n}$

Embedded use of Alamo



$$X_{Al}^{O} = \beta t^{2} + \beta t^{2.2} + \beta t^{2.5} + \beta t^{2.7}$$
$$X_{Ti}^{O} = \beta t^{1.2} + \beta t^{2.5} + \beta$$

$$X_{Al}^{R} = \beta t^{2} + \beta t^{1.2}$$
$$X_{Ti}^{R} = \beta t^{0.5} + \beta$$

RIPE Solution Statistics

Oxidation Kinetic Parameters

Catalyst	$f(X)$	k	$+/-$	$R^2(rate)$	$R^2(X)$
NiO/Al_2O_3	$X(1-X)$	**5.62**	**0.31**	0.854	0.99
NiO/Al_2O_3*	$4(1-X)(-\log(1-X))^{\frac{3}{4}}$	**0.62**		<0	0.98
$NiO/Ti\ _2$	$\frac{3}{2}(1-X)(-\ln(1-X))^{\frac{5}{6}}$	**1.65**	**0.03**	0.96	0.99
$NiO/Ti\ _2$*	$2(1-X)(-\log(1-X))^{\frac{1}{2}}$	**1.66**		<0	0.98

Reduction Kinetic Parameters

Catalyst	$f(X)$	k	$+/-$	$R^2(rate)$	$R^2(X)$
NiO/Al_2O_3	$(1-X)$	**0.79**	**0.04**	0.85	0.99
NiO/Al_2O_3*	$(1-X)^{\frac{2}{3}}$	**0.77**		0.68	0.99
NiO/TiO_2	$(1-X)^{\frac{2}{3}}$	**1.2**	**0.14**	0.61	0.99
NiO/TiO_2*	$(1-X)^{\frac{2}{3}}$	**1.15**		0.6	0.99

Accurate kinetic parameters with associated confidence intervals

Modeling Tool Contributions

- **Pyomo models are automatically generated**
  - Data-driven algebraic models for use in the IDAES framework
    - EOS models, Kinetic network, or data-driven surrogate models
  - Provenance for updating and tracking solution quality

- **Adaptive design of experiments**
  - Error maximization sampling extended acquisition of new data

- **Sensitivity of estimated parameters**
  - Interfacing with UQ to facilitate propagation of uncertainty through IDAES framework

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Motifs & Structure

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Transmission Data
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Representative Dispatch Days
Supply/Demand Models

Multi-scale Infrastructure
Planning Model

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Transformations
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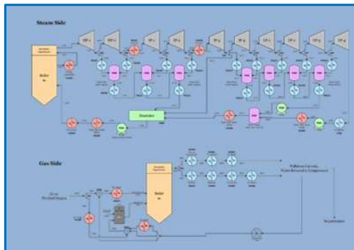
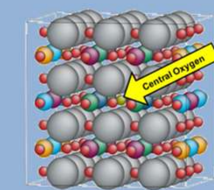


Process Systems



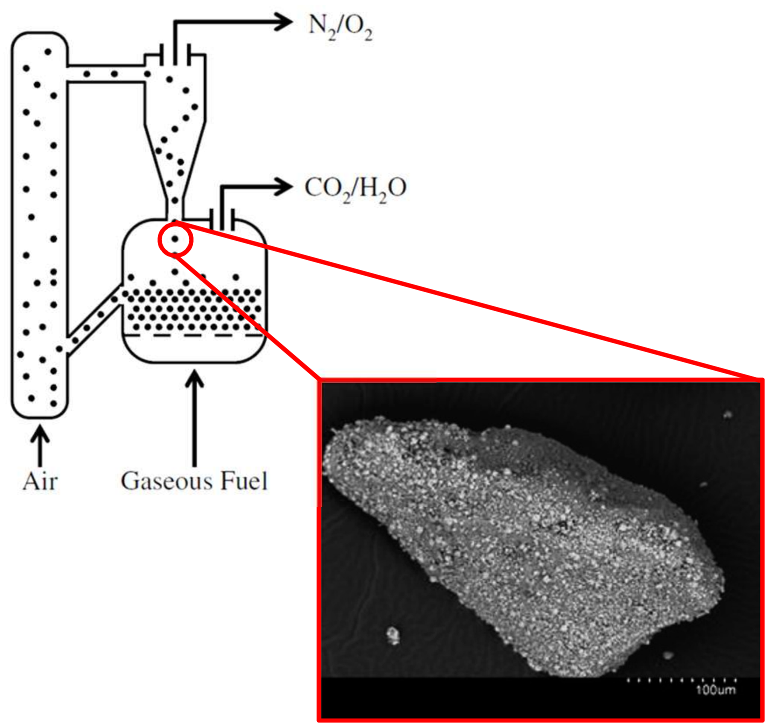
Materials Optimization

Energy Market Model

Importance of Oxygen Carriers for CLC

- CLC provides a variety of benefits over traditional fossil fuel combustion
  - Easy **recovery of CO_2** from waste streams
  - Potential for **co-generation of H_2** for liquid fuel (via SR-CLC)
  - Access to **higher thermodynamic efficiencies**

- Performance is currently limited by the **tradeoff of reactivity against stability** for oxygen carrier being cycled through the reactors
  - High activity oxygen carriers tend to experience high attrition
  - Low activity oxygen carriers will require large solids recycle streams



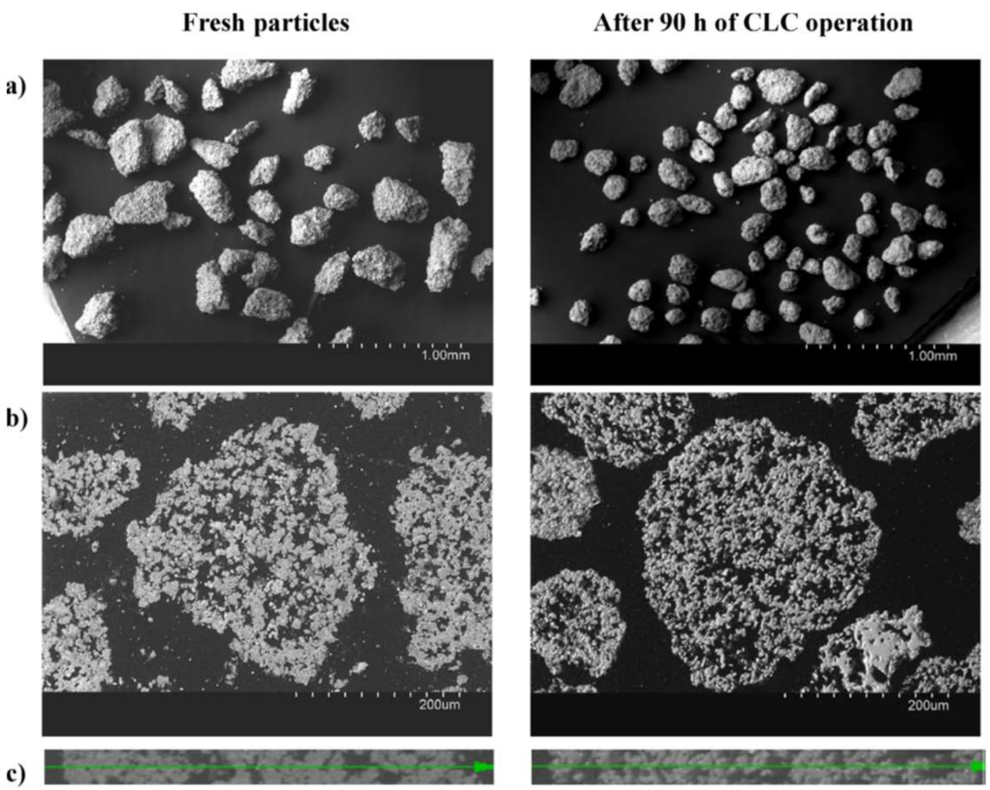
L.F. de Diego *et al.*, *Fuel*, 86(7-8):1036–1045, 2007

J. Adanez *et al.*, *Progress in Energy and Combustion Science*, 38(2):215–282, 2012.

Current Status of Oxygen Carrier Development

- Large body of experimentally synthesized oxygen carriers
  - Ni/NiO
  - Fe/FeO/Fe_2O_3
  - $BaFeO_3$ (perovskite)
- Experimental studies focused on characterizing oxygen carriers before & after time on stream
- Novel **atomic-scale support & dopant interactions** lead to best performance
  - Ni/$NiAl_2O_4$
  - $BaFe_{1-x}In_xO$

Potential for advances via atomic-scale materials design



Cabello A., Gayan P., Garcia-Labiano F., Diego L. F. de, Abad A., Izquierdo M. T., Adanez J., *Applied Catalysis B: Environmental*, 147:980–987, 2014.

Materials Design via Mathematical Optimization

- Current design paradigms:
  - Experiments & expert intuition
  - Database interpolation

- Proposed paradigm: Design **bottom-up** by explicitly arranging building blocks of matter via **mathematical optimization**, supporting high-throughput discovery of materials

Material Information →

Conceptual Design Process

$$\max_{s} \quad F(s)$$
$$\text{s.t.} \quad s \in S$$

→ **Design Variables & Constraints** →

Mathematical Optimization Model

$$\max_{x} \quad f(x)$$
$$\text{s.t.} \quad g(x) \leq 0$$
$$h(x) = 0$$

→ **Optimal Solutions & Novel Materials**

Mathematical optimization provides a rigorous, systematic way to explore the entire material design space

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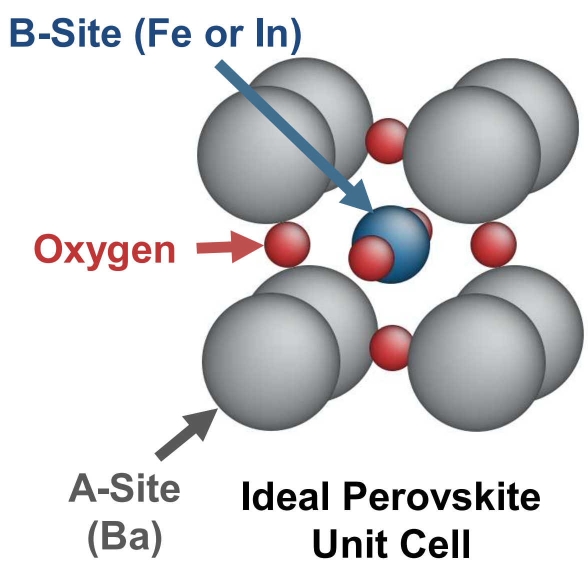
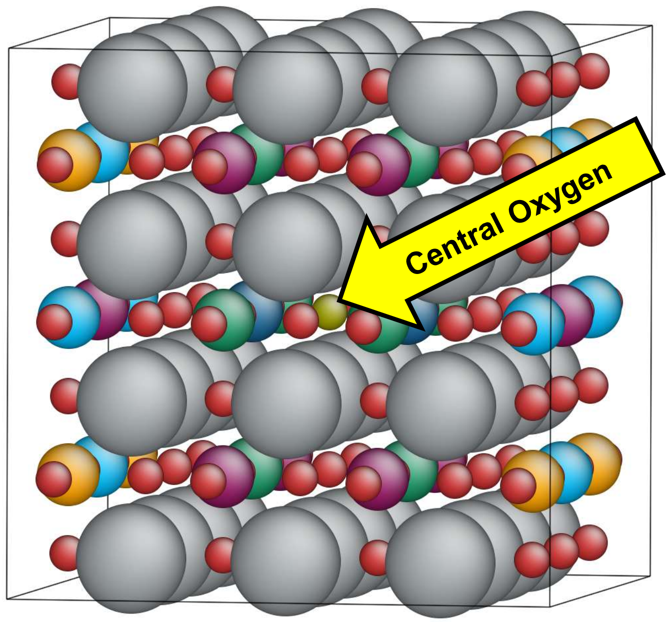
$BaFe_{1-x}In_xO_{3-\delta}$ Perovskite



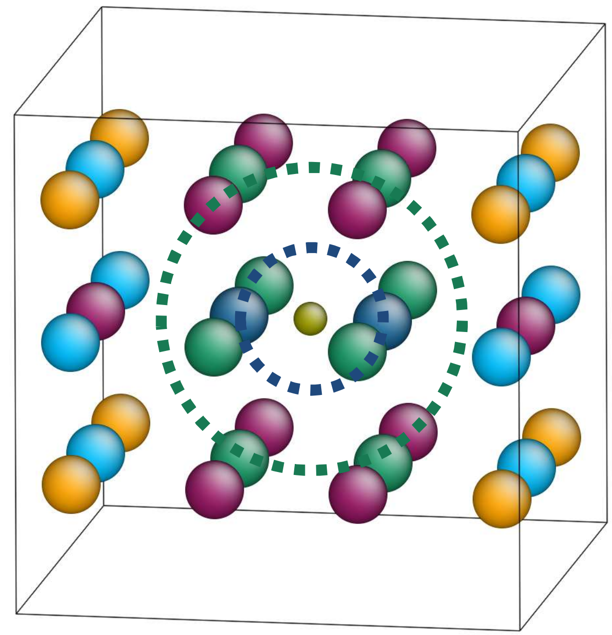
- Interesting oxygen carrier properties
  - Fast reduction and oxidation
  - Temperature tunability based on In content
- Key Hypothesis:
  - In atom **weakens Fe-O bonds** of neighboring B-sites
- Key Metric:
  - Oxygen excess energy ≈ perovskite reducibility
- Can we identify patterns of In doping that **minimize oxygen excess energy**?

Lekse J. W., Natesakhawat S., Alfonso D., Matranga C., *Journal of Materials Chemistry A*, 2(7):2397–2404, 2014.

Defining a Perovskite Motif



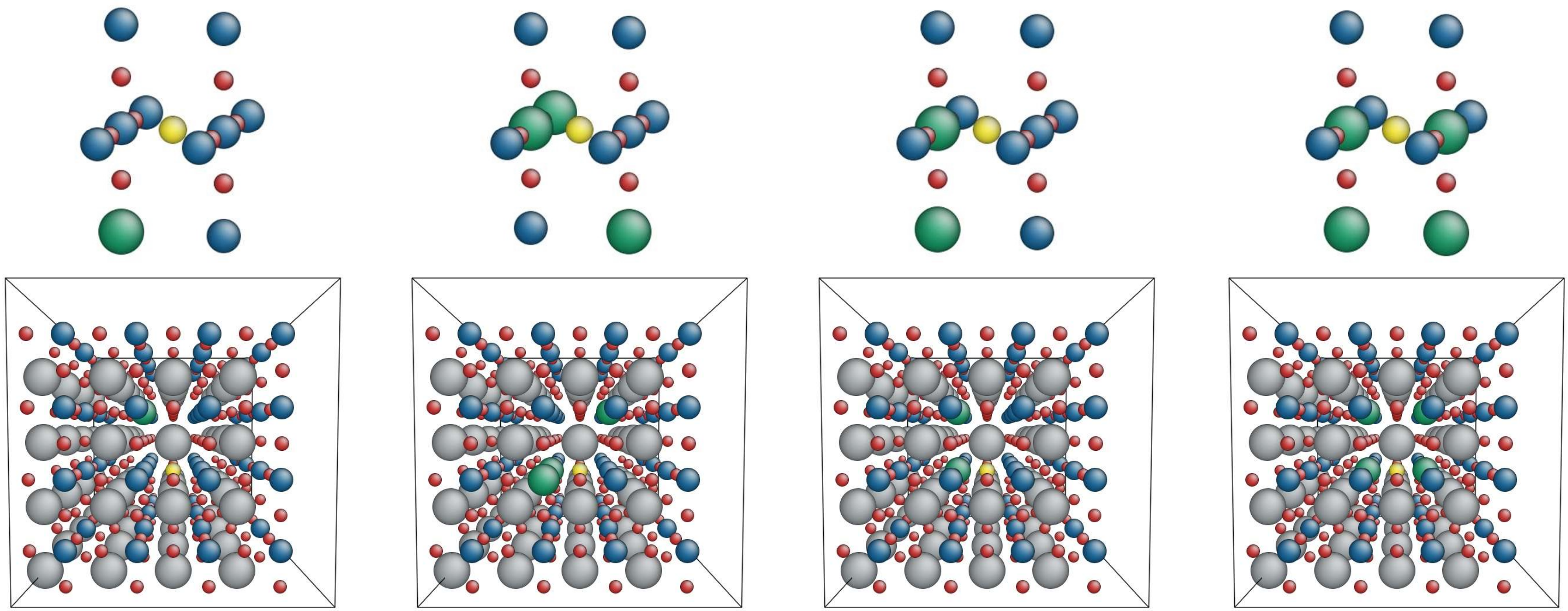
Perovskite supercell, focused on a particular oxygen



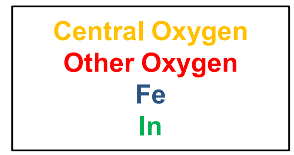
Perovskite supercell, focusing on neighboring B-sites

Chosen Motif: Ten nearest B-sites to central oxygen

Automatically Generated Motifs & Supercells



74 Rotationally-unique motifs identified

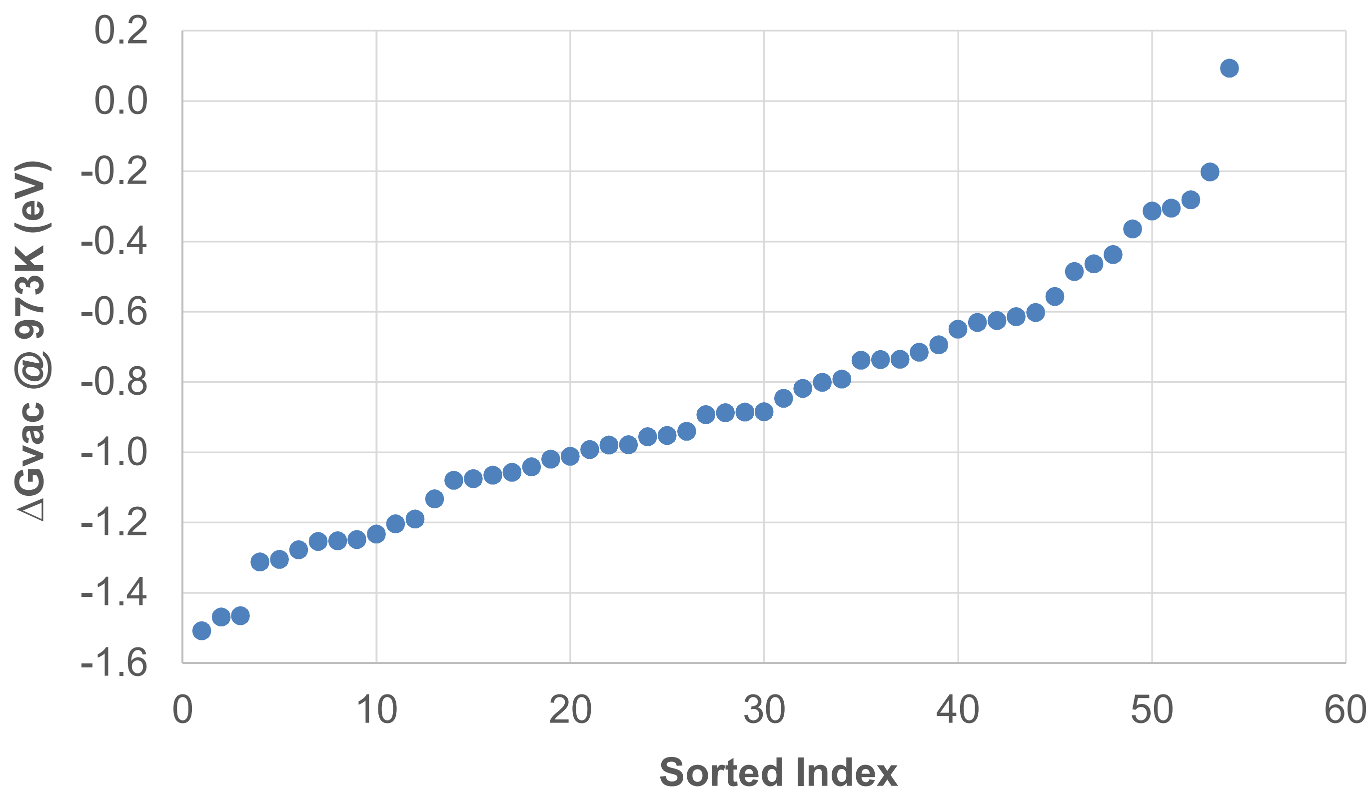


Distribution of Oxygen Excess Energies

Iteratively improve detail of DFT evaluations to prove convergence to "true" evaluation

Oxygen Excess Energy @ 0K

Vacancy Formation Energy @ 973K (near process conditions)



DFT Calculations using DFT+U in VASP by: Dominic Alfonso, De Nyago Tafen @ NETL

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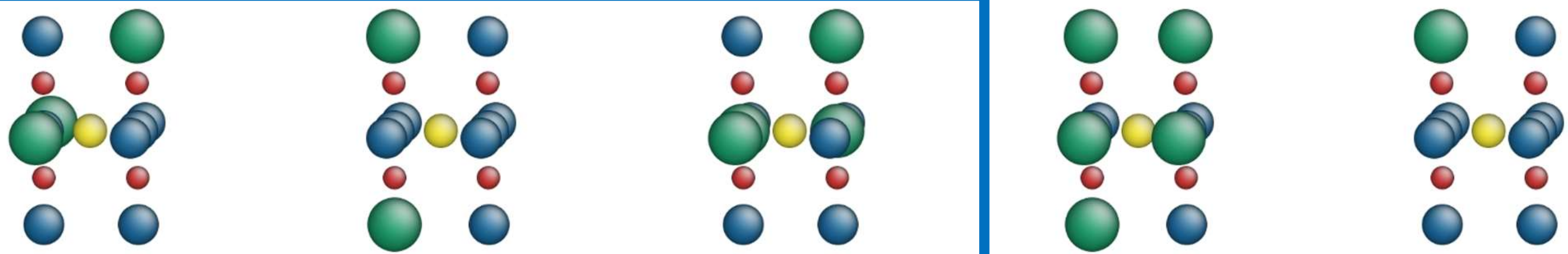
Ranking of Oxygen Excess Energy

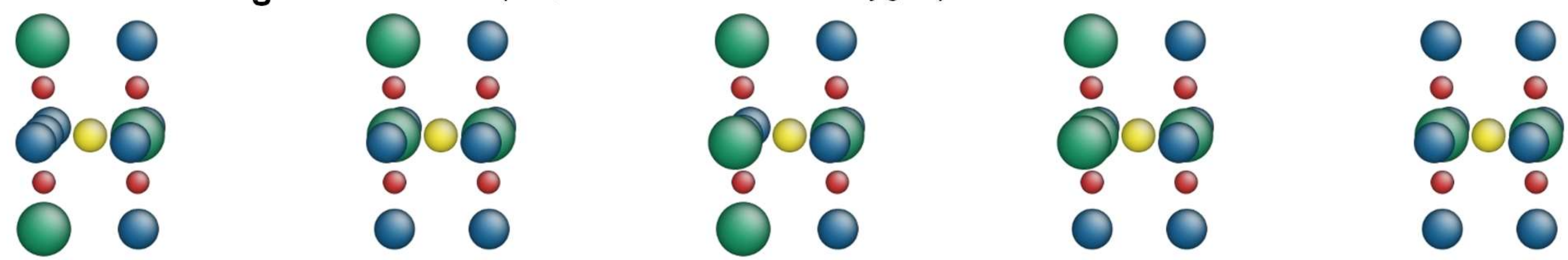
O
Central O
Fe
In

5 Motifs with Lowest: *(i.e., easier to remove oxygen)*



-1.51 eV **-1.47 eV** **-1.47 eV** **-1.31 eV** **-1.31 eV** **@ 973K**

5 Motifs with Highest: *(i.e., harder to remove oxygen)*



-0.31 eV **-0.31 eV** **-0.28 eV** **-0.20 eV** **0.09 eV** **@ 973K**

Oxygen sites directly next to Indium tend to have higher excess energy
Oxygen sites with Indium in the second-nearest shell have lower excess energy

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Dopant Design Optimization Model

$\max\limits_{Y_j, Z_{ic}}$ **Total number of targeted oxygen conformations**

s.t. **Indication of target oxygen conformations**

Local dopant concentration bounds

Global dopant concentration bounds

$Z_{ic} \in \{0,1\} \quad \forall i \in I, \quad \forall c \in C$

$Y_j \in \{0,1\} \quad \forall j \in J$

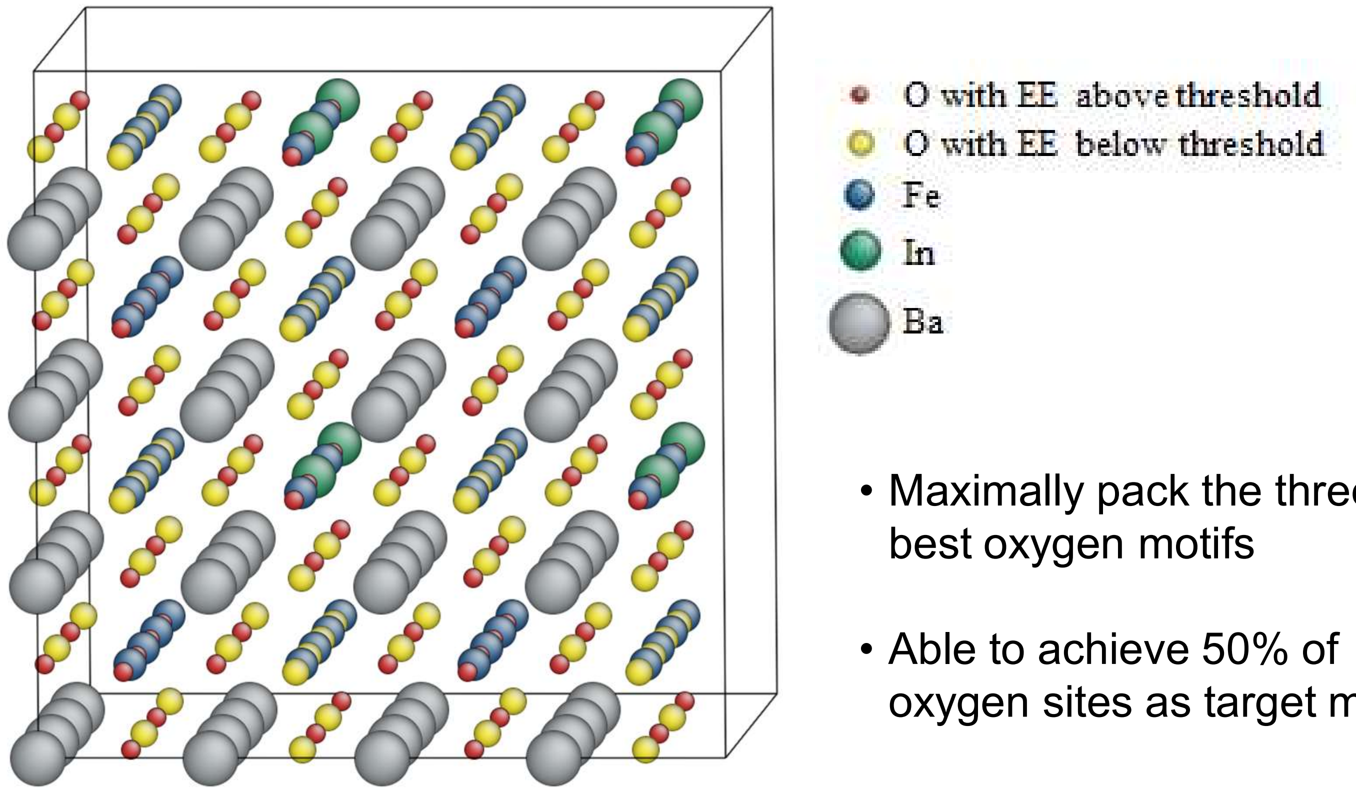
Presence of oxygen conformation → Z_{ic}

Presence of dopant → Y_j

<u>Based on optimization model developed in previous milestone, published in:</u>

Hanselman C. L., Gounaris C. E., "A Mathematical Optimization Framework for the Design of Nanopatterned Surfaces," *AIChE Journal*, 62(9):3250–3263, 2016.

Example Results: 4x4x4 Supercell



- Maximally pack the three best oxygen motifs
- Able to achieve 50% of oxygen sites as target motifs

Next Steps

- **Compare performance** of optimized designs against randomly-formed dopant patterns
- Solve dopant design model over **larger crystal domains**
  - Resulting in higher-quality material patterns
  - Requiring development of effective mathematical decomposition strategies
- Model **stability** of perovskite structure more explicitly in model
  - Resulting in guaranteed stable designs
  - Requiring translation of material stability into mathematical constraints

Perovskite-Specific Conclusions

- Identified relevant motifs and developed framework to evaluate perovskite oxygen excess energy
- Developed several approaches for **linking perovskite reducibility to dopant placement**
- Generated mathematical optimization model to **optimize dopant placement** with respect to oxygen excess energy

Key Benefit: Greater understanding of perovskite dopant impact on reducibility; Targets for experimental synthesis

Approach-Generic Conclusions

- Created framework for identifying, codifying, and enumerating material motifs
- Developed routines for identifying **simplified structure-function relationships** that can be embedded directly into mathematical optimization models
- Established an **application-generic mathematical optimization** model to optimize placement of desirable features in a nanostructured material

Key Benefit: Mathematical optimization accelerates discovery of materials for efficient, clean energy production

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IDAES Approach to Modeling & Optimization

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Expanding the scope of electric power infrastructure planning

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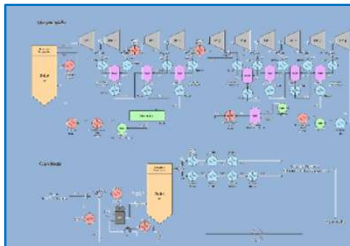
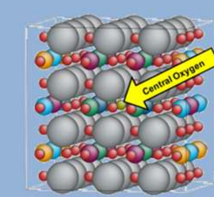

Process Systems



Materials Optimization


Energy Market Model

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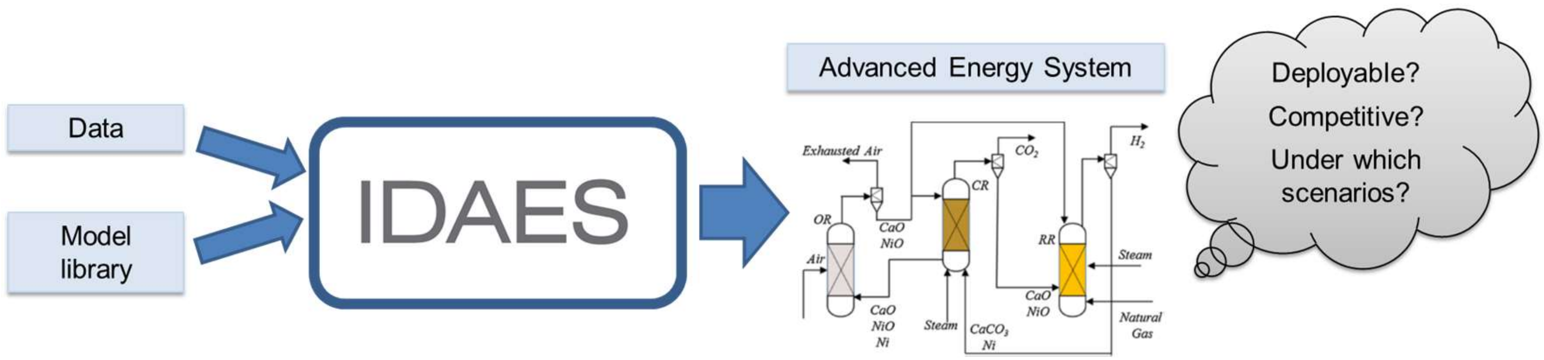
Energy Infrastructure Planning Model

- Evaluate the changes in **generation** and **transmission infrastructure** required to meet the projected **demand for electricity** over the next few decades.
  - Support decision-making process in the energy sector.
  - Evaluate various scenarios of future energy demand growth.
  - Ensure robustness of the energy system.
  - Study the impact of resource cost trends and policy shifts.

- Test the *deployability* of the **new technologies** proposed by IDAES under different scenarios.



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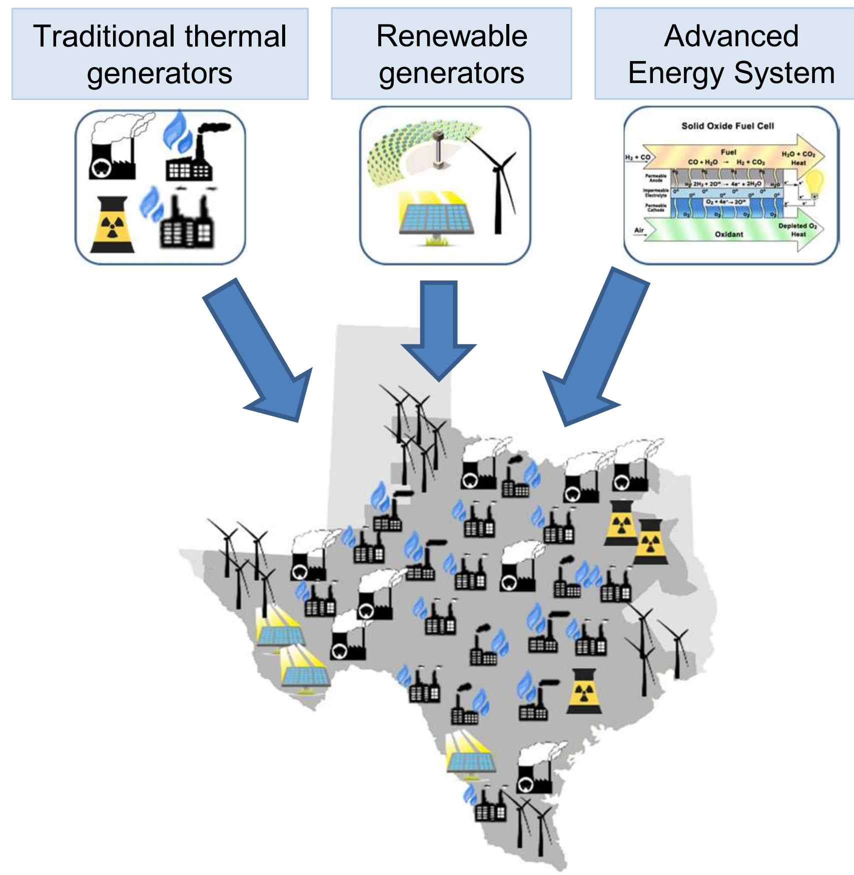
Proposed planning problem

Given an area with:

A set of **existing** and **potential** generators with the respective:

- energy sources (coal, natural gas, nuclear, solar, wind)
- generation technology
- location, if applicable
- nameplate capacity
- age and expected lifetime
- CO_2 emission
- operating costs
- investment cost, if applicable
- operating data
  - <u>thermal generators</u>: ramping rates, operating limits, spinning and quick-start maximum reserve (**unit commitment data**)
  - <u>renewable generators</u>: capacity factor

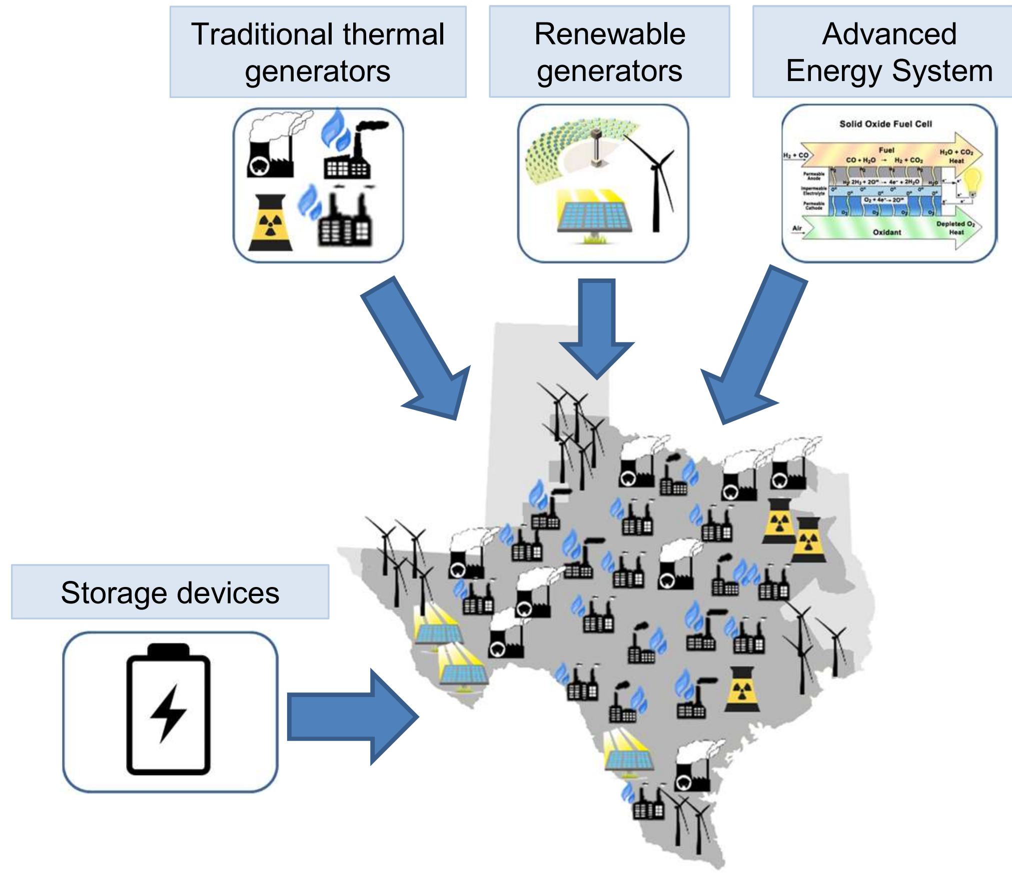


Proposed planning problem

Given an area with:

A set of **potential storage devices**, with specified:

- technology:
  - lithium-ion, lead-acid, and flow batteries
- investment cost,
- power rating,
- rated energy capacity,
- charge and discharge efficiency,
- storage lifetime.



Proposed planning problem

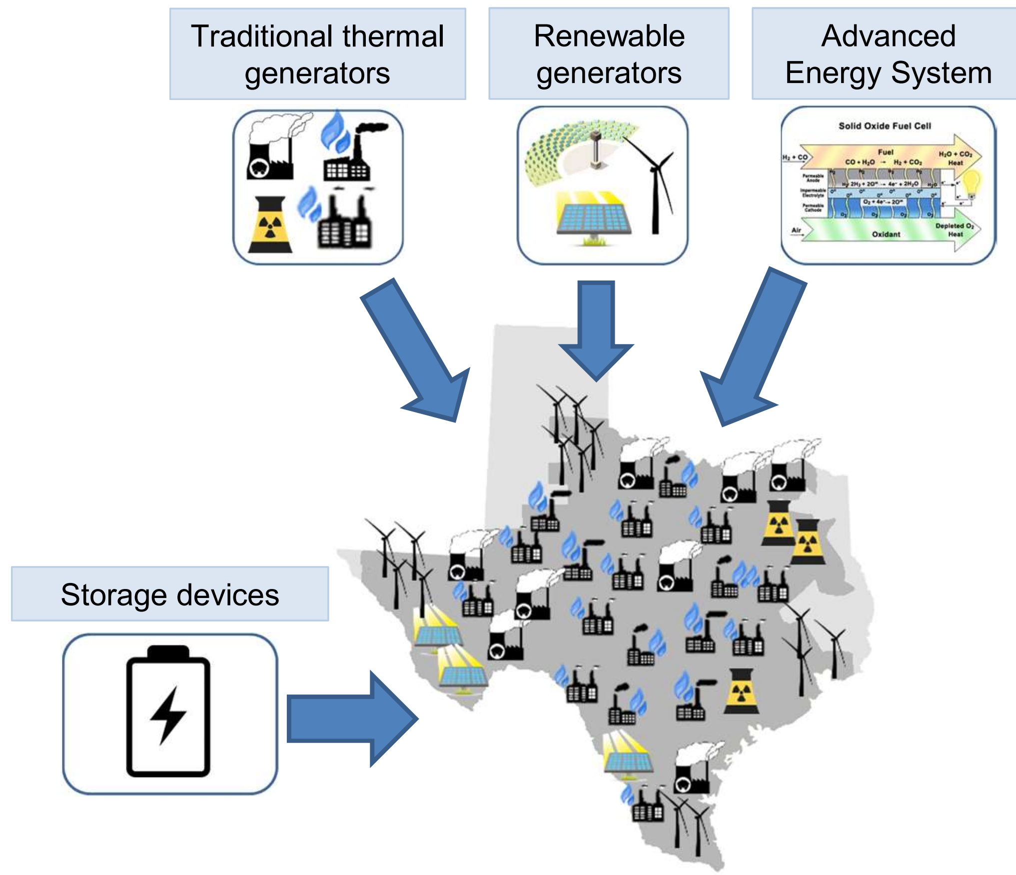
Given:

- Projected load demand over the time-horizon at each location
- Distance between locations
- Transmission loss per mile

Find:

- The **location**, **year**, **type** and **number** of generators and storage devices to **install**;
- When to **retire** the generators;
- Whether or not to **extend their lifetime**;
- Power flow between locations;
- Approximate operating schedule;

in order to minimize the overall operating and investment costs



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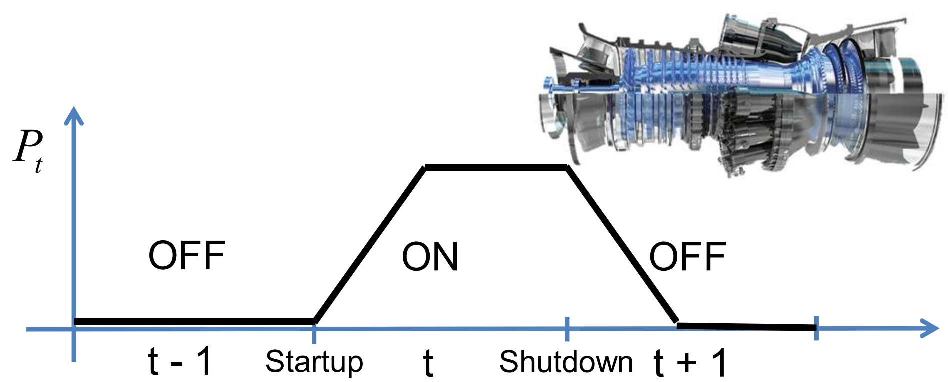
Unit commitment of thermal units

Natural Gas and Coal

What is unit commitment?

- "Unit commitment (UC) is an optimization problem used to determine the **operation schedule** of the generating units at **every hour interval** with varying loads under different constraints and environments."



Why to include unit commitment in a planning model?

- Accounts for the need of fast **ramping rates** in a system with high renewable penetration.
- Helps ensuring **flexibility** and **robustness** of the system.
- Accounts for **startup cost** in the total cost.

Very important for systems with **increasing share of renewables**

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Better than currently available commercial software

(e.g., Markal, TIMES, ReEDS) .

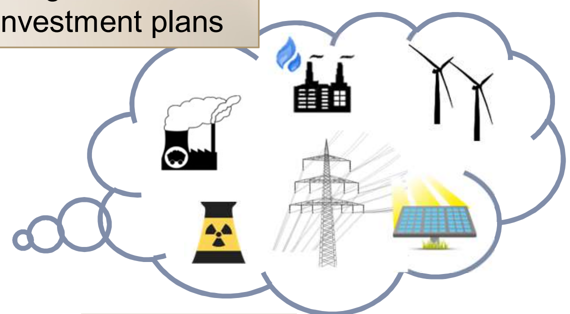
- Mixed-integer Linear Programming model.
  - Helps determine what is built when over long term horizon (20-40 years)
- Allows **hourly** and **sub-hourly** representation of time.
  - Captures the dynamics of the renewable generation and load demand.
  - Includes **unit commitment** of thermal generators.
- Detailed representation of **retirement** and **retrofit** of old generators
  - Important for regions with **aging** generation and transmission **infrastructure** (e.g., United States).

- **Open source**.
  - Researchers will have **access** to all the code and will be able to modify it within the platform.
- Allows the solution of **large instances** without the need of a supercomputer.
  - Due to algorithmic strategies (Nested Decomposition algorithm).
- As a **future step**, it will be extended to **handle uncertainties** in:
  - fuel price;
  - renewable generation;
  - new technology costs and performance.

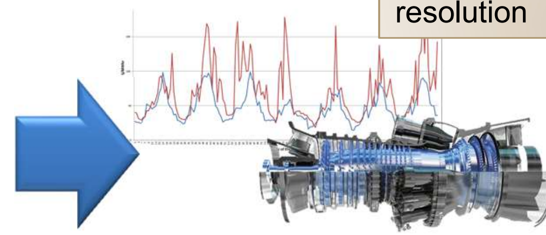
Modeling Challenges

- **Temporal multi-scale aspect of the problem:**
  - For a 30 year horizon, there are **262,800** hourly sub-periods of time
- **Spatial multi-scale aspect of the problem**
  - Large number of potential locations
  - Large number of generators

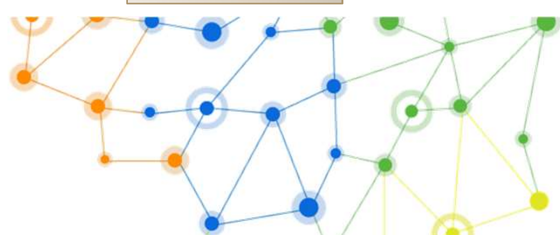
Long term investment plans



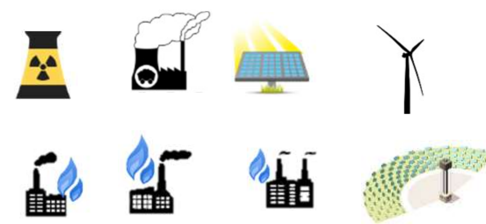
Hourly time resolution



Large region



Individual generators



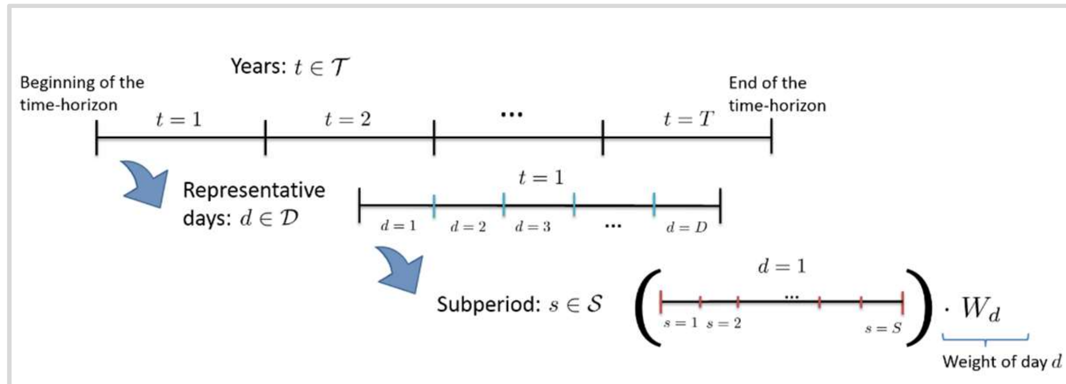
- **Very large-scale models** (million to tens of millions of equations and variables)
- Performance/cost targets are not easy to come up with
  - These models have million **co-depended parameters** regarding different aspect such as investment and operations cost in the generation and transmission level, load demand, renewable source availability, and environmental constraints.

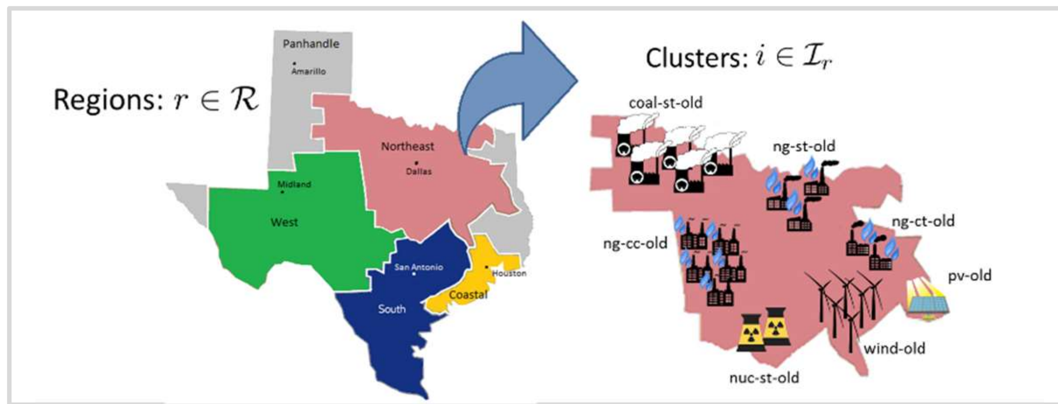
Modeling Strategies

- **Time scale approach:**
  - *d* representative days per year with hourly level information
- **Region and cluster representation**
  - Area represented by a few zones
  - Potential locations are the midpoint in each zone
  - Clustering of generators*

*Palmintier, B.S., Webster M.D., *Heterogeneous unit clustering for efficient operational flexibility modeling,* 2014

- **Transmission representation**
  - Flow in each line is determined by the energy balance between each region r.





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Formulation and Solution Strategy

MILP Multi-period Model

- Energy balance
- Capacity factor of the renewable generators
- Unit commitment constraints
- Operating reserve constraints
- Investment constraints.
- Generators balance

Objective function:

Minimization of the net present cost over the planning horizon comprising:

- Operating, startup, investment and retrofit costs
- Fuel consumption
- Environmental costs (if applicable)

Nested Decomposition Algorithm

Basic Idea

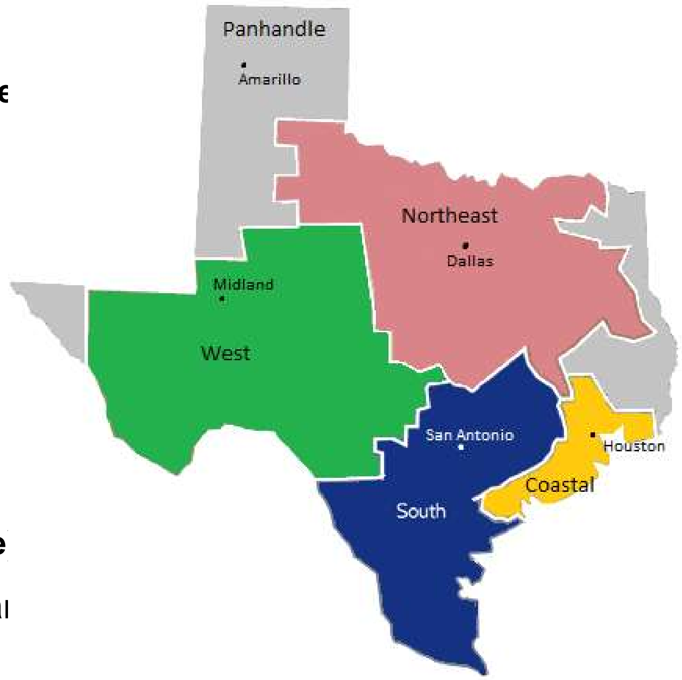
- This algorithm decomposes the problem by time period, which in this case is **by year**.
- It consists of **Forward** and **Backward Passes**.
- The **Forward Pass** solves the problem in myopic fashion (1 year time horizon).
- The **Backward Pass** projects the problem onto the subspace of the linking variables by adding cuts.

Multiple valid cuts to be chosen by the user.

Provides **massive computational savings**.

Case Study: ERCOT (Texas)

- **30 year time horizon (1st year is 2015)**
- **Data from ERCOT database**
- **Cost information from NREL (Annual Technology Baseline (ATB) Spre 2016**
- **All costs in 2015 USD**
- **Regions:**
  - Northeast (midpoint: Dallas)
  - West (midpoint : Glasscock County)
  - Coastal (midpoint: Houston)
  - South (midpoint : San Antonio)
  - Panhandle (midpoint : Amarillo)
- **Fuel price data from EIA Annual Energy Outlook 2016 (reference case**
- **Advanced fossil fuel data from Iyengar et al. (2014), and Newby ar (2013).**
- **Storage device data from Schmidt et al. (2017), and Luo et al. (2015).**



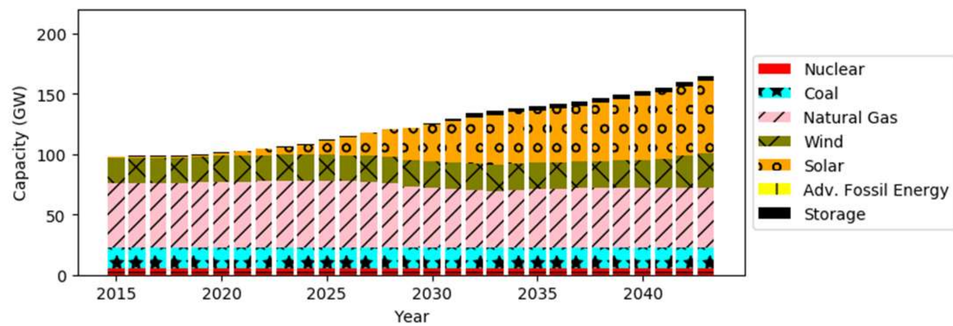
ERCOT, 4 representative days per year

Discrete variables: **500,500**
Continuous variables: **810,181**
Equations: **1,730,491**
Solver: Gurobi

PYOMO

- Scenario 1: No **carbon tax**.

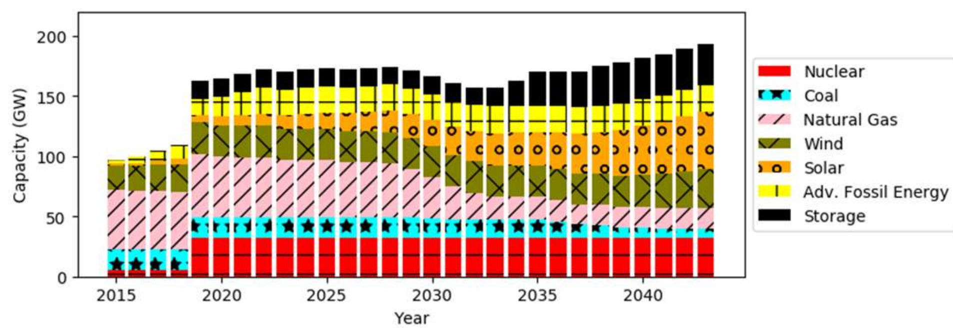
Solution time
Full-space: 10.1 hours
Nested Decomposition: 5.2 hours



Natural gas favored to handle renewable generation and load demand

- Scenario 2: **Carbon tax** starting at $10/tonne in year 2020, and increasing linearly to $100/tonne in 2029.

Solution time
Full-space: 4.0 hours
Nested Decomposition: 2.8 hours



Advanced fossil fuels, nuclear and storage favored instead of natural gas

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Conclusions

- Powerful multiscale optimization model for planning electric power infrastructures
- Potential for evaluating new IDAES technologies under a variety of scenarios.
- Massive computational savings through algorithmic improvements.

Future steps

- Improve the representation of the transmission.
- Test the model for other U.S. ISOs.
- Perform a sensitivity analysis with an actual technology developed by IDAES.
- Extend the formulation to multi-stage stochastic programming

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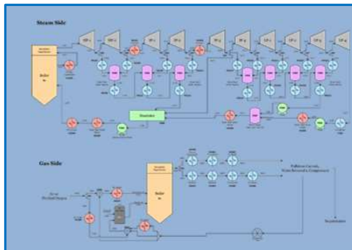
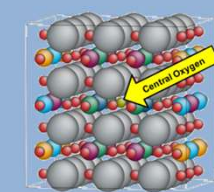


Process Systems



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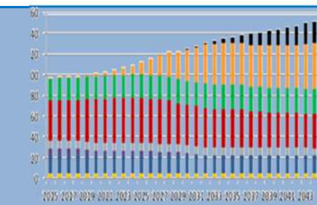

Energy Market Model

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Acknowledgements/Co-authors for specific sections:

ALAMO/RIPE: Nikolaos Sahinidis, Marissa Engle

Molecular Design: Chrysanthos E. Gounaris, Dominic Alfonso, Jonathan W. Lekse, De Nyago Tafen, Christopher Matranga

Infrastructure Planning: Ignacio Grossmann, Ben Omell, Joel Theis