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IDAES
Institute for the Design of Advanced Energy Systems

Advances in computational technology for process systems

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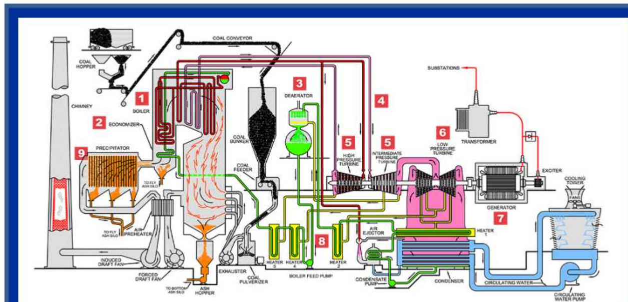
IDAES: Next generation modeling and optimization platform

Challenge: Develop and utilize multi-scale models and computational tools to accelerate innovation through the design, analysis, optimization, operation and troubleshooting of advanced fossil energy systems (process and markets)

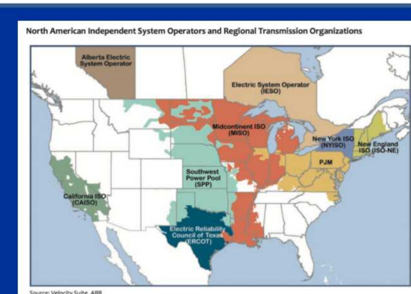


Rigorous Modeling and Optimization of Existing Fleet

- Model library of steady-state and dynamic unit models
- Full flowsheet models to support design and operation improvements of existing fleet (efficiency, flexibility, load)

Grid-integration and infrastructure planning

- Grid-level operational models and production cost modeling
- Targets for existing fleet improvements (efficiency, flexibility, markets)
- Multi-scale infrastructure planning



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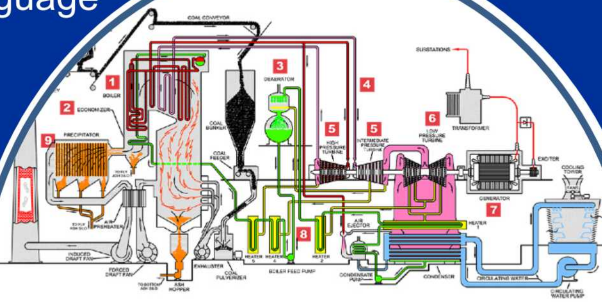
Core Enabling Technologies for IDAES

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

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



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

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

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

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

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Other Presentations

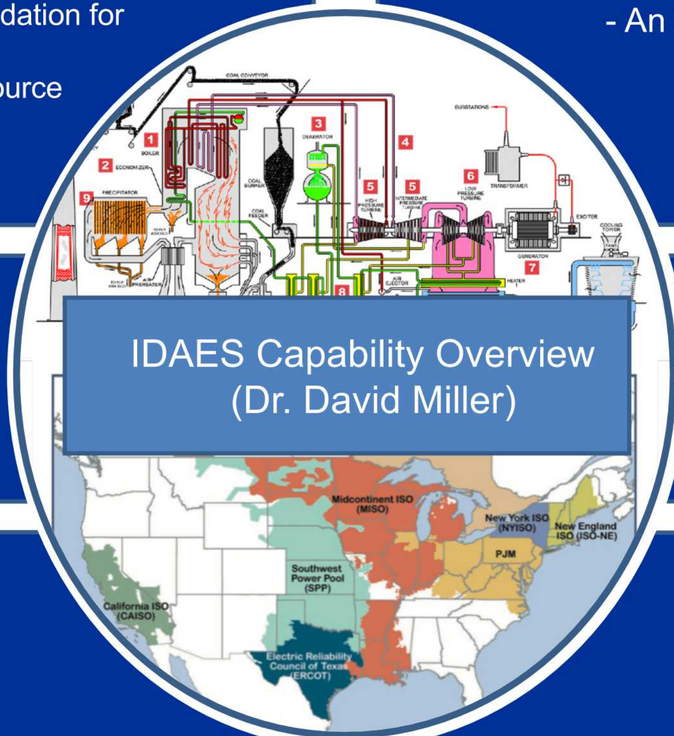
- Introduction to Pyomo: The optimization foundation for IDAES (Dr. John Siirola)
- Making IDAES Products Available – Open Source Release Approach and Plans (Keith Beattie)
- Demonstration: Jupyter Notebook/DMF: how to use the tools (Dan Gunter)

- An advanced approach to integrated process optimization (Prof. Larry Biegler)

- Dynamic Modeling, Optimization and Control (Dr. Bethany Nicholson)

- Power Plants and Advanced Combustion Systems: Current Status and Future Opportunities (Dr. Anthony Burgard)

- Process Modeling - IDAES Integrated Approach (Dr. Andrew Lee)



IDAES Capability Overview (Dr. David Miller)

- Conceptual Design of New Energy Technologies (Prof. Ignacio Grossmann)

- Grid-level Modeling: Opportunities and Program Plan (Dr. John Siirola)

- Machine learning approaches to properties and reaction models (Prof. Nikolaos Sahinidis)

- Poster: Robust Optimization (Natalie Isenberg)

- Poster: Parallel Computing Needs and Capabilities in IDAES (Dr. Carl Laird)

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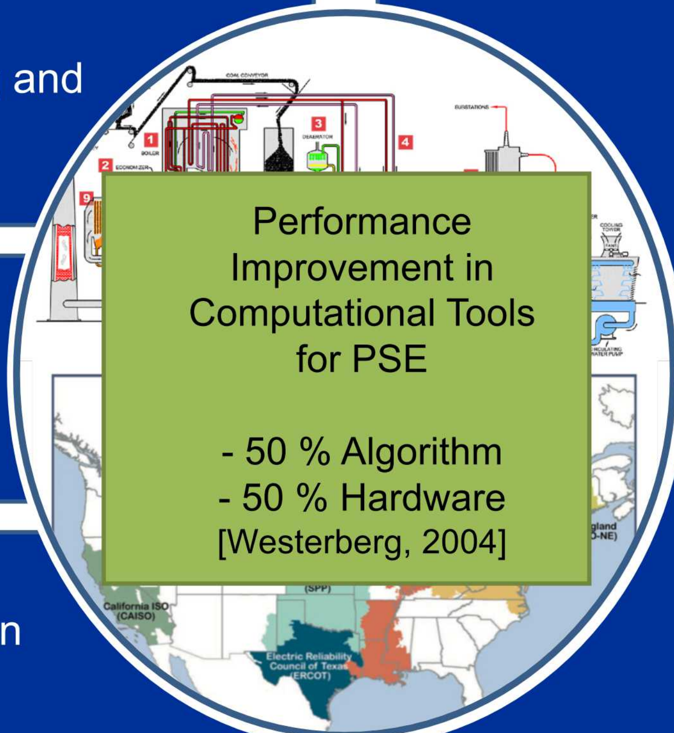
IDAES: Built on fundamental advances in PSE

Transition to glass-box modeling and analysis (algebraic, glass-box)

Advances in continuous nonlinear optimization (dynamics, uncertainty)

Advances in discrete optimization (algorithms and formulation)



Performance Improvement in Computational Tools for PSE

- 50 % Algorithm
- 50 % Hardware
[Westerberg, 2004]

Open-source, extensible algebraic modeling platforms

Emerging computational architectures and high-performance computing

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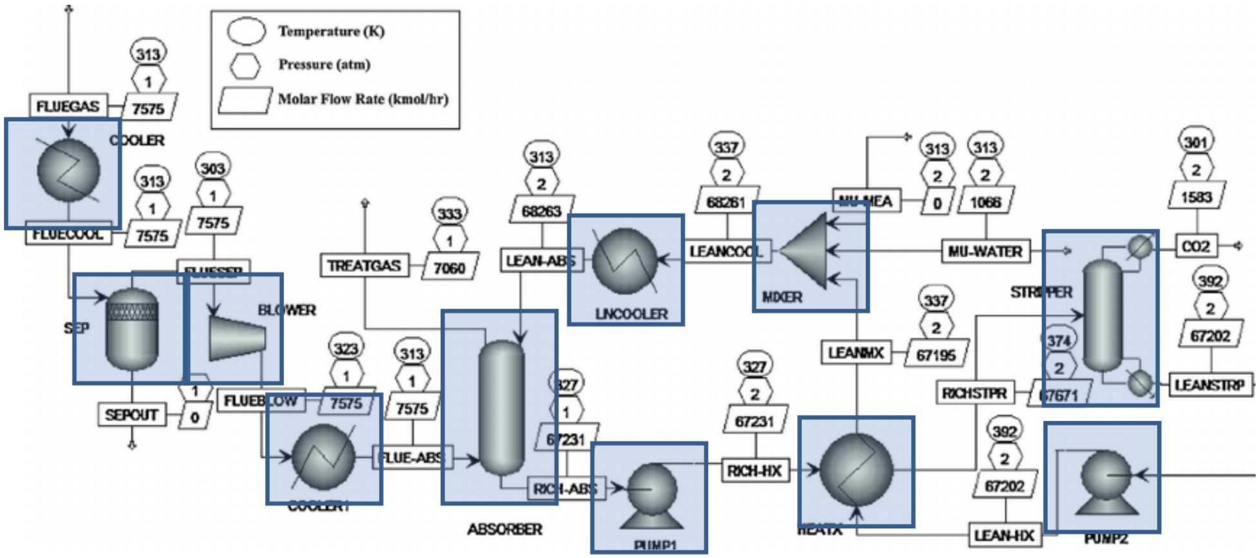
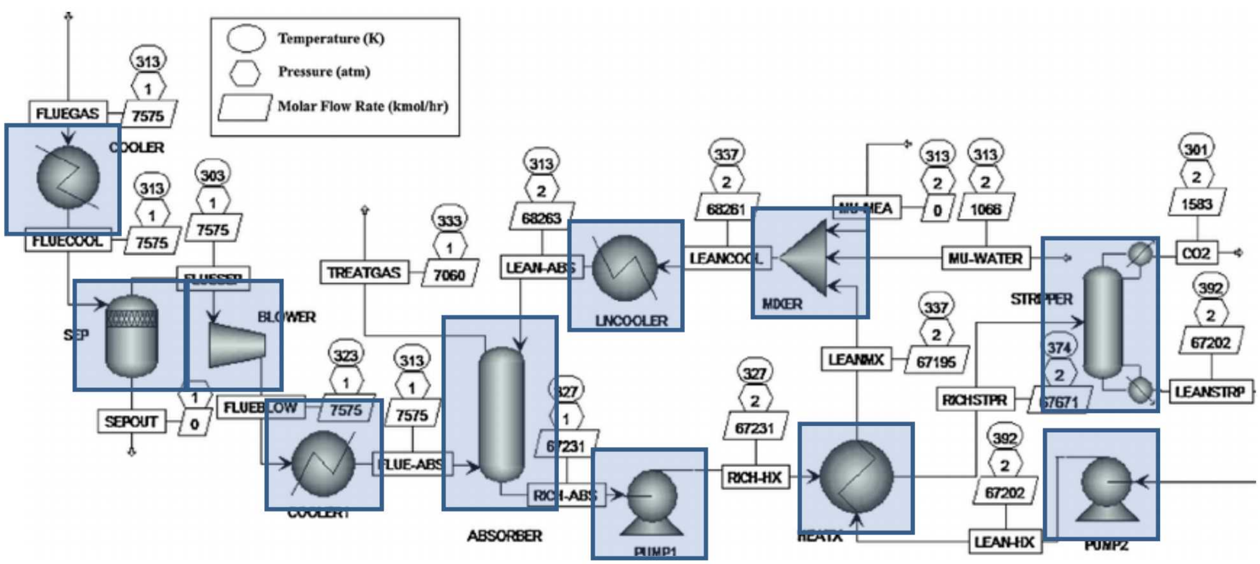
Sequential Modular Process Flowsheet Simulation



Kundu, Prodip & Chakma, Amit & Feng, Xianshe. (2014). Effectiveness of membranes and hybrid membrane processes in comparison with absorption using amines for post-combustion CO2 capture. International Journal of Greenhouse Gas Control. 28. 248–256.

Sequential Modular Process Flowsheet Simulation



- Specialized solution approaches for each individual unit
- Improved convergence reliability
- Reduces peak computational effort (unit-by-unit)

- Computationally slow
- Analysis beyond traditional simulation → Black-box only

Kundu, Prodip & Chakma, Amit & Feng, Xianshe. (2014). Effectiveness of membranes and hybrid membrane processes in comparison with absorption using amines for post-combustion CO2 capture. International Journal of Greenhouse Gas Control. 28. 248–256.

Process Optimization: Transition to EO (algebraic) models

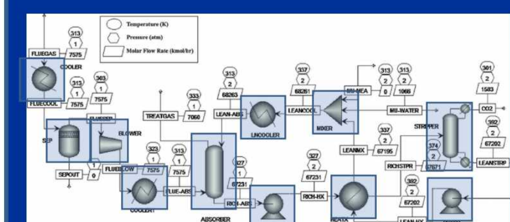
Optimization over degrees of freedom only

$$\min_{u} \quad f(u)$$

$$u^L \leq u \leq u^U$$

u ↓ ↑ f

Simulator



Black-box optimization (DFO)
~ 100-1000 simulations

[Adapted from Biegler, 2017]

Process Optimization: Transition to EO (algebraic) models

Optimization over degrees of freedom only

$$\min_{u} \quad f(u)$$

$$u^L \leq u \leq u^U$$

$u \downarrow$ $\quad$ $\uparrow f$

Simulator

$$h(x,u)=0$$

Black-box optimization (DFO)

~ 100-1000 simulations

$$\min_{x,u} \quad f(x,u)$$

$$x^L \leq x \leq x^U$$

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Optimization with embedded algebraic model as constraints

$$\min_{x,u} \; f(x,u)$$

$$h(x,u)=0$$

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Process Optimization: Transition to EO (algebraic) models

Optimization over degrees of freedom only

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Simulator

$$h(x, u) = 0$$

Black-box optimization (DFO)
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Optimization with embedded algebraic model as constraints

$$\min_{x,u} \; f(x, u)$$
$$h(x, u) = 0$$
$$x^L \leq x \leq x^U$$
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Glass-box optimization
~ 1-5 STE

[Adapted from Biegler, 2017]

Equation-Oriented (algebraic) models: Benefits

$$h(x,u)=0$$

$$\min_{x,u} \; f(x,u)$$
$$h(x,u)=0$$
$$x^L \le x \le x^U$$
$$u^L \le u \le u^U$$

- Explicit equations exposed to general numerical solvers and analysis tools
- Significantly faster computational performance: automatic differentiation, exposed structure
  - Fully integrated complex facilities (enterprise-wide)
  - DAE and uncertainty can be addressed in this form
- Separation of model from solver
  - Supports a wide range of Newton-based solvers
  - Same model used for different analyses (simulation, optimization, sensitivity, UQ)
- Automatic model transformation and reformulation (e.g., MPEC, GDP, DAE, Stochastic Programming)
- MINLP / global optimization with explicit expressions

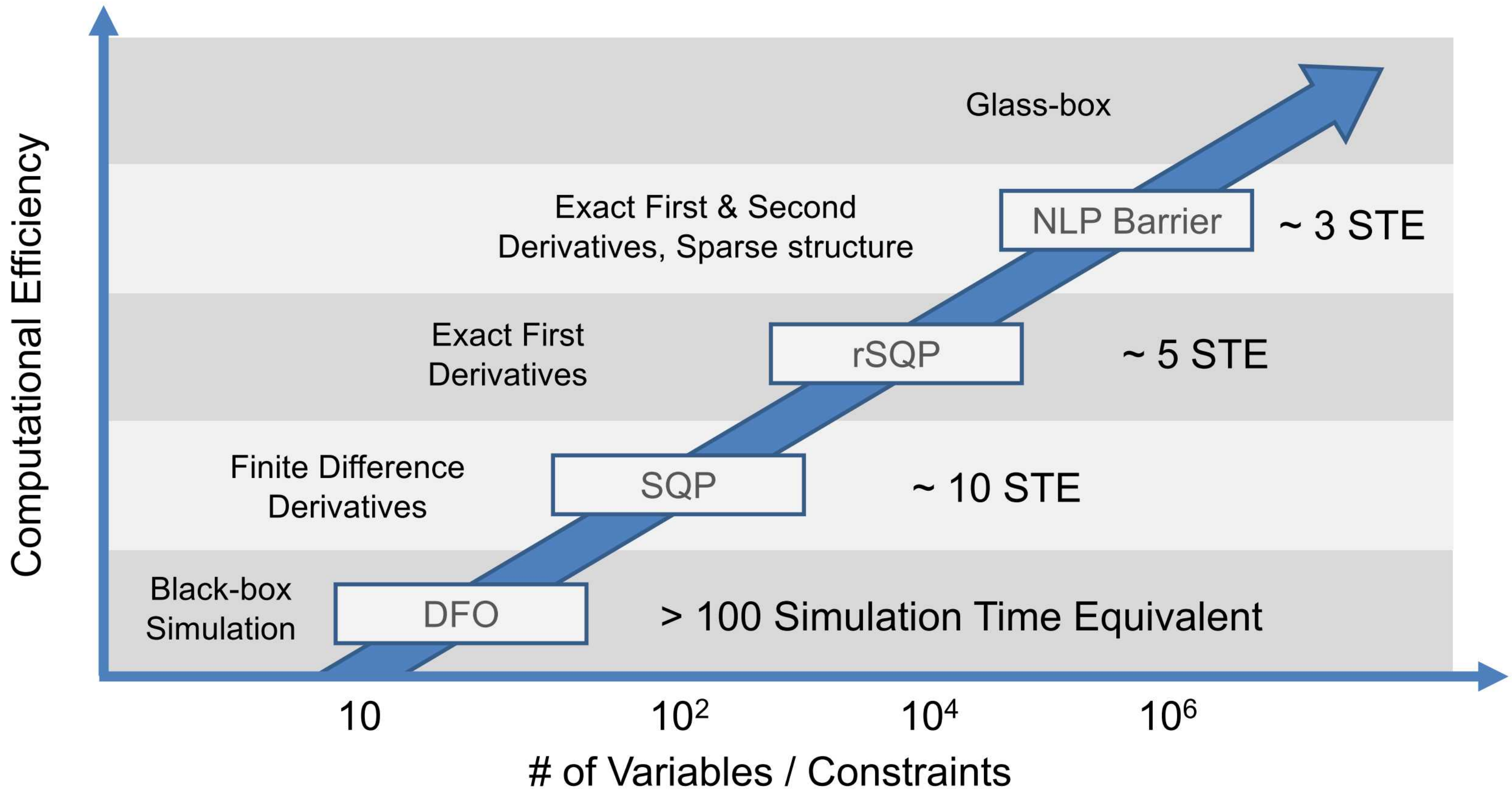
Equation-Oriented (algebraic) models: Challenges

$$h(x,u)=0$$

$$\min_{x,u} \; f(x,u)$$
$$h(x,u)=0$$
$$x^L \leq x \leq x^U$$
$$u^L \leq u \leq u^U$$

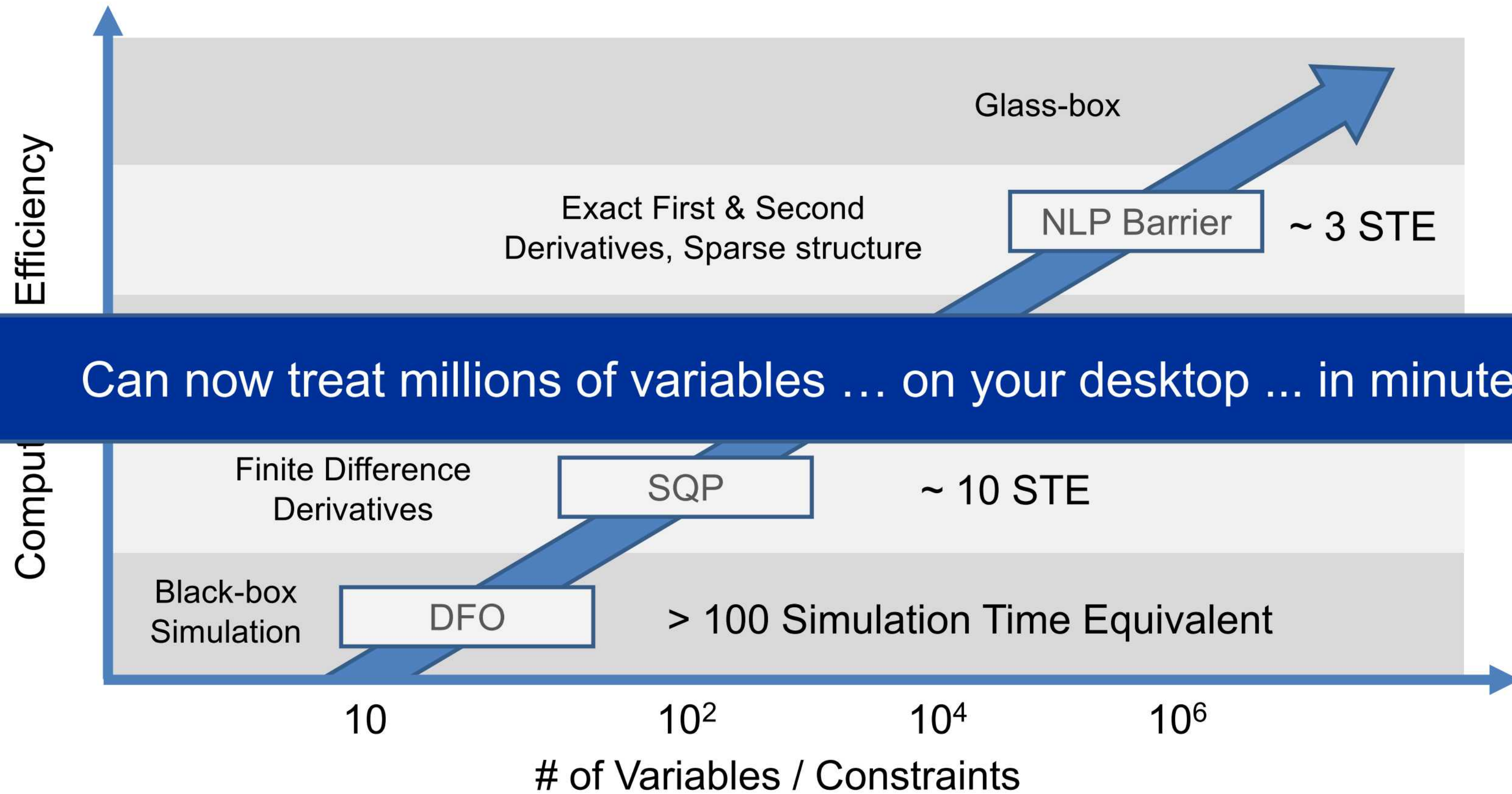
- Effective initialization critical for reliable convergence
- Not everything can (easily) be made equation-oriented
  – Need a strategy for black-box sub-components
- Strong formulations for multi-phase physics (structural changes to gthe model)
- Nonlinear simulation and optimization formulations are much larger than black-box counterparts

Process Optimization Environments and NLP Solvers



[Adapted from Biegler, 2017]

Process Optimization Environments and NLP Solvers



Can now treat millions of variables … on your desktop ... in minutes

[Adapted from Biegler, 2017]

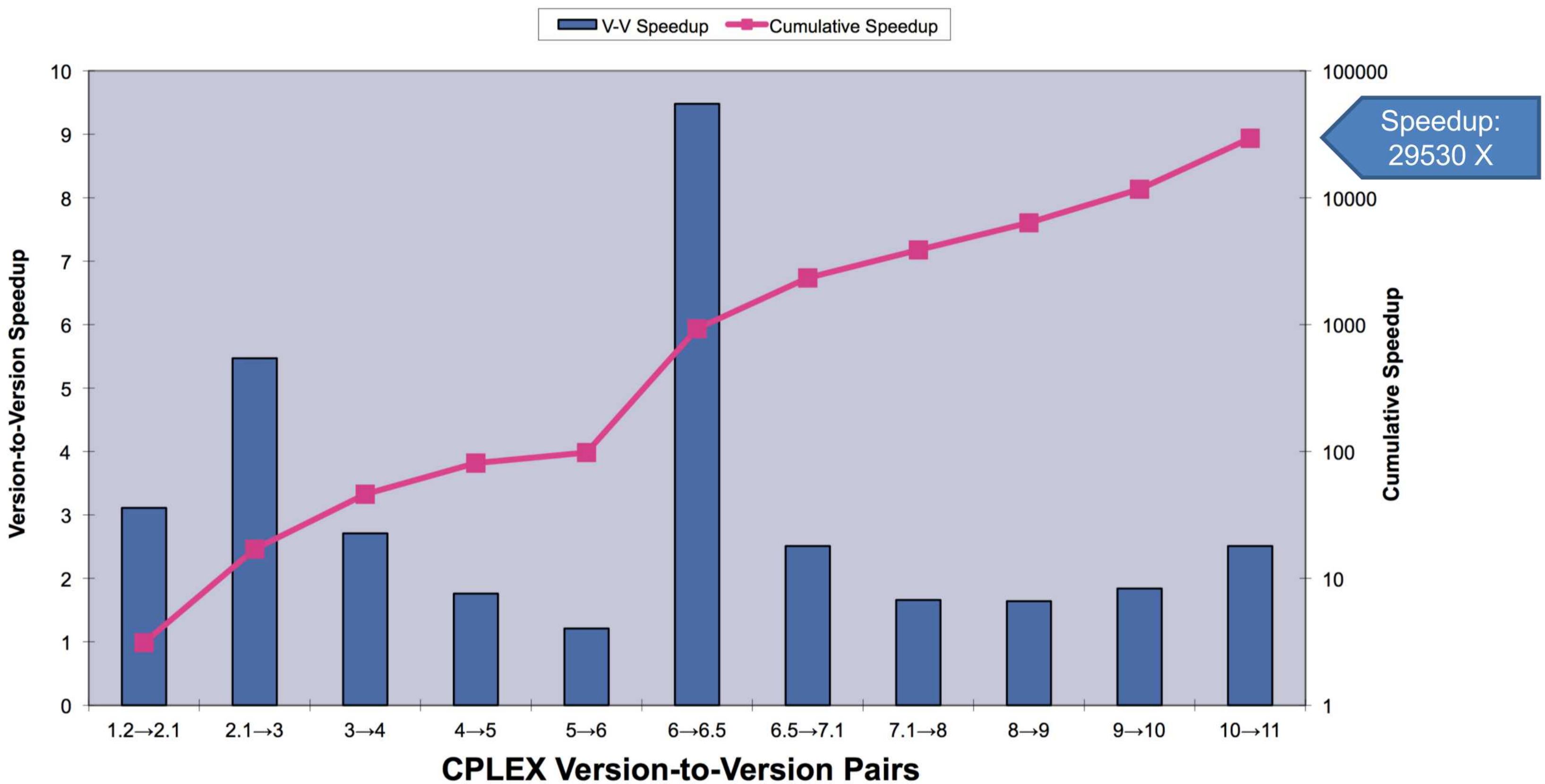
Discrete Optimization (MILP, MINLP)

- Mixed-integer programming adds extremely powerful discrete capabilities
  - Yes/No, On/Off decisions (e.g., build / not build, produce/don't produce)
  - Constraint & model structure (e.g, laminar / turbulent, reactor / no reactor)
  - Logical conditions (e.g., implication, cardinality, if-this-then-that)
  - Countable quantities, whole numbers (e.g., stages in distillation column)

- Discrete optimization needs within IDAES
  - Process synthesis, conceptual design
  - Process integration and intensification (e.g., HENS, MENS)
  - Grid operation, infrastructure planning, and production cost modeling
  - Machine learning approaches for fitting correlations and surrogate models

- Strong off-the-shelf solvers for MILP, MIQP, MISOCP, MINLP
- Algorithms have seen dramatic improvement in recent years

50% Algorithm, 50% Hardware: A Notable Exception



[R. E. Bixby, "A Brief History of Linear and Mixed-Integer Programming Computation", Documenta Math., Extra Volume ISMP, 2012, 107–121.]

50% Algorithm, 50% Hardware: A Notable Exception

Improvement in MIP Software from 1988-2017

- Algorithms: 147650x
- Machines: 17120x

  http://preshing.com/20120208/a-look-back-at-single-threaded-cpu-performance/
- NET: (Algorithm $\times$ Machine): 2,527,768,000x

What Does This "Mean"?

- A "typical" MILP that would have taken 124 years to solve in 1988 will solve in 1 second now.
- This is amazing, but your mileage may vary

[Linderoth, FOCAPO 2017]

Power Industry Example from Robert E. Bixby

Example 1: A Unit-Commitment Story

Electrical Power Industry, ERPI GS-6401, June 1989:
Mixed-integer programming (MIP) is a powerful modeling tool, "They are, however, theoretically complicated and computationally cumbersome"

In Other Words: MIP is an interesting "toy", but it just isn't going to work it practice.

9-Jun-10 © 2010 Gurobi Optimization 4

An Example Unit-Commitment Model
California 7-Day Model

`UNITCAL_7`: 48939 constraints, 25755 variables (2856 binary)

Reported Results 1999 – machine unknown
2 Day model: 8 hours, no progress
7 Day model: 1 hour to solve initial LP

9-Jun-10 © 2010 Gurobi Optimization 5

[R. E. Bixby. Mixed-integer programming: It works better than you may think. In FERC Conference, 2010. Retrieved 5/20/18: https://www.ferc.gov/CalendarFiles/20100609110044-Bixby,%20Gurobi%20Optimization.pdf]

Solved in 2010 in just over 3 minutes

Summary of Mathematical Programming in PSE

- Advances in mathematical programming, coupled with effective problem formulation, allow efficient solution to real-world problems

Applications of mathematical programming in process systems engineering

	LP	MILP	QP, LCP	NLP	MINLP	Global	SA/GA
Design and synthesis							
HENS	×	×		×	×	×	×
MENS	×	×		×	×	×	×
Separations		×			×		
Reactors	×			×	×	×	
Equipment Design				×	×		×
Flowsheeting				×	×		
Operations							
Scheduling	×	×			×		×
Supply chain	×	×			×		
Real-time optimization	×		×	×			
Control							
Linear MPC	×		×				
Nonlinear MPC				×		×	
Hybrid		×		×	×		

[L. T. Biegler, I. E. Grossmann, “Retrospective on optimization”, Computers & Chemical Engineering, Volume 28, Issue 8, 2004, Pages 1169-1192.]

Realizing the Benefits of Mathematical Programming Advances

- Needs:
  - Glass-box models for efficiency (derivatives, sparsity)
  - Explicit access to model equations (model transformation for DAE, GDP, logic)
  - Library of modeling components (and parameterized system models)
    - Reusability, Reliability
  - Ability to model novel energy systems

Algebraic modeling language ⇄ Domain-specific modeling library and software framework

1. Add glass-box capabilities to an existing domain-specific package (request)
2. Add domain-specific modeling capabilities to an algebraic modeling language

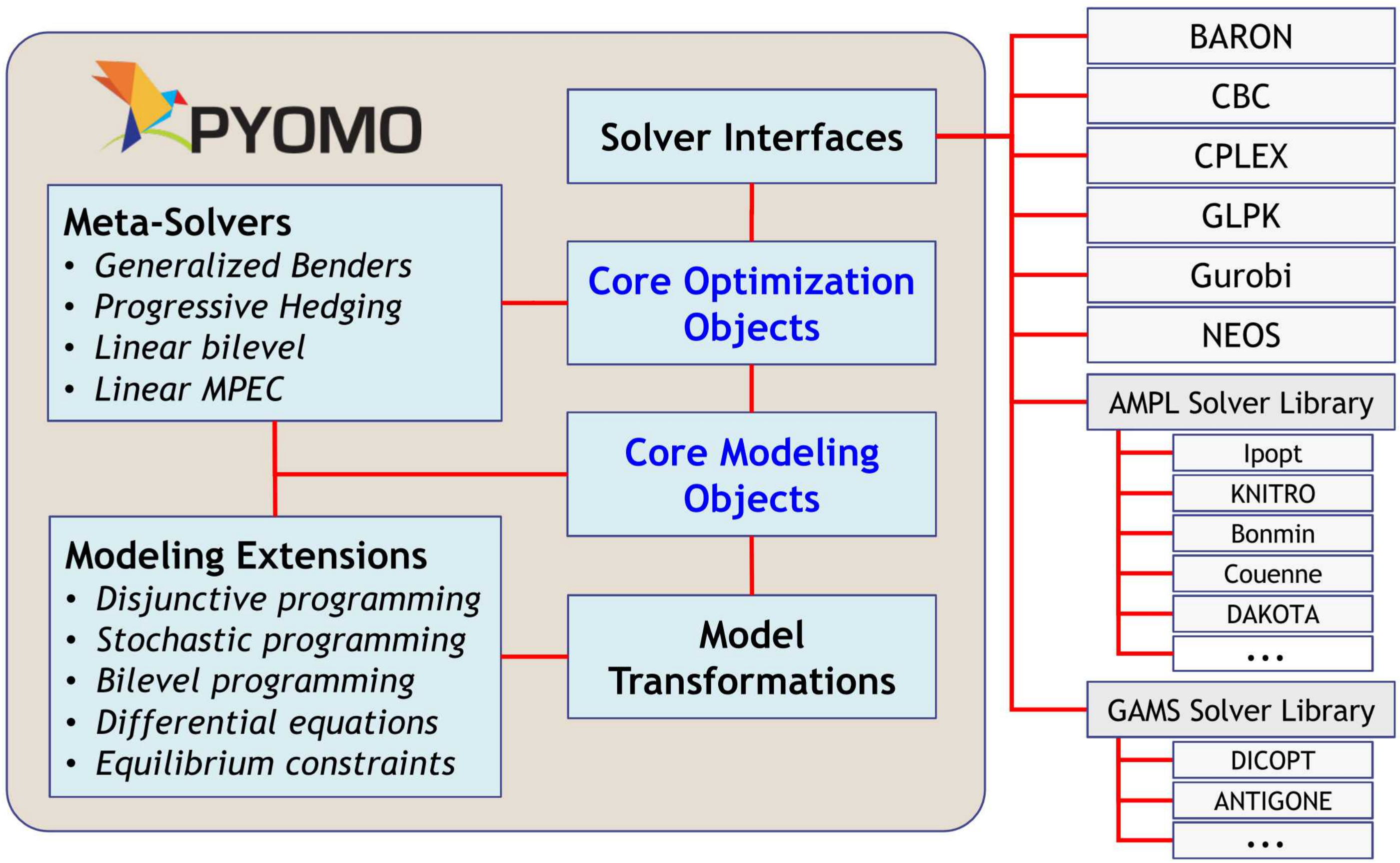
Pyomo: Python Optimization Modeling Objects

- A fully equation-oriented modeling environment
- Built with Python – rich, well-supported programming environment
- Extensible, object-oriented (high-level, hierarchical modeling)
- Access to large body of Python libraries (e.g., SciPy, Pandas) for workflows
- Open-source (BSD Licensed)
- Full support for model transformations and meta-algorithms

PYOMO PYOMO DAE PySP

- Foundation for IDAES modeling framework in Python
  - Unit models inherit off of Pyomo components
  - Other IDAES modules integrated through Python

Pyomo: Python Optimization Modeling Objects



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Landscape of Computing Hardware

Mobile Architectures

Multi-core,
Specialized arch. (GPU, SOC),

Focused on performance and power efficiency

Parallel Architectures

Multi-core,
Specialized architectures (GPU),
HPC clusters, Cloud

Focused on performance and power efficiency

Landscape of Computing Hardware

Mobile Architectures

Performance (Geekbench):

iPhone X: 4206

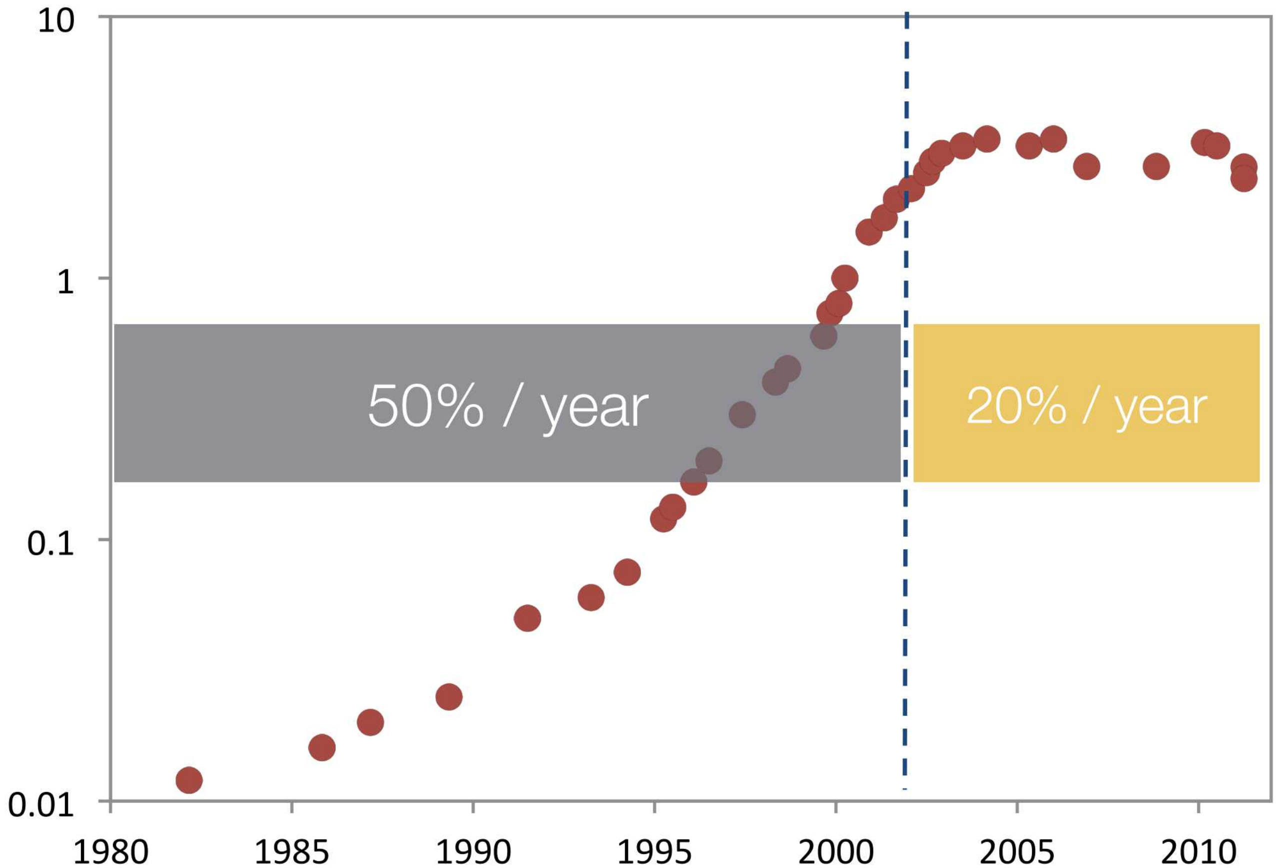
iPhone 8: 4216

Parallel Architectures

Multi-core,
Specialized architectures
(GPU),
HPC clusters, Cloud

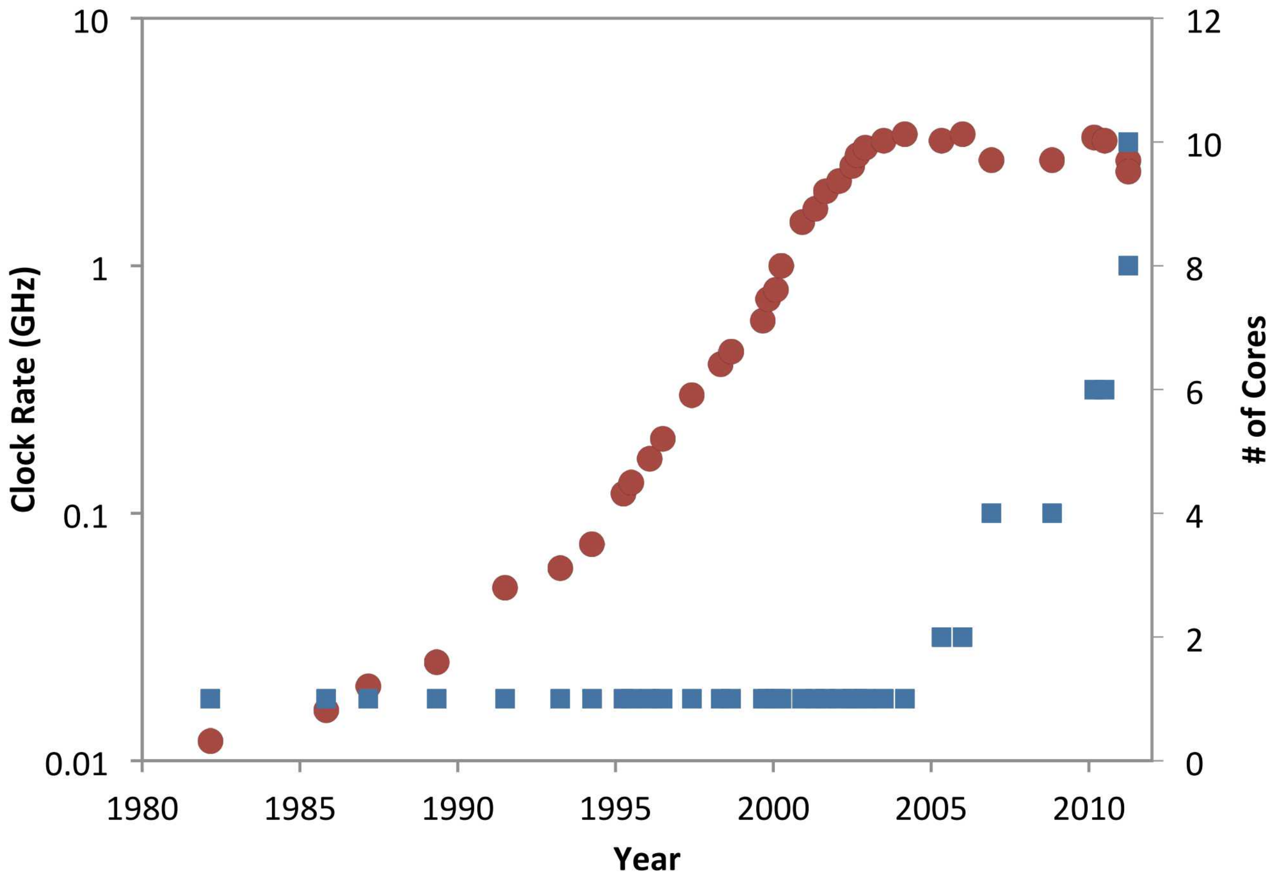
Focused on performance and
power efficiency

Landscape of Computing Hardware



[Steven Edwards, Columbia University]

Landscape of Computing Hardware



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Parallel Computing Architectures

	Single Data	Multiple Data
Single Instruction	SISD	SIMD
Multiple Instruction	MISD	MIMD

Alternative architectures (e.g, Graphics Processing Unit)

- Affordable -- 1000's cores
- Specialized compilers and tools (CUDA, OpenCL)
- Several complexities and limitations

Desktop Multi-core (MIMD)

- Affordable hardware
- Standard tools (threads/openMP)
- Fast communication (no network)

- Low # of cores (relatively)
- Bottleneck: Memory access/# CPU

HPC Cluster (MIMD)

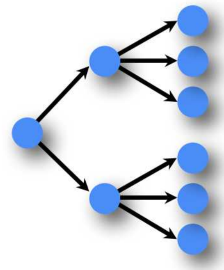
- Distributed computing (networked)
- Standard tools (MPI)
- Scalable: 100-1000s of cores

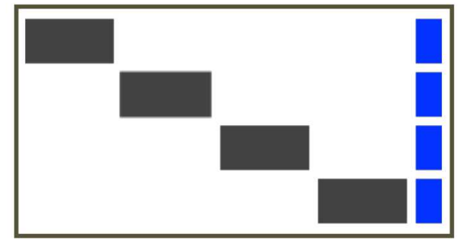
- Bottlenecks: communication

- IDAES utilizing both MIMD and SIMD architectures
- Fine-grained and coarse-grained parallelism
- Inherently parallel algorithms
- Parallel because of problem structure

Exploiting Problem Structure

- Optimization Under Uncertainty
  - two-stage stochastic programming formulation
  - block structure because of coupled scenarios
  - common structure of many applications (parameter estimation, spatial decomposition)

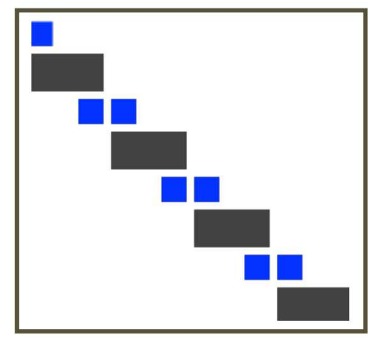




Kang, J., Word, D.P., and Laird, C.D., "An interior-point method for efficient solution of block-structured NLP problems using an implicit Schur-complement decomposition", Computers and Chemical Engineering, 2014.

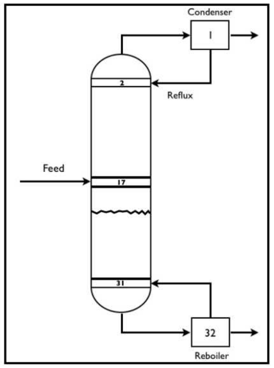
- Dynamic Optimization
  - Simultaneous approach (discretization using OCFE)
  - block structure because of finite element discretization
  - pass-on variables couple neighboring blocks

$$
\begin{aligned}
\min_{u} \int_{t_0}^{t_f} & L(x,y,u)\, dt \\
\text{s.t.} \quad F(\dot{x}, x, y, u) &= 0 \\
x(t_0) &= x_0 \\
(x,y,u)^L \leq (x,y,u) &\leq (x,y,u)^U
\end{aligned}
$$



Word, D.P., Kang, J., Akesson, J., and Laird, C.D., "Efficient Parallel Solution of Large-Scale Nonlinear Dynamic Optimization Problems", Computational Optimization and Applications, 2014.

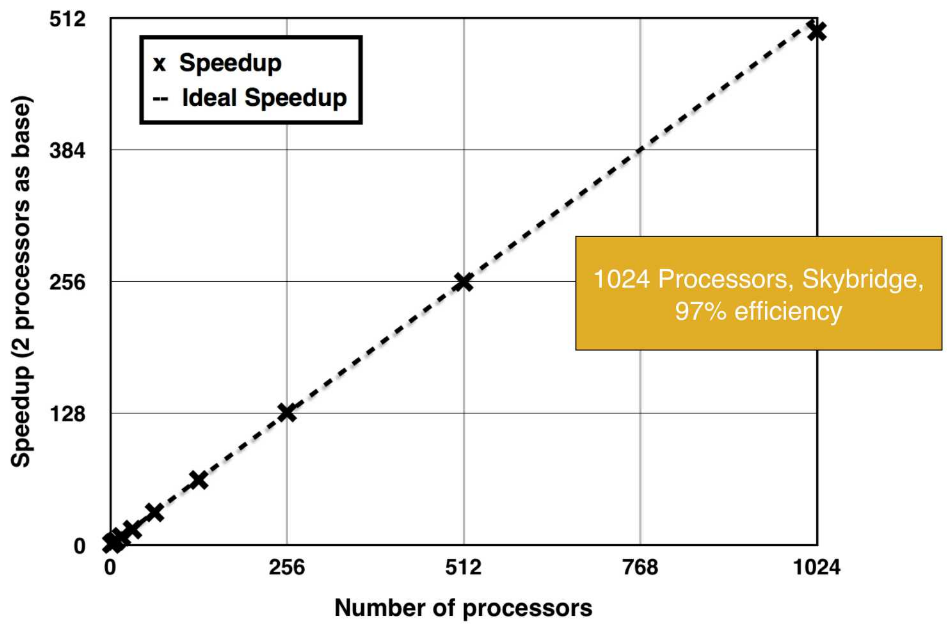
Parallel Algorithm Performance



- 32 state vars, 35 algebraic vars
- Discretize model (OCFE)
- Uncertainty in mole fraction of the feed stream
- 96 scenarios, 32 processors

[Benallou, Seborg, and Mellichamp (1986)]

Case	# Vars.	# Coupling Vars.	FS-S time(s)	ESC-P time(s)	PCGSC-P time(s)
1	1430550	150	10.3	2.6	0.6
2	2861100	300	-	10.8	1.1
3	4291650	450	-	32.1	2.4
4	5722200	600	-	70.3	3.2
5	7152750	750	-	90.5	4.3
6	8583300	900	-	160.5	5.3
7	10013850	1050	-	218.0	6.3
8	11444400	1200	-	286.6	8.1



- N-1 Contingency Constrained Economic Dispatch

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IDAES: Why now?

- Transition from specialized simulation methods to equation-oriented modeling
- Improvement in computational performance of nonlinear solvers
- Tremendous advances in efficiency of MIP, MIQP, MISOCP, MINLP
- Open-source, extensible modeling tools within a rich programming language
- Efficient solution of advanced simulation, optimization and analyses on laptop, support for emerging computational architectures for HPC

IDAES: Why now?

- Transition from specialized simulation methods to EO modeling
  - **derivatives, sparsity, expressions**
- Improvement in computational performance of nonlinear solvers
  - **Large-scale optimization enables simultaneous (cost of a few sim.)**
  - **Rigorous treatment of DAEs and uncertainty**
  - **Process design and optimization, dynamics and control**
- Tremendous advances in efficiency of MIP, MIQP, MISOCP, MINLP
  - **With effective problem formulations → powerful decision making tools**
  - **Conceptual design, infrastructure operation and planning**
- Open-source, extensible modeling tools within a rich programming language
  - **Development platform for next-generation modeling and optimization tools**
- Emerging computational architectures for HPC
  - **computational architectures to solve larger problems faster**
  - **enable solution of problems not previous tractable.**