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IDAES Institute for the Design of Advanced Energy Systems

Parallel Computing Needs and Capabilities in IDAES

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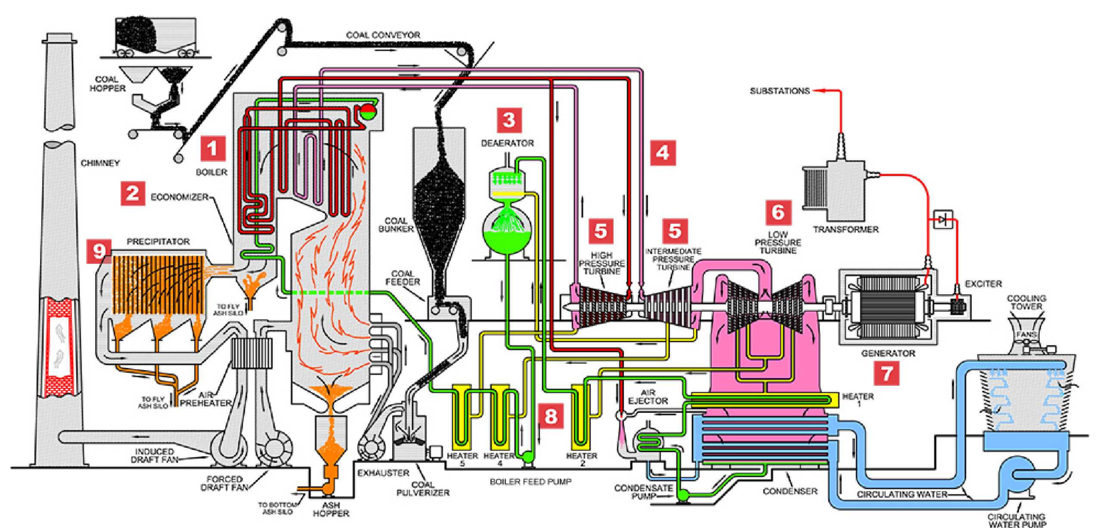
Motivation

IDAES framework brings advanced modeling, optimization, and analysis of energy and chemical process systems

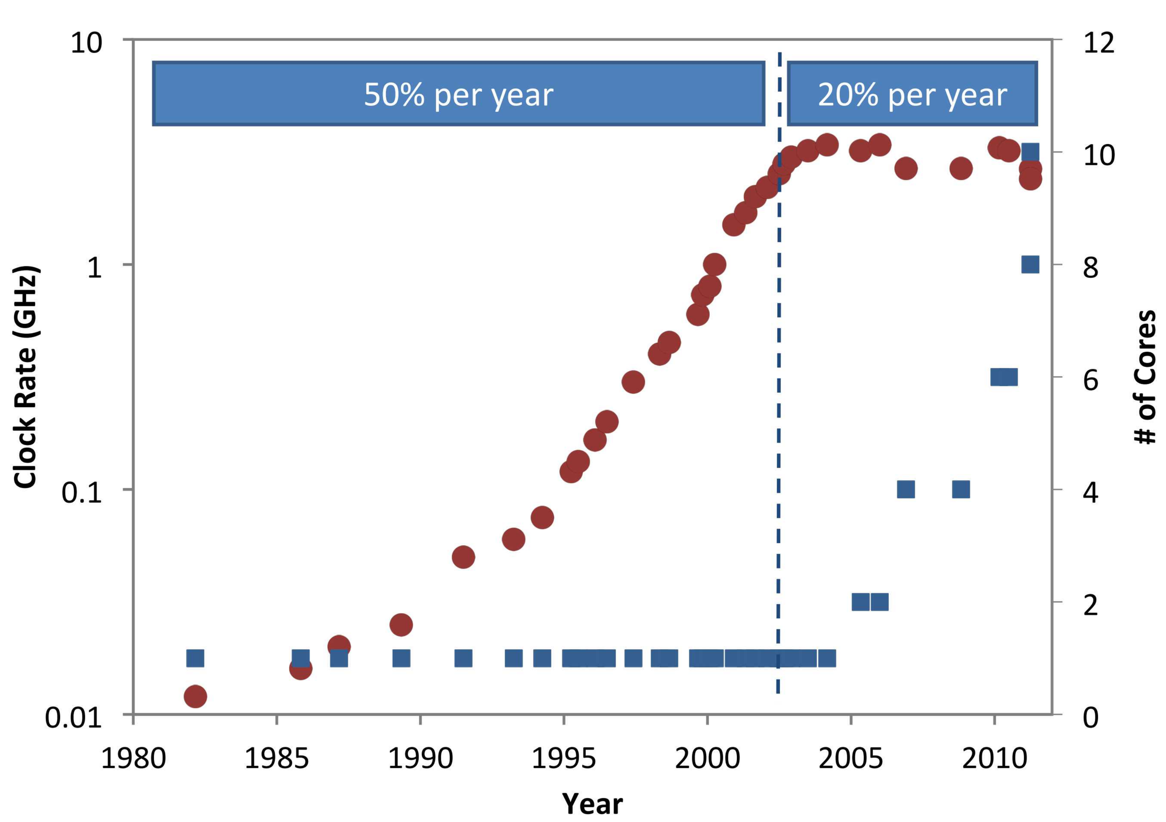
- Equation-oriented modeling framework with suite of unit models supporting separation of models and algorithm or solution approach
- Enables efficient composition, simulation, and optimization of process systems through flexible python frameworks.



Motivating example: Improve the efficiency and reliability of existing coal-fired power plants while accelerating development of a broad range of advanced fossil energy systems.

Challenge: Computational effort of some advanced analyses

Landscape of desktop and scientific computing



32 nm	Tick	Early 2010: Westmere
	Tock	Early 2011: Sandy Bridge
22 nm	Tick	Early 2012: Ivy Bridge
	Tock	Mid 2013: Haswell
	-	Mid 2014: Haswell refresh
14 nm	Tick	Late 2014: Broadwell
	Tock	Mid 2015: Skylake
	-	Early 2017: Kaby Lake
	-	Late 2017: Coffee Lake

Performance improvement in PSE applications

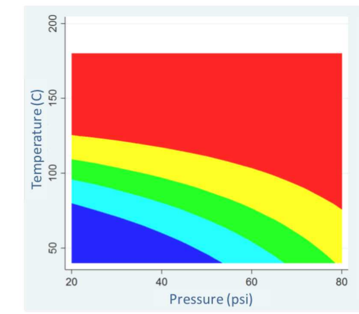
50% Hardware
50% Algorithms

Continued performance improvement demands high-efficiency parallel algorithms

Large-scale IDAES Application Needs and Capabilities in Pyomo

Solution of ensembles of problems

- Parameter sweeps
- Convergence reliability testing
- Global sensitivity analysis, UQ

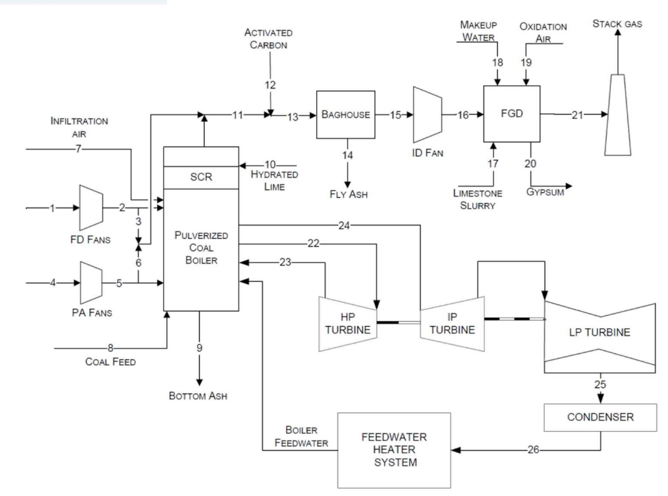


Pyomo DAE

PySP

Rapid solution of large flowsheets

- Parallel model evaluation, linear algebra
- Modular decomposition (units/tearing)
- (Planned summer 2018)



Decomposition of structured problems

- Dynamic optimization
  (structure from discretization of differential equations)
- Optimization under uncertainty
  (structure from multi-scenario formulation)
- Parameter estimation
  (structure from multiple data sets)

Parallel execution through MPI (mpi4py)

- Parallel bounds tightening
- Convergence reliability evaluation

Parallel optimization under uncertainty

- PySP: Stochastic programming capability
- Progressive hedging (Pyro, bundling, etc.)
- Combined with other packages (Pyomo.DAE)

Suite of parallel interfaces in Pyomo

- In progress
- Exemplar algorithmic use cases (branch & bound, PH, Schur-complement, uncertainty quant.)
- Testing existing python packages for usability, parallel scalability, and general efficiency
  - Pyro, mpi4py, celery, multiprocessing
  - Synchronized (blocking) and asynchronous

Overview of Parallel Architectures and Performance

	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

Cloud

Serial Execution Time = 10 min

Parallel Time = 5.5 min

2 Processors
1.8 Times Speedup
~90% Efficiency

Parallel Time = 1.0 min

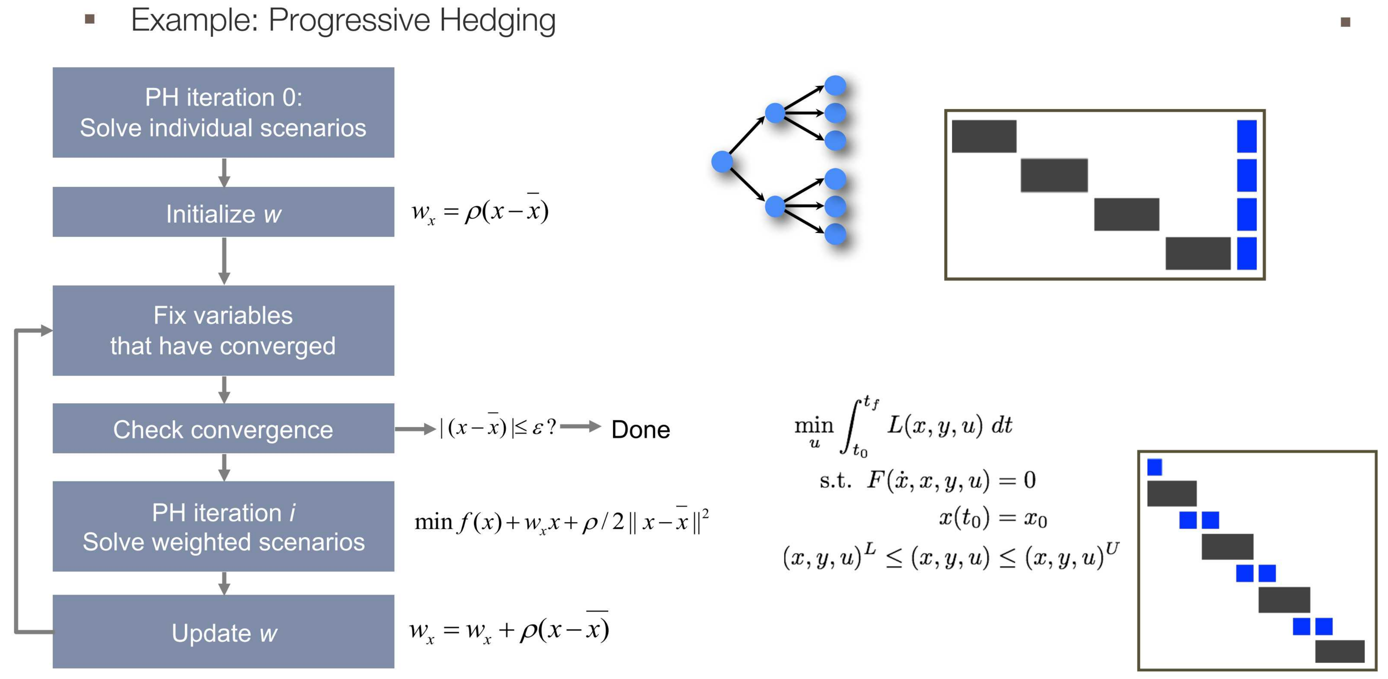
Infinite Processors
10 Times Speedup

Amdahl's Law $S_\infty = \frac{1}{\phi_s}$

Decomposition Strategies for Parallel Solution of Structured Optimization Problems

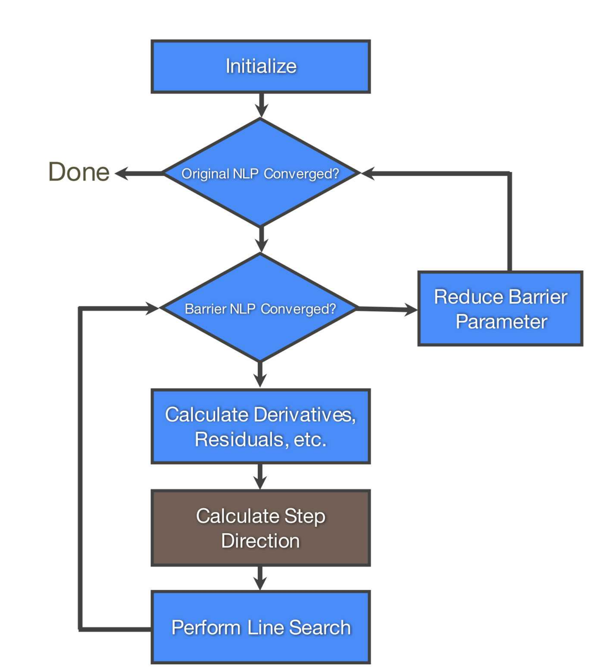
Decomposition strategies allow for parallel solution through iterative solution of smaller subproblems (with coordination)

- Example: Progressive Hedging



Internal linear decomposition approaches start with a "host" algorithm and parallelize the linear algebra

- Example: Schur-complement decomposition



Structure in the optimization problem induces structure in the linear algebra

Parallelize all scale-dependent operations

- Vector and matrix operations
- Model evaluation

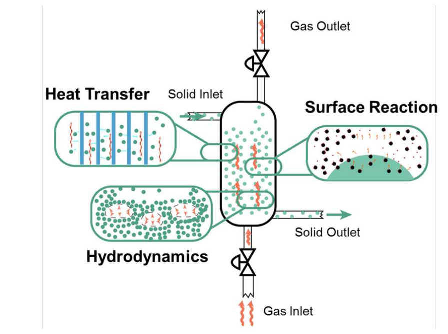
Compared with problem-level decomposition, implementation is time consuming

Retain convergence properties of serial algorithm

Parallel Performance Examples

Progressive hedging to parallelize parameter estimation on a Bubbling Fluidized Bed (BFB) model

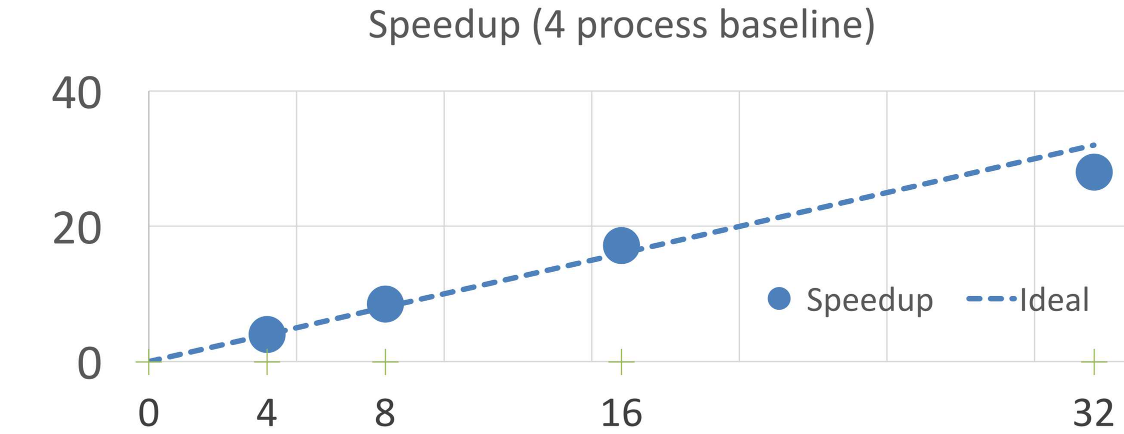
- 1D Spatial model, 3 regions (particle, cloud-wake, emulsion)
- (Lee and Miller, 2013, Ind. Eng. Chem. Res.)



	C_r	a_h	h_w	Time (s)
Actual	1.0	0.8	1500.0	-
PH (Serial)	0.9824	0.7850	1501.74	7050.85
PH (15 processors)	0.9824	0.7850	1501.74	610.98
PH (30 processors)	0.9824	0.7850	1501.74	459.10

Parallel timing for convergence evaluation tool in IDAES

- Solution of ensemble of simulations / optimizations for evaluation of convergence reliability
- 40 CPU machine



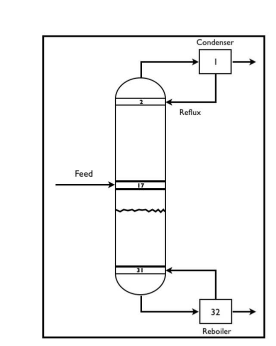
PySP for power grid planning problem (progressive hedging)

- Contingency constrained two-stage optimization formulation

Case Name	# Cont.	PH Iter	Time (s)
case6ww	11	12	2 s
case57	79	21	12 s
case118	117	14	2m 3s
case300	322	8	2m 54s
case2383wp	2252	6	4m 50s

Implicit Schur-complement for Optimization Under Uncertainty

- Distillation system model: [Benallou, Seborg, and Mellichamp (1986)]
- 32 states, 96 scenarios, 32 proc.



Case	# Vars.	# Coupling Vars.	FS-S time(s)	ESC-S time(s)	ESC-P time(s)	PCGSC-S time(s)	PCGSC-P time(s)
1	1430550	150	10.3	79.1	2.6	17.9	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

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, vol 71, Dec. 2014, pp 563-573.

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