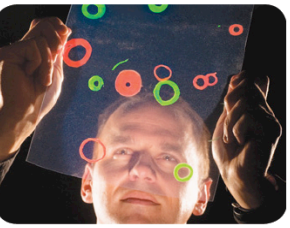

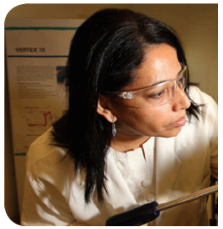

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Structured Modeling and Decomposition Methods in Pyomo

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U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration | CCR Center for Computing Research

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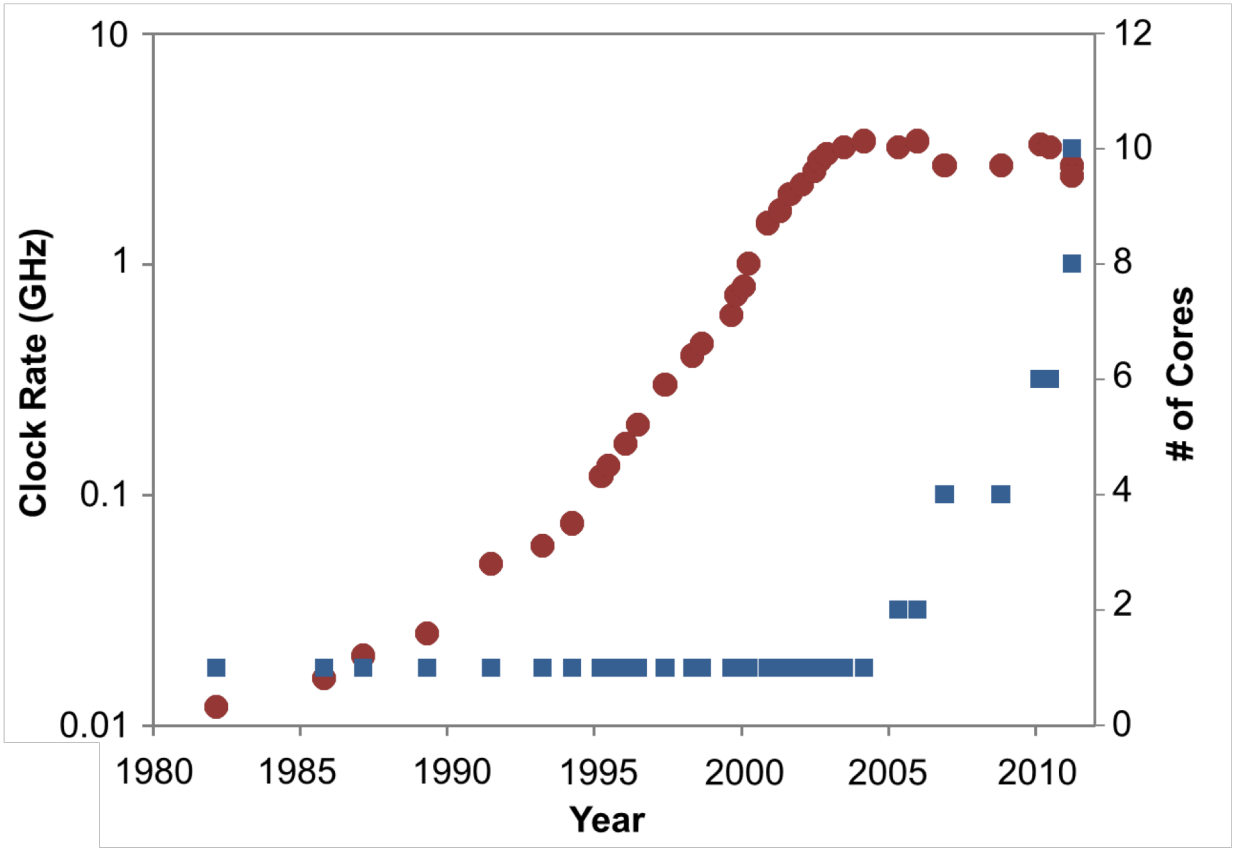
Landscape of Computing Hardware

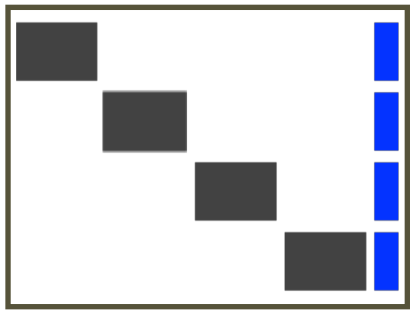


- Improvements in computing clock rates have slowed
- Increased focus on parallel computing architectures

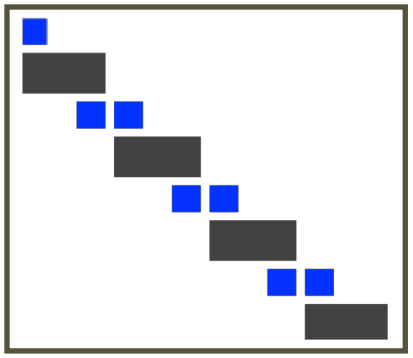
[Steven Edwards, Columbia University]

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)



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



[Laird, 2018]

Overview of Decomposition Algorithms

- Decomposition approaches allow for parallel/distributed computing
  - External decomposition
    - Progressive Hedging (PH)
    - Alternating direction method of multipliers (ADMM)
    - Benders decomposition, dual decomposition
  - Internal decomposition
    - Schur-complement decomposition
    - Block cyclic reduction
    - Reduced-space decomposition

External Decomposition	Internal Decomposition
Break full NLP into subproblems and coordinate solutions	*Build full NLP and decompose at linear algebra level of host algorithm*
Highly flexible and easier to implement	Harder to implement
Typically linear convergence	Convergence rates of host algorithm
Convergence not well understood for general nonconvex NLPs	Convergence properties host algorithm

[Rodriguez, AIChE 2018]

The Unspoken Implementation Challenge

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- Despite having well-established decomposition methods for exploiting common problem structures, there are very few general implementations of these approaches interfaced with popular algebraic modeling languages

- Why?
  - Few algebraic modeling languages are capable of capturing the high-level model structure that can be exploited by these algorithms

Software platform

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- Pyomo: Python Optimization Modeling Objects
- Formulate optimization models within Python


```
from pyomo.environ import *

m = ConcreteModel()

m.x1 = Var()
m.x2 = Var(bounds=(-1,1))
m.x3 = Var(bounds=(1,2))

m.obj = Objective(sense = minimize,
    expr = m.x1**2 + (m.x2*m.x3)**4 + m.x1*m.x3
     + m.x2 + m.x2*sin(m.x1+m.x3) )
```

- Utilize high-level programming language to write scripts and manipulate model objects
- Leverage third-party Python libraries

    e.g. SciPy, NumPy, MatPlotLib, Pandas

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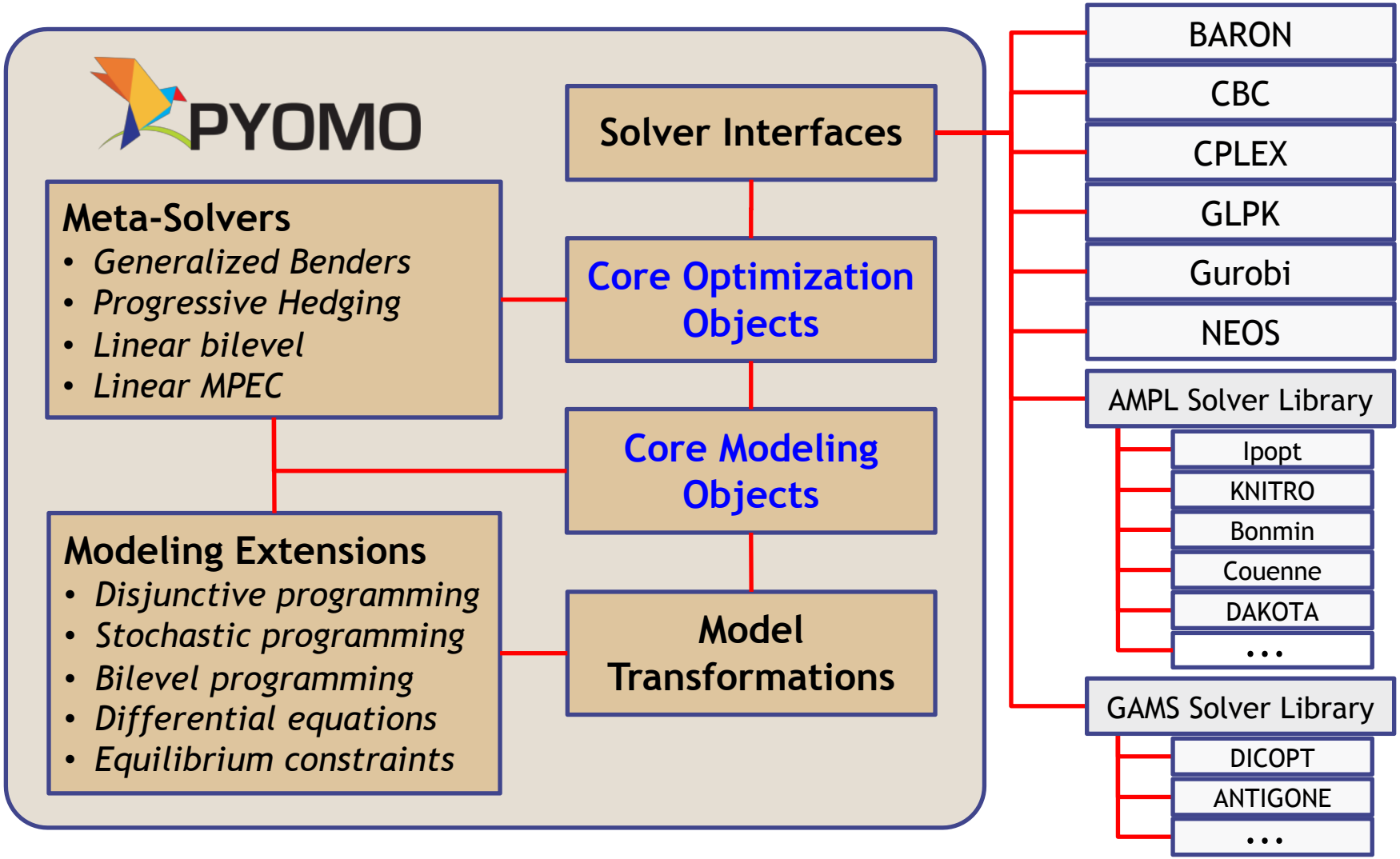
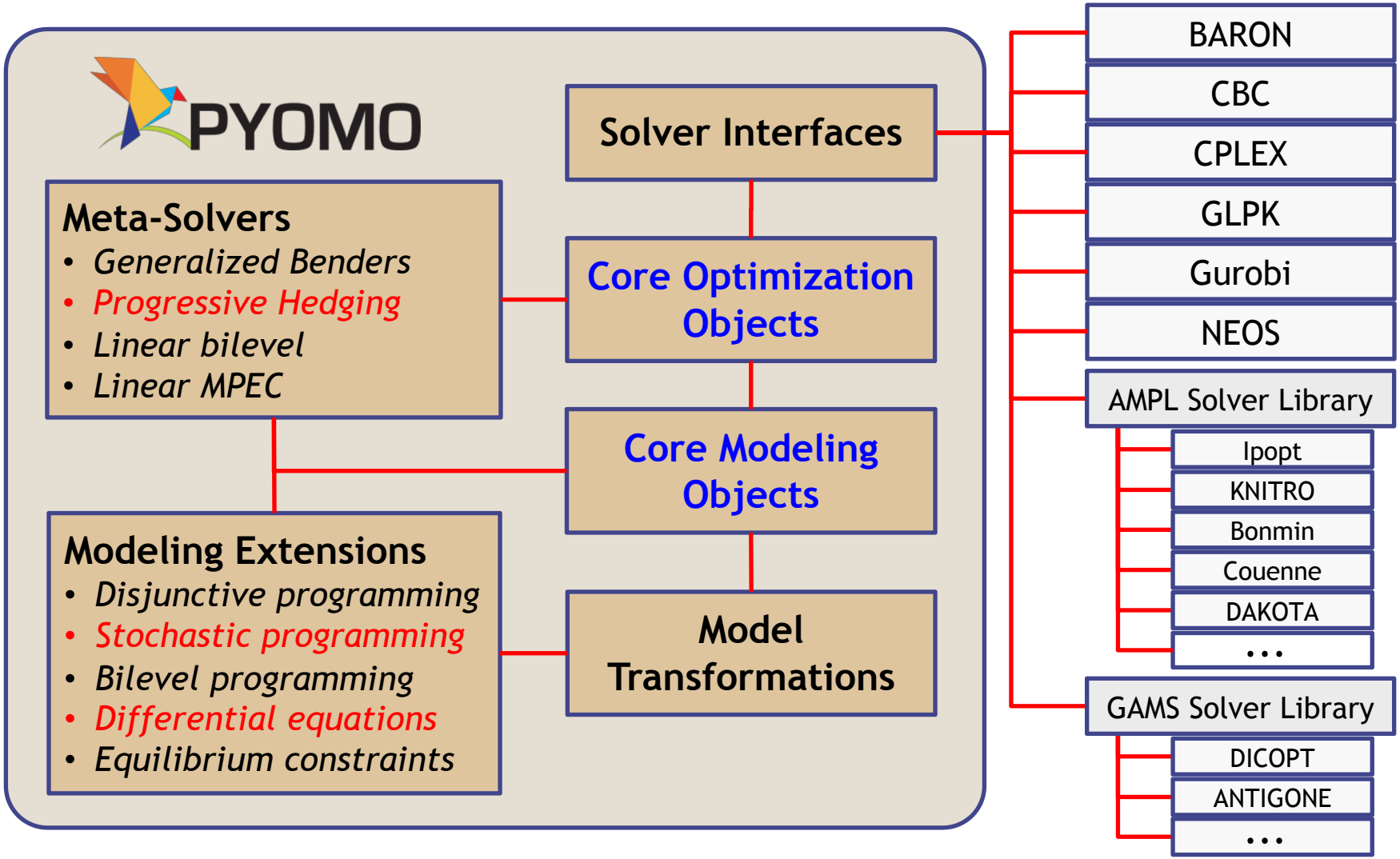
Pyomo at a Glance



Pyomo at a Glance



- Extend Pyomo syntax to represent:
  - Continuous domains
  - Ordinary or partial differential equations
  - Systems of differential algebraic equations (DAEs)
- Available discretization schemes:
  - Finite difference methods (Backward/Forward/Central)
  - Collocation (Lagrange polynomials with Radau or Legendre roots)
- Extensible framework
  - Write general implementations of custom discretization schemes
  - Build frameworks/meta-algorithms including dynamic optimization
- Interface with numerical simulators
  - Scipy for simulating ODEs
  - CasADi for simulating ODEs and DAEs

Simple Example

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$$\frac{dz}{dt} = z^2 - 2z + 1$$

$$z(0) = -3$$

```
from pyomo.environ import *
from pyomo.dae import *

model = m = ConcreteModel()
m.t   = ContinuousSet(bounds=(0, 1))

m.z    = Var(m.t)
m.dzdt = DerivativeVar(m.z, wrt=m.t)

def _zdot(m, t):
    return m.dzdt[t] == m.z[t]**2 - 2*m.z[t] + 1
m.zdot = Constraint(m.t, rule=_zdot)

def _init_con(m):
    return m.z[0] == -3
m.init_con = Constraint(rule=_init_con)

# Discretize model using backward finite difference
discretizer = TransformationFactory('dae.finite_difference')
discretizer.apply_to(m,nfe=10,scheme='BACKWARD')
```

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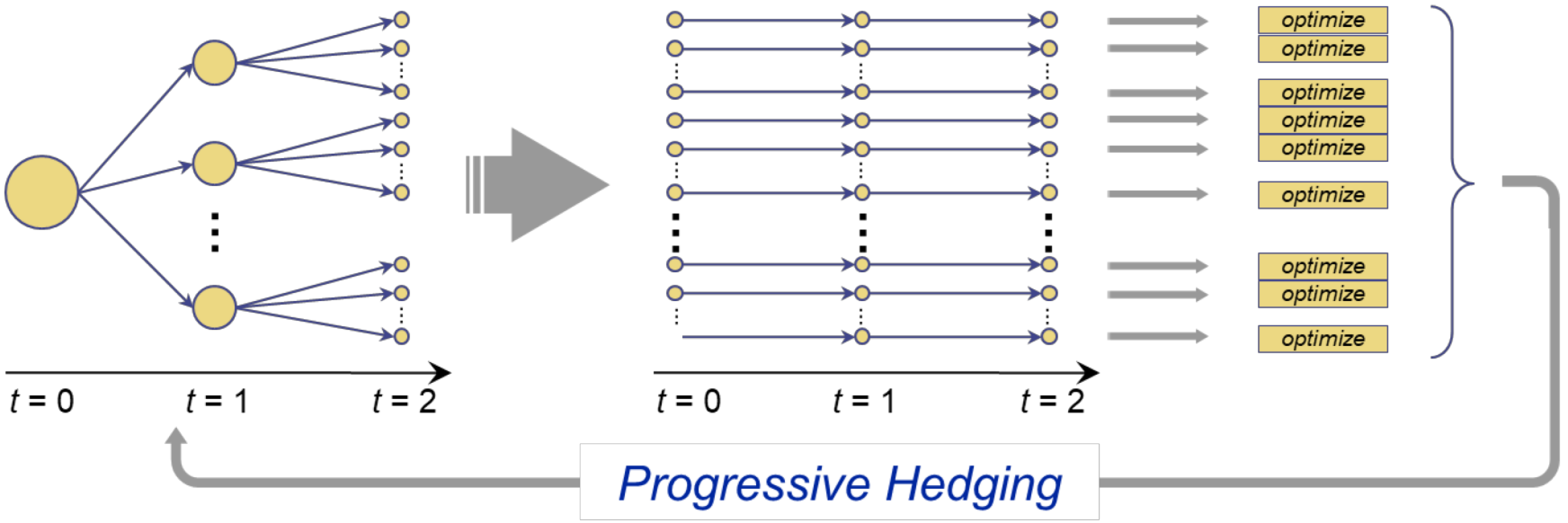
- Framework for representing stochastic programming models, only requiring:
  - deterministic base model
  - scenario tree defining the problem stages and uncertain parameters
- PySP provides two primary solution strategies
  - build and solve the deterministic equivalent (extensive form)
  - Progressive Hedging
  - (plus beta implementations of others, including 2-stage Benders and an interface to DDSIP)
- Parallel infrastructure for generating and solving subproblems on parallel (distributed) computing platforms

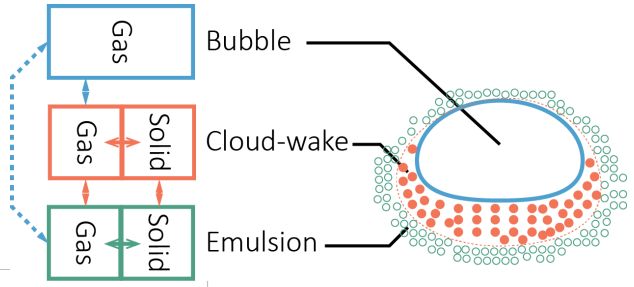
Progressive Hedging

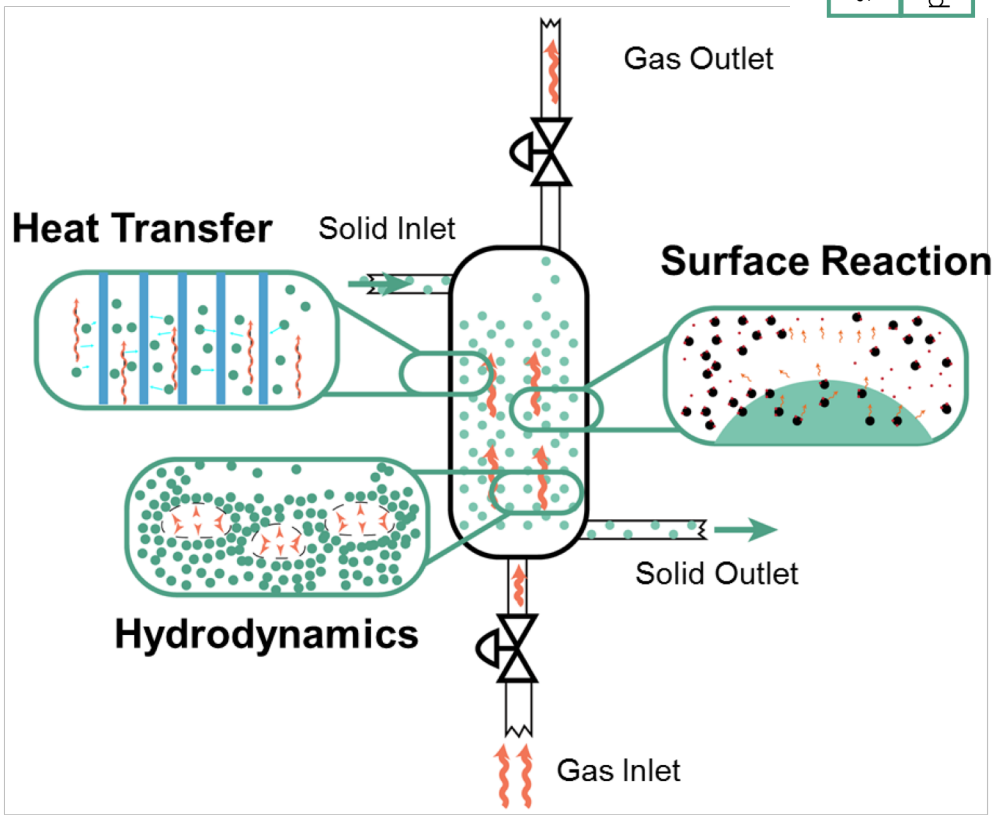
- Scenario-based decomposition algorithm
- Iteratively converge coupling constraints (non-anticipativity constraints) by penalizing deviation from consensus



Bubbling Fluidized Bed (BFB) Model

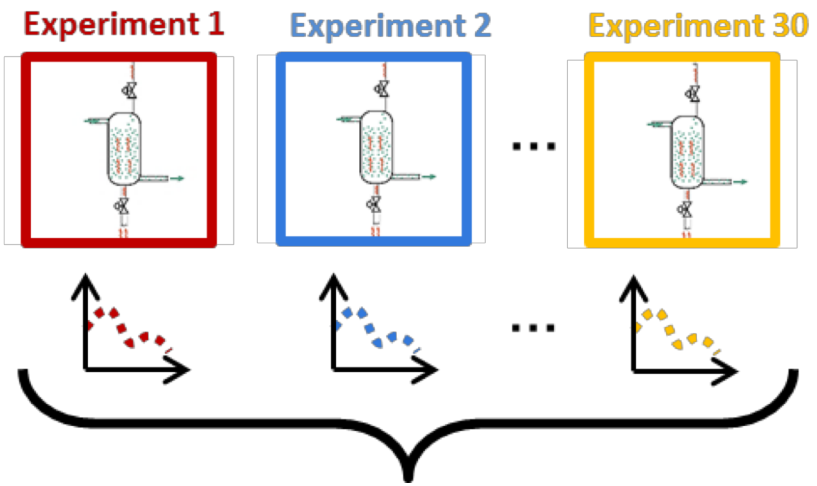
- Gas-solid, 3 region model [3]
- Steady state model with 1-D spatial variation





[Lee and Miller, Ind. Eng. Chem. Res., 2013]

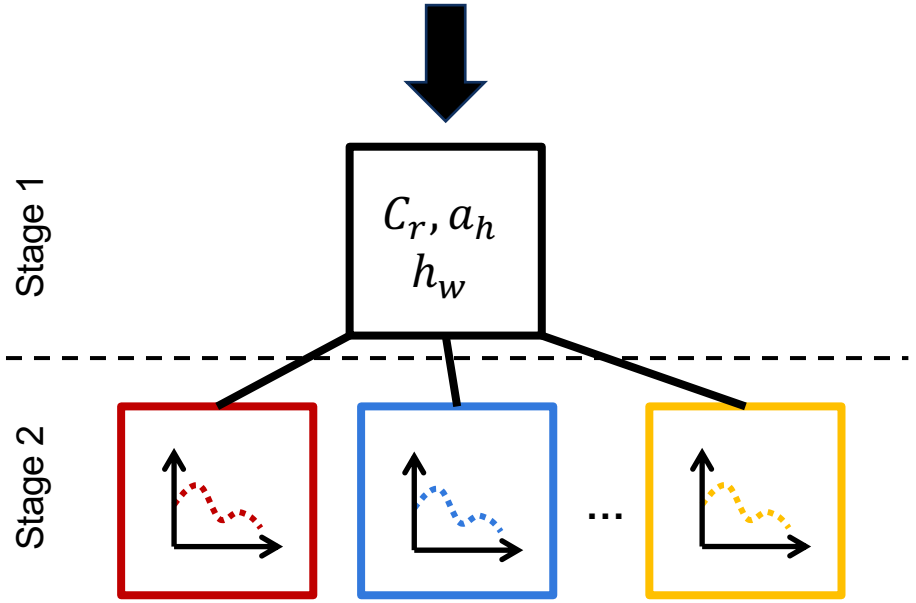
BFB Parameter Estimation



Heat Exchanger Model Parameters	
C_r	Average correction factor for tube model
a_h	Empirical factor for tube model
h_w	Heat transfer coefficient of tube walls

$$\min_{\{C_r, a_h, h_w\}} \sum_{exp.} (error_{meas})^2$$

$$s.t. \quad BFB\ model\ equations$$



Stochastic structure implementation in PySP

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```
def pysp_scenario_tree_model_callback():
    from pyomo.pysp.scenariotree.tree_structure_model \
        import CreateConcreteTwoStageScenarioTreeModel

    st_model = CreateConcreteTwoStageScenarioTreeModel(scenarios)

    first_stage = st_model.Stages.first()
    second_stage = st_model.Stages.last()
    # First Stage
    st_model.StageCost[first_stage] = 'FirstStageCost'
    st_model.StageVariables[first_stage].add('cr')
    st_model.StageVariables[first_stage].add('ah')
    st_model.StageVariables[first_stage].add('hw')
    # Second Stage
    st_model.StageCost[second_stage] = 'SecondStageCost'

    return st_model

def pysp_instance_creation_callback(scenario_name, node_names):
    experiment = int(scenario_name.replace('Scenario',''))
    explist = [1,2,3] # Different data sets

    experiment = explist[experiment-1]
    instance = generate_model_paramest(experiment)

    return instance
```

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BFB Parameter Estimation

- Create and solve extensive form

```
runef --solve --solver ipopt --output-solver-log -m bfb_param.py
```

- Solve using progressive hedging

```
runph --solver ipopt --output-solver-log -m bfb_param.py --default-rho=.25
```

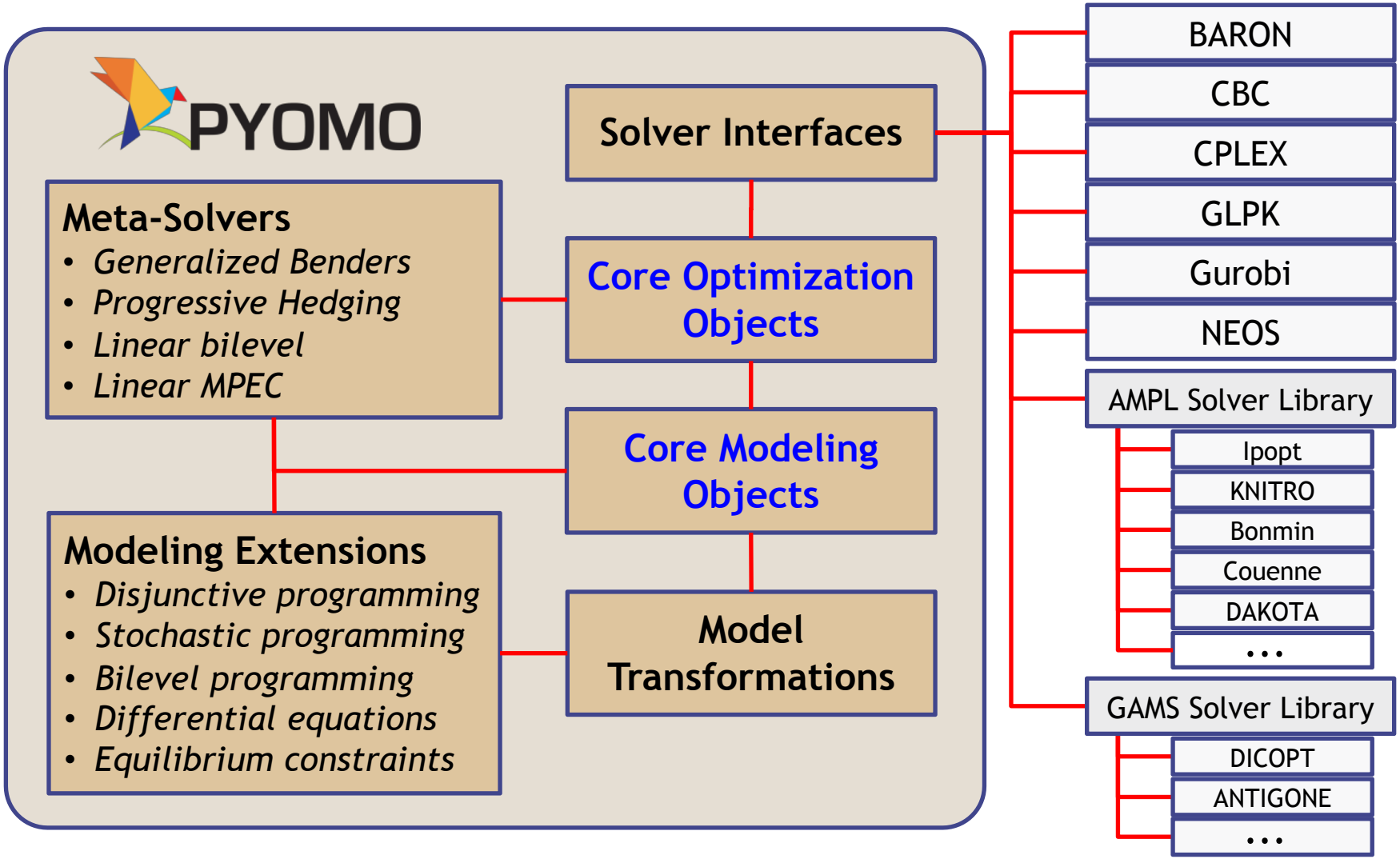
- Solve using progressive hedging in parallel

```
mpirun -np 1 pyomo_ns : -np 1 dispatch_srvr : -np 30 phsolverserver : \
    -np 1 runph --solver-manager=phpyro --shutdown-pyro \
    -m bfb_param.py --solver=ipopt --default-rho=0.25
```

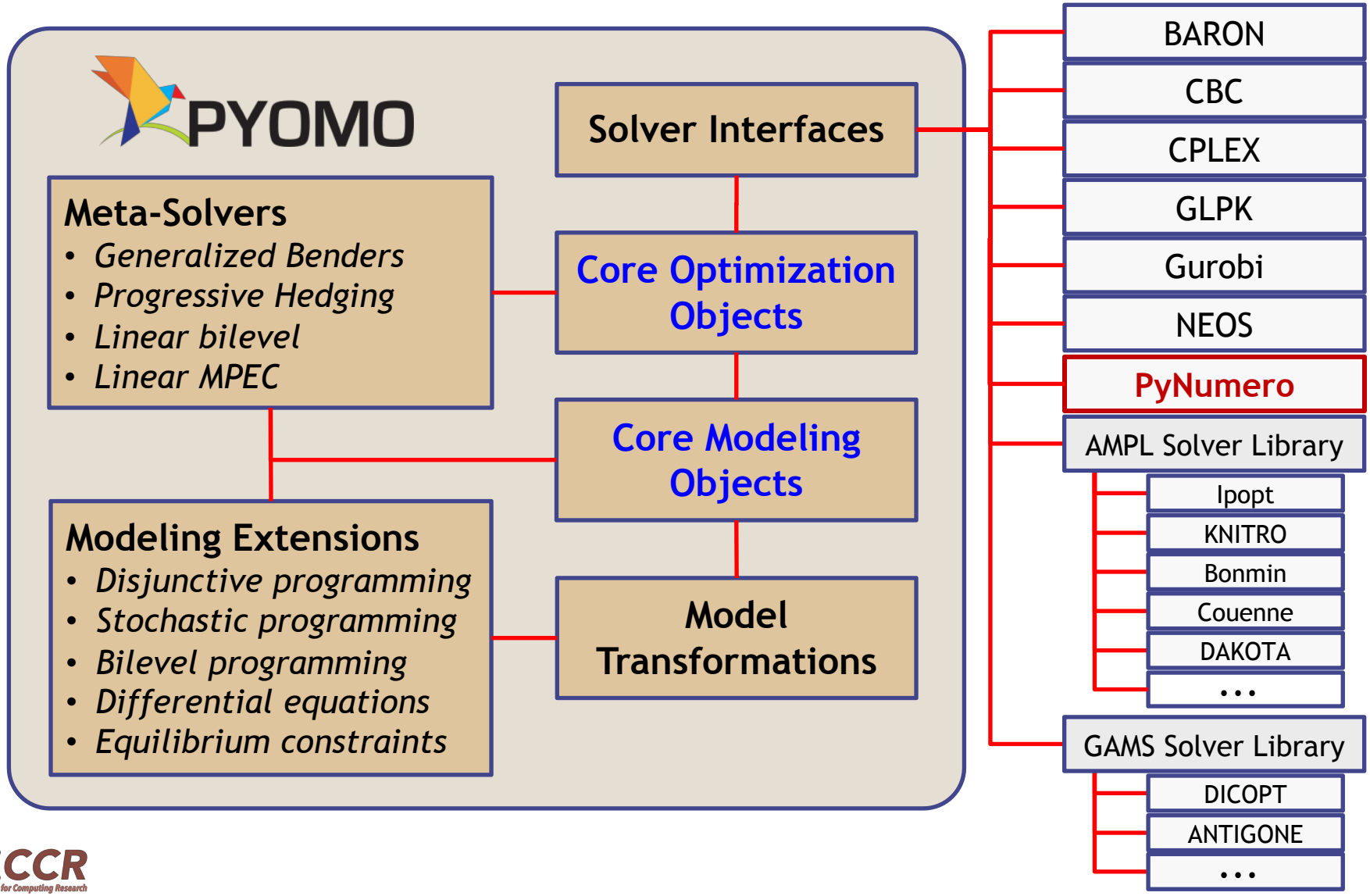
	C_r	a_h	h_w	Solve Time (s)
Actual	1.0	0.8	1500.0	-
Extensive Form	1.016	0.51	1450.35	604.45
Progressive Hedging (15 processors)	0.9824	0.7850	1501.74	610.98
Progressive Hedging (30 processors)	0.9824	0.7850	1501.74	459.10

Extensive form problem size ~400,000 variables and constraints
PH subproblem size ~13,000 variables and constraints

Pyomo at a Glance



Pyomo at a Glance



Purpose of PyNumero

- High-level Python framework for rapid development of nonlinear and parallel decomposition algorithms without large sacrifices in computational performance

- Dramatically reduce time required to prototype new algorithms while minimizing the performance penalty

- Develop a framework for the low-level numerical treatment of Pyomo models that can be used to:
  - Calculate efficient numerical derivatives
  - Implement algorithms that are natively aware of Pyomo model structure

[Rodriguez, AIChE 2018]

PyNumero

- Python C/C++ extension for nonlinear programming
  - Provides first and second derivatives via ASL
  - Interfaces with Numpy/Scipy for all array-operations
  - Supports python calls to HSL linear solver (MA27)
  - Computationally expensive operations performed in C/C++
  - Distributed with Pyomo and conda-forge

```
from pyomo.contrib.pynumero.interfaces import PyomoNLP
import pyomo.environ as aml

m = aml.ConcreteModel()
m.x = aml.Var([1, 2, 3], bounds=(0.0, None))
m.phys = aml.Constraint(expr=m.x[3]**2 + m.x[1] == 25)
m.rsrc = aml.Constraint(expr=m.x[2]**2 + m.x[1] <= 18.0)
m.obj = aml.Objective(expr=m.x[1]**4-m.x[3]*m.x[2]**3)

def my_algorithm(model):
    nlp = PyomoNLP(model)
    x = nlp.create_vector_x()
    c = nlp.evaluate_c(x)
    Jc = nlp.jacobian_c(x)
    …
```

PyNumero Performance

- Equality Constrained Problem with 100K variables

$$\text{minimize} \quad \int_{t_0}^{t_f} \alpha(y_{A,1} - y_{\text{ref}})^2 + \beta(u - u_{\text{ref}})^2 dt$$

$$\text{subject to} \quad \frac{dx_{A,0}}{dt} = \frac{1}{A_{\text{cond}}} V(y_{A,1} - x_{A,0})$$

$$\frac{dx_{A,i}}{dt} = \frac{1}{A_{\text{tray}}} [L_1(y_{A,i-1} - x_{A,i}) - V(y_{A,i} - y_{A,i+1})] \qquad \forall \ i \in \{1, ..., FT-1\}$$

$$\frac{dx_{A,FT}}{dt} = \frac{1}{A_{\text{tray}}} [F x_{A,\text{feed}} + L_1 x_{A,FT-1} - L_2 x_{A,FT} - V(y_{A,FT} - y_{A,FT+1})]$$

$$\frac{dx_{A,i}}{dt} = \frac{1}{A_{\text{tray}}} [L_2(y_{A,i-1} - x_{A,i}) - V(y_{A,i} - y_{A,i+1})] \qquad \forall \ i \in \{FT+1, ..., NT\}$$

$$\frac{dx_{A,NT+1}}{dt} = \frac{1}{A_{\text{reboiler}}} [L_2 x_{A,NT} - (F-D) x_{A,NT+1} - V y_{A,NT+1}]$$

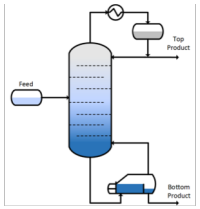
$$x_{A,i} = x_{0_{A,i}} \qquad \forall \ i \in \{0, ..., NT+1\}$$

$$V = L_1 + D$$

$$L2 = L_1 + F$$

$$u = \frac{L_1}{D}$$

$$\alpha_{A,B} = \frac{y_A(1 - x_A)}{x_A(1 - y_A)}$$



Basic SQP ~10% slower than IPOPT

Alternating Direction Method of Multipliers

Algorithm 2: Alternating Direction Method of Multipliers

Given barrier parameter $\rho > 0$, tolerances $\epsilon_r > 0, \epsilon_s > 0$, and estimates y^0, z^0

for $k = 0, 1, 2, \ldots$ **do**

  update partition variables:

  foreach $i \in \mathcal{P}$ **do**

$$x_i^{k+1} = \underset{x_i \in \mathcal{X}_i}{\arg\min}\, f_i(x_i) + \left(A_i x_i + B_i z^k\right)^T y_i^k + \frac{\rho}{2}\|A_i x_i + B_i z^k\|^2$$

  update coupling variables:

$$z^{k+1} = \underset{z}{\arg\min}\, \mathcal{L}_\rho(x^{k+1}, z, y^k)$$

  compute primal residual:

$$r^{k+1} = Ax^{k+1} + Bz^{k+1}$$

  compute dual residual:

$$s^{k+1} = \rho A^T B \cdot (z^{k+1} - z^k)$$

  update dual variables:

$$y^{k+1} = y^k + \rho \cdot r^{k+1}$$

  if $\|r^{k+1}\| \leq \epsilon_r$ *and* $\|s^{k+1}\| \leq \epsilon_s$ **then**

    stop

```python
from pyomo.contrib.pynumero.interfaces.nlp_transformations
import AdmmNLP
# …
for k in range(max_iter):

    # Step 3. Update partition variables
    for bid, nlp in enumerate(nlps):
        xs[bid] = basic_sqp(nlp, tee=False)

    # Step 6. Compute coupling variables
    z = [None] * len(nlps)
    for bid, nlp in enumerate(nlps):
        zi[bid] = xs[bid][nlp.zid_to_xid]
    z = np.mean(z, axis=0)

    # Step 8/10. Compute residuals
    r = [None] * len(nlps)
    for bid, nlp in enumerate(nlps):
        ri[bid] = xs[bid][nlp.zid_to_xid] - z
    s = z - old_z_estimates

    # Update estimates
    for bid, nlp in enumerate(nlps):
        nlp.z_estimates = z
        nlp.w_estimates = nlp.w_estimates + nlp.rho * r[bid]
        nlp.init_x = xs[bid]
        nlp.init_y = ys[bid]
    old_z_estimates = z

    # Step 14. Compute infeasibility norms
    r_norm = np.linalg.norm(np.concatenate(r))
    s_norm = np.linalg.norm(s)

    if r_norm < rtol and s_norm < stol:
        break
```

[J. S. Rodriguez, B. Nicholson, C. D. Laird, V. M. Zavala, "Benchmarking ADMM in nonconvex NLPs", Computers & Chemical Engineering, 2018.]

Summary

- Explicitly capturing high-level structure leads to significantly easier, faster, and more flexible implementations
- Pyomo provides high-level modeling constructs for capturing exploitable structure (www.pyomo.org)
- PyNumero is a promising tool for prototyping general implementations of decomposition algorithms

On-going work:

- Implementations of several internal decomposition methods using PyNumero (Schur-complement, cyclic reduction, etc.)
- Interface to the Rapid Optimization Library (ROL) to access several parallel-in-time algorithms under development