# The Future of Process Optimization

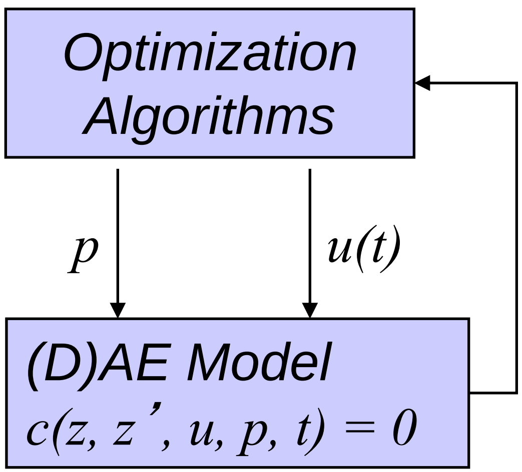
L. T. Biegler
Chemical Engineering Dept.
Carnegie Mellon University

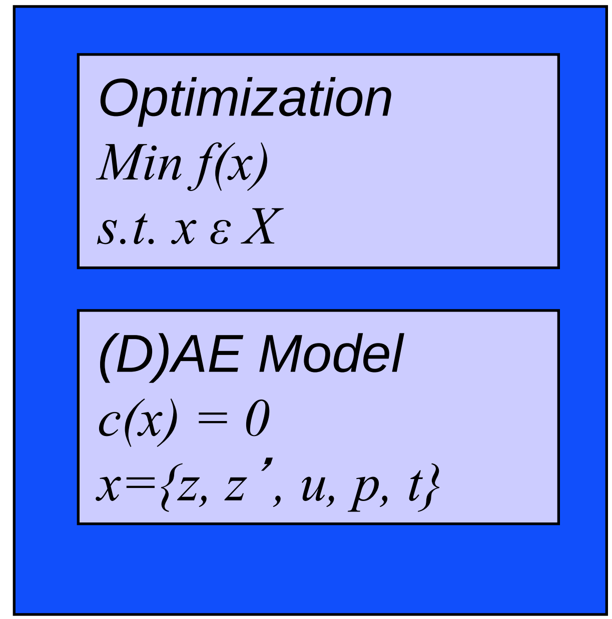
June, 2017

*Congratulations George!*

# Why Process Optimization?

- Equipment and Flowsheet Design
- Process Operations, Transients and Upsets
- Parameter Estimation and Model Discrimination




- Optimization Gives Better Results than with “Experience”
- Consistent Results among all Practitioners
- Reduce Solution Time by Orders of Magnitude
- Support and Enhance Process Understanding

# A Look Back in Optimization
# Early Work (1975)

The Use of Hestenes' Method of Multipliers to Resolve Dual Gaps in Engineering System Optimization[1]

G. STEPHANOPOULOS[2] AND A. W. WESTERBERG[3]

Synthesis of Optimal Process Flowsheets By an Infeasible Decomposition Technique in the Presence of Functional Non-Convexities

*GEORGE STEPHANOPOULOS*

*Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455 U.S.A.*

*and*

*ARTHUR W. WESTERBERG*

*Department of Chemical Engineering, University of Florida, Gainesville, Florida 32611 U.S.A.*

# Evolution of Gradient-Based (NLP) Algorithms & Tasks

’80s: Flowsheet optimization
~ 100 variables and constraints

**SQP**

’90s: Static real-time optimization (RTO)
over 100 000 variables & constraints

**rSQP**

’00s: Simultaneous dynamic optimization
over 1 000 000 variables and constraints

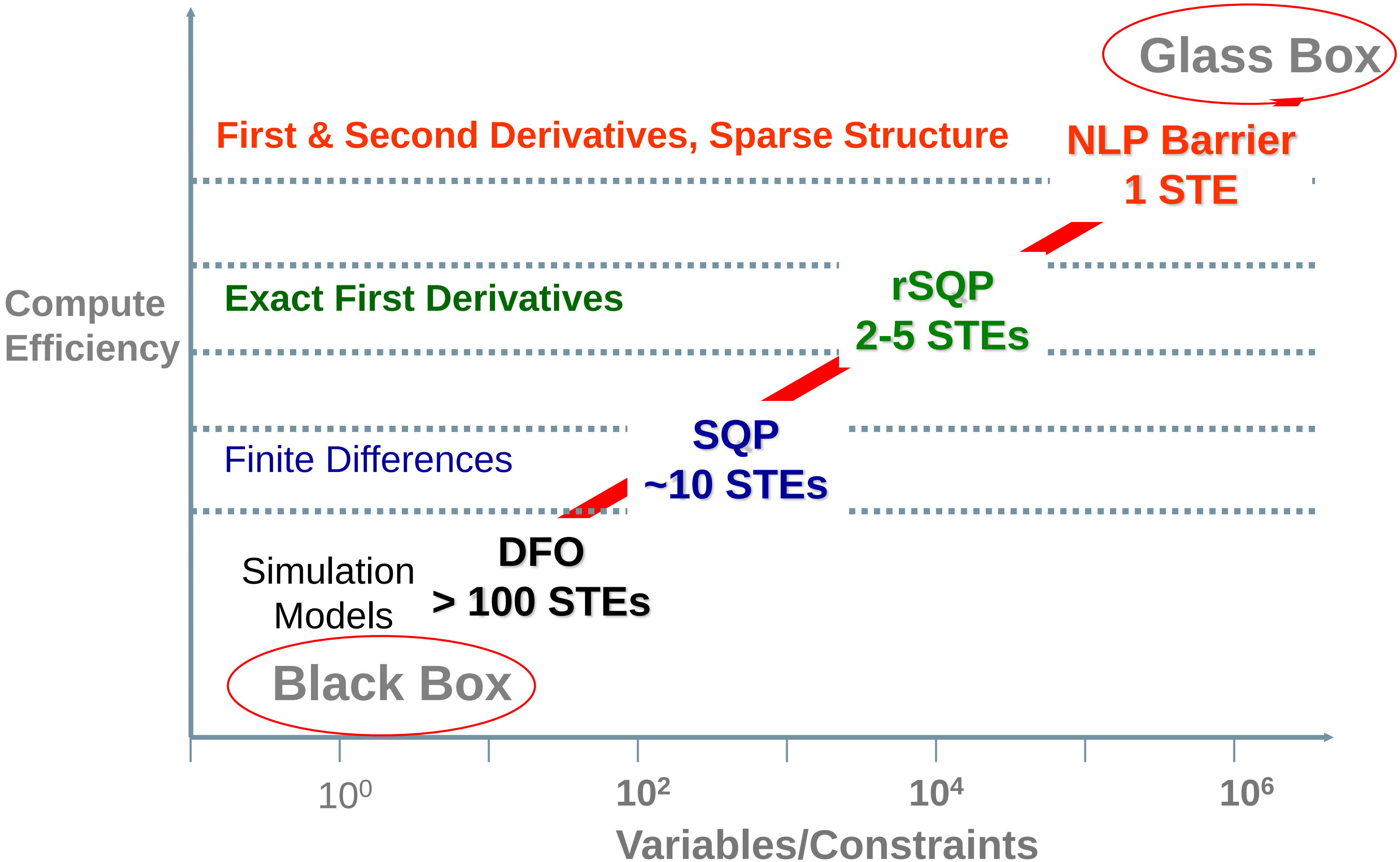
**Barrier (IPOPT)**

‘10s: Sensitivity-based dynamic on-line optimization for large NLPs: < 1 CPUs

**sIPOPT**

The most efficient NLP tools now handle millions of variables and constraints with modest computational effort

# Process Optimization Environments and NLP Solvers

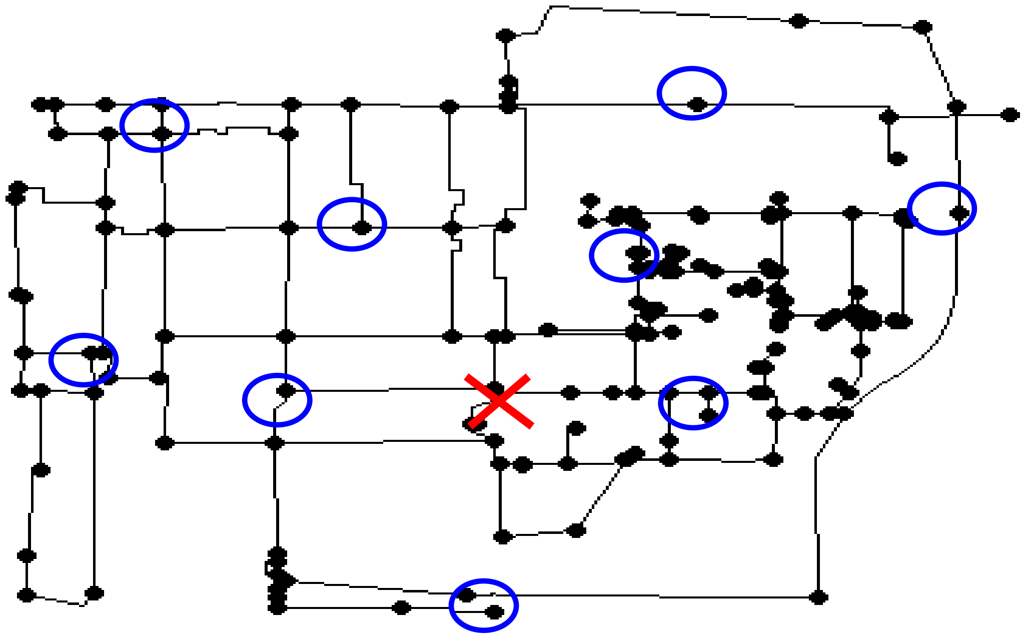


# Equation-Oriented Utopia for Process Optimization

- Glass Box Models - Exact Jacobians/Hessians and sparse equation structure
- Fast Newton-based NLP solvers
- NLP sensitivity (post-optimality and interpretation, multi-level opt., …)
- EO-Modeling Enables:
  - Efficient MINLP Strategies
  - Deterministic Global Optimization
  - Robust and Stochastic Optimization for Uncertainty
- NLP Reformulation for MPECs/MPCCs (for nonsmooth models, bi-level problems, phase changes,…)

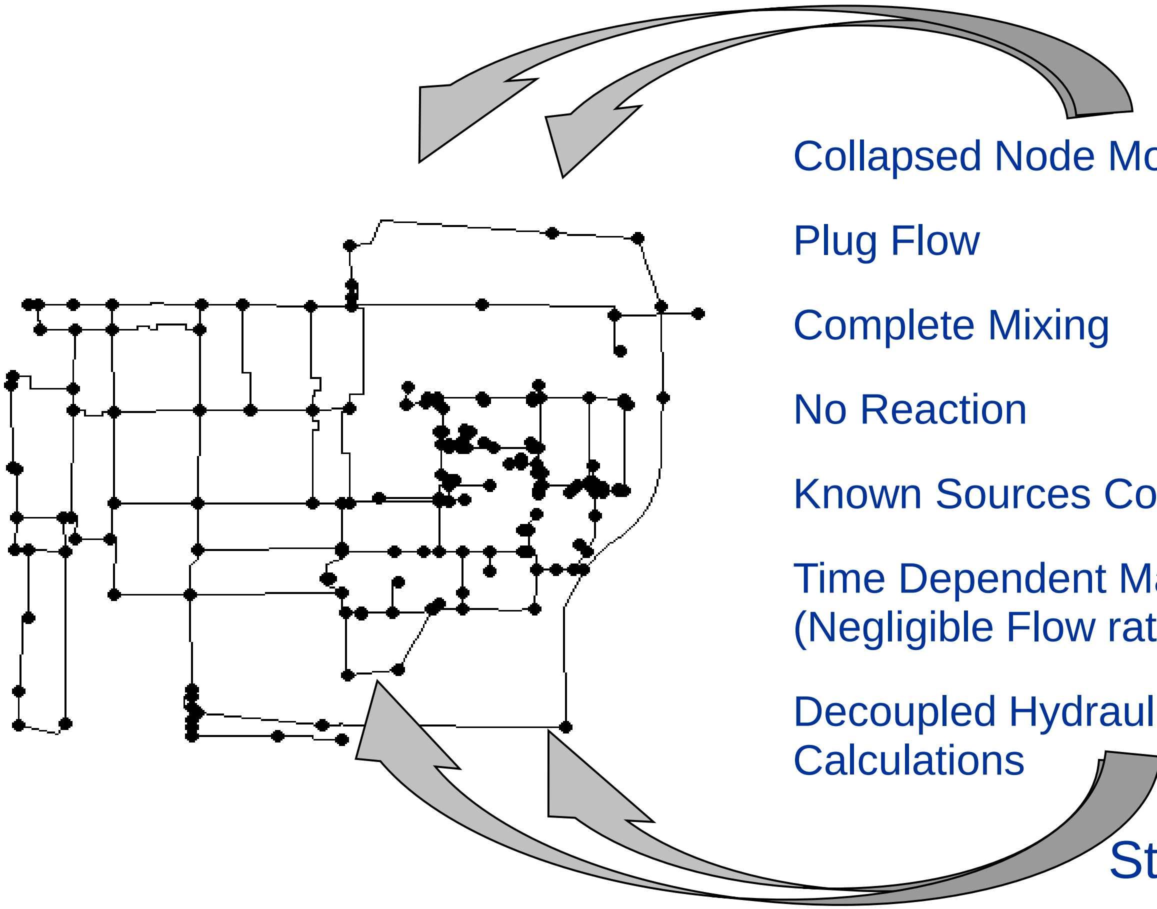
# Early Warning Detection System
# Municipal Water Networks

(Laird, B., 2005, 2006)



- Installed sensors provide an early warning of contamination
- System provides only a coarse measure of contamination time and location
- Desired: Accurate and fast time & location information

# Water Quality Model




Collapsed Node Models

Plug Flow

Complete Mixing

No Reaction

Known Sources Contaminant Free

Time Dependent Mass Injections at All Nodes (Negligible Flow rates)

Decoupled Hydraulics and Water Quality Calculations

# Equation-Oriented Optimization Formulation

**Node Concentrations & Injection Terms Only**

$$\min_{m(t),\bar{c}(x,t),\hat{c}(t)} \Psi = \sum_{r\in\Theta_s} \sum_{k\in\mathcal{N}_s} \frac{1}{2}\int_0^{t_f} w_k(t)\,(\hat{c}_k(t) - \hat{c}_k^\star(t))^2\;\delta(t-t_r)\;dt + \frac{\rho}{2}\int_0^{t_f} m_k(t)^2 dt$$

$$\left.\begin{aligned} \frac{\partial \bar{c}_i(x,t)}{\partial t} + u_i(t)\frac{\partial \bar{c}_i(x,t)}{\partial x} &= 0, \\ \bar{c}_i(x{=}\mathcal{I}_i(t),t) &= \hat{c}_{k_i(t)}(t), \\ \bar{c}_i(x,t{=}0) &= 0, \end{aligned}\right\} \forall i \in \mathcal{P},$$

Only Constraints with Spatial Dependence

$$\hat{c}_k(t) = \frac{\left(\sum_{i\in\Gamma_k(t)} Q_i(t)\;\bar{c}_i(x{=}\mathcal{O}_i(t),t)\right) + m_k(t)}{\left(\sum_{i\in\Gamma_k(t)} Q_i(t)\right) + Q_k^{ext}(t) + Q_k^{inj}(t)}, \qquad \forall k \in \mathcal{J},$$

**Pipe Boundary Concentrations**

$$\left.\begin{aligned} V_k(t)\frac{d\hat{c}_k(t)}{dt} &= \left(\sum_{i\in\Gamma_k(t)} Q_i(t)\;\bar{c}_i(x{=}\mathcal{O}_i(t),t)\right) + m_k(t) - \left[\left(\sum_{i\in\Gamma_k(t)} Q_i(t)\right) + Q_k^{ext}(t) + Q_k^{inj}(t)\right]\hat{c}_k(t), \\ \hat{c}_k(t{=}0) &= 0, \end{aligned}\right\} \forall k \in \mathcal{S},$$

$$m_k(t) \geq 0, \qquad \forall k \in \mathcal{N}.$$

**Injection Terms Only**

# Pipeline Simulation Techniques

## Eulerian

Discretize in time and space

Track concentration at fixed points or volumes

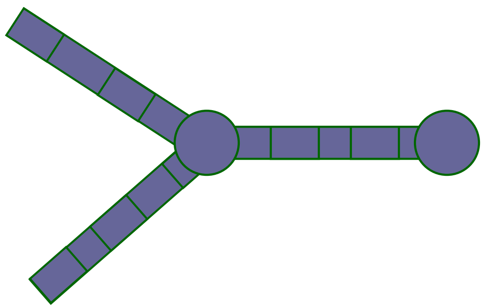
Local process for simulation, but global treatment needed for simultaneous optimization

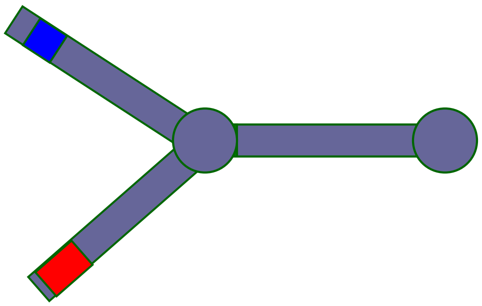
## Lagrangian

Discretize in time alone

Track concentration of elements as they move

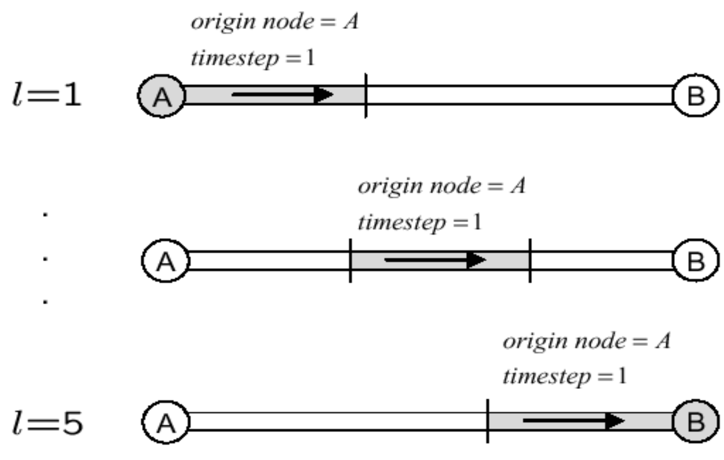
Algorithmic in nature





Review of methods by Rossman and Boulos, 1996.

# Origin Tracking Algorithm



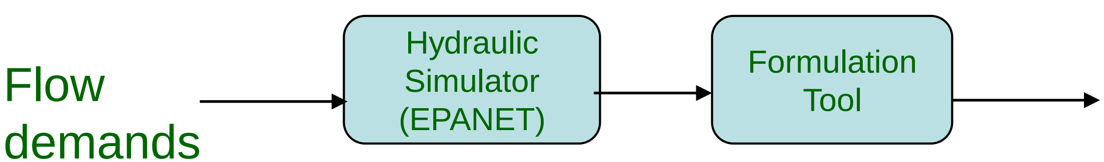

$$\bar{c}(x{=}\mathcal{I}_i(t_1), t_1) = \hat{c}_A(t_1)$$
$$\bar{c}(x{=}\mathcal{O}_i(t_1), t_1) = 0$$

$$\bar{c}(x{=}\mathcal{I}_i(t_5), t_5) = \hat{c}_A(t_5)$$
$$\bar{c}(x{=}\mathcal{O}_i(t_5), t_5) = \hat{c}_A(t_1)$$

Known Hydraulics – Function of Time
Pipe Network PDEs Linear in Concentration
Pipe by Pipe PDEs

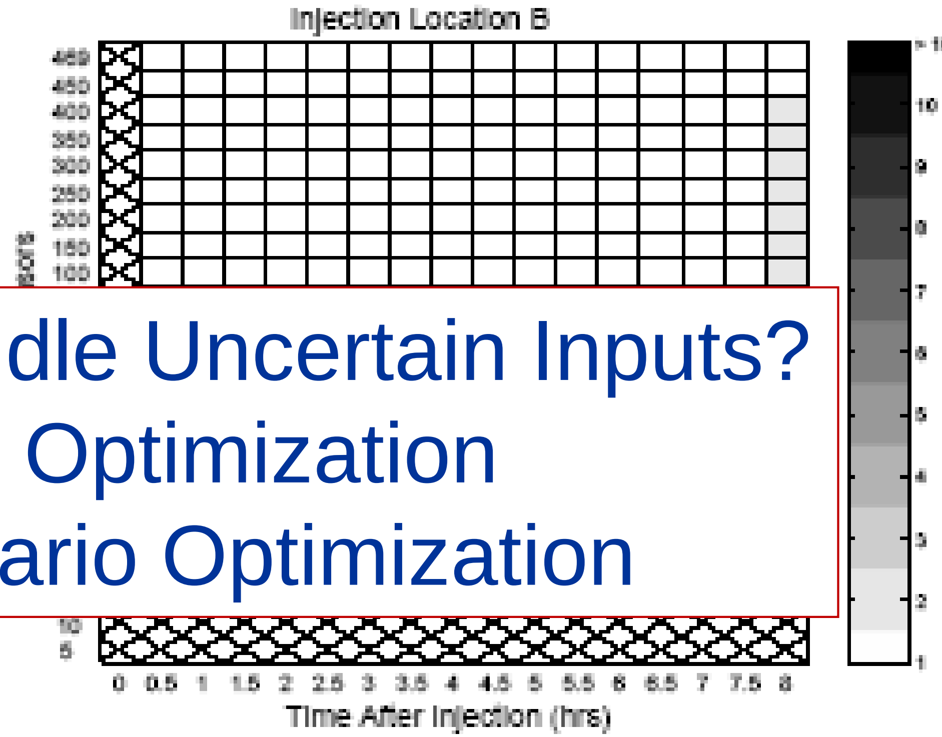
- Efficient for Large Networks
- Convert PDEs to DAEs with variable time delays

Removes Need to Discretize in Space




$$\begin{aligned} \min_{\bar{c},c,m} \quad & f(c,m) \\ \text{s.t.} \quad & \bar{c} - Pc = 0, \\ & \bar{N}\bar{c} + Nc + Mm = 0, \\ & m \geq 0 \end{aligned}$$

# Municipal Source Detection Example


How do we handle Uncertain Inputs?
Robust Optimization
Multi-Scenario Optimization

Alg
networks

Links to existing water flow network simulator ➔ variable time delays

Solution time < 2 CPU minutes for ~ 250,000 variables, ~45,000 degrees of freedom ➔ Effective in a real time setting

Can impose unique solutions through an extended MIQP formulation (post-processing phase)

# Multi-scenario Optimization

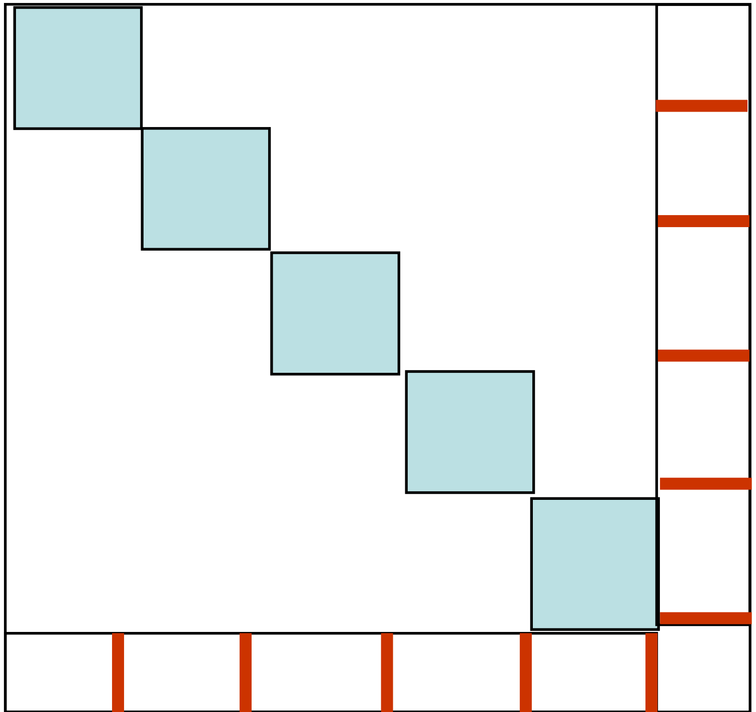
$$Min\ f_0(d) + \Sigma_i f_i(d, x_i)$$
$$s.t.\ h_i(x_i, d) = 0,\ i = 1, \dots N$$
$$g_i(x_i, d) \leq 0,\ i = 1, \dots N$$
$$r(d) \leq 0$$

Variables:

x: state (z) and decision (y) variables for each scenario

d: common variables (e. g. equipment parameters) used

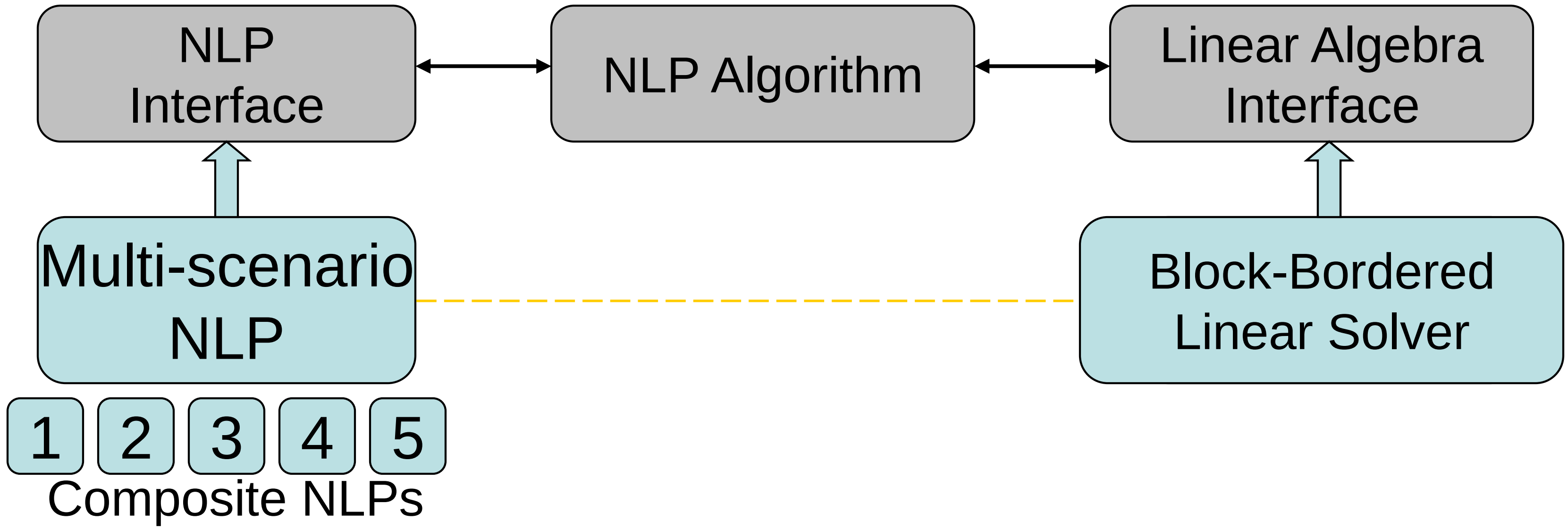
$\delta_i$: substitute for d in each period and add $\delta_i = d$

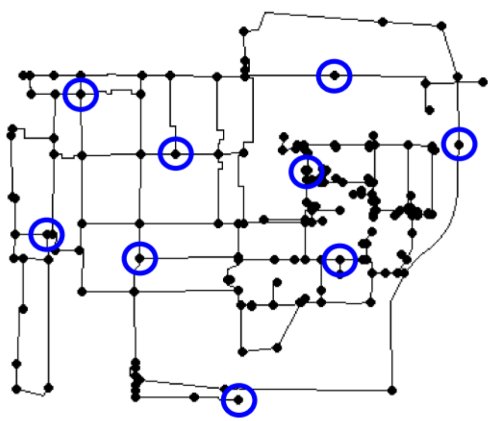


***Composite NLP***

$$Min\ \Sigma_i (f_i(\delta_i, x_i) + f_0(\delta_i)/N)$$
$$s.t.\ h_i(x_i, \delta_i) = 0,\ i = 1, \dots N$$
$$g_i(x_i, \delta_i) + s_i = 0,\ i = 1, \dots N$$
$$0 \leq s_i,\ \underline{d - \delta_i = 0},\ i = 1, \dots N$$
$$r(d) \leq 0$$

# IPOPT Decomposition for Linear Algebra Multi-scenario Implementation (Laird, B.)



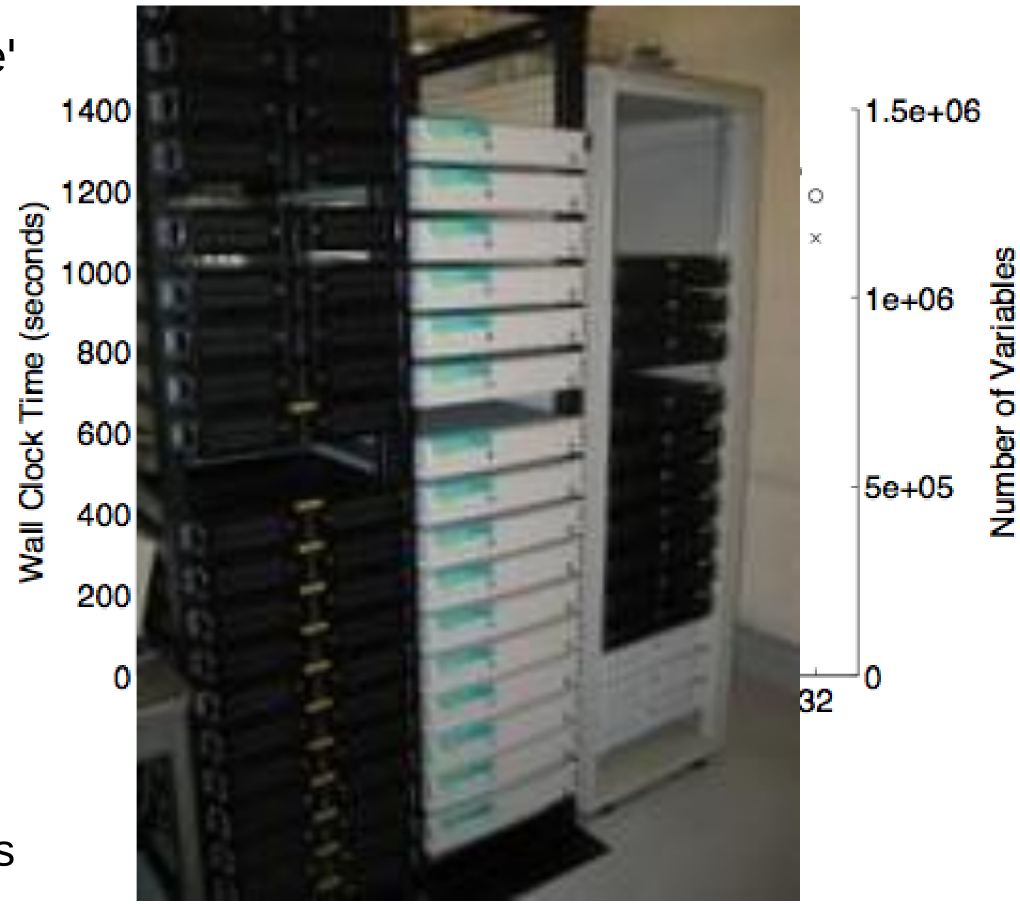
- Water Network Base Problem
  - 36,000 variables
  - 600 common variables
- Testing
  - Vary # of scenarios (data sets)
  - Vary # of common variables

# Parallel Schur-Complement Scalability

- Multi-scenario Optimization
  - Single Optimization over many scenarios, performed on paralle' cluster

  Water Network Case Study
  - 1 basic model
    - Nominal design optimization
  - 32 scenarios (operating data)
    - Form individual blocks

- Determine Injection time profiles as common variables
- Characteristics
  - 36,000 variables per scenario
  - 600 common variables
  - Solution with $1.2 \times 10^6$ variables (20 CPU min)



# Dynamic Optimization in Parallel Architectures

**Exploit Structure of KKT Matrix –** *Nicholson, Wan, B. 2017*

$$\min_{\Pi,\pi_{k,j}} \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM(j)} \left(y_{k,j}(z_i)-y^M_{k,j,i}\right)^T \mathbf{V}_{\mathbf{y}}^{-1}\left(y_{k,j}(z_i)-y^M_{k,j,i}\right)$$
$$+\sum_{k=1}^{NS}\left(w_{k,NZ}-w^M_{k,NZ}\right)^T \mathbf{V}_{\mathbf{w}}^{-1}\left(w_{k,NZ}-w^M_{k,NZ}\right)$$

$s.t.$

$$\mathbf{F}_{k,j}\left[\frac{dy_{k,j}(z)}{dz}, y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$
$$\mathbf{G}_{k,j}\left[y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$
$$y_{k,j}(0)=\phi(y_{k,j-1}(z_{L_{k,j-1}}), F_{f_{k,j}})$$
$$j\in\{1..NZ\},\quad k\in\{1..NS\}$$

$$\begin{aligned}\min\quad & \varphi(x)\\ \text{s.t.}\quad & c(x)=0\\ & x\in X\end{aligned}$$

$$\begin{aligned}\min\quad & \textstyle\sum_{k=1}^{N}\varphi(x_k,u_k)\\ \text{s.t.}\quad & x_{k+1}=f(x_k,u_k)\\ & x_k\in X, u_k\in U\end{aligned}$$

$$\begin{bmatrix} H_k & A_k & -I\\ A_k^T & 0 & 0\\ V_k & 0 & X_k\end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta\lambda\\ \Delta\nu\end{bmatrix}=-\begin{bmatrix} r_x\\ r_\lambda\\ X_kV_ke-\mu_\ell e\end{bmatrix}$$

$$\begin{bmatrix}
W_{u_1u_1} & f_{u_1} & & & & & & & & \\
f_{u_1}^T & 0 & -I & & & & & & & \\
 & -I & W_{x_2x_2} & W_{x_2u_2} & f_{x_2} & & & & & \\
 & & W_{u_2x_2} & W_{u_2u_2} & f_{u_2} & & & & & \\
 & & f_{x_2}^T & f_{u_2}^T & 0 & -I & & & & \\
 & & & & -I & W_{x_3x_3} & W_{x_3u_3} & f_{x_3} & & \\
 & & & & & W_{u_3x_3} & W_{u_3u_3} & f_{u_3} & & \\
 & & & & & f_{x_3}^T & f_{u_3}^T & 0 & \ddots & \\
 & & & & & & & \ddots & \ddots & -I\\
 & & & & & & & & -I & W_{x_Nx_N}
\end{bmatrix}$$

**Sparse LBL Factorization**

**Memory Bottlenecks**

**Factorization Time *Scales Superlinearly* with Data sets**

**Block Tridiagonal Systems**

**Develop Tailored Decomposition?**

Carnegie Mellon

# Cyclic Reduction (CR) for Dynamic Optimization

$$\begin{bmatrix} A_1 & C_1 & & & \\ B_2 & A_2 & C_2 & & \\ & B_3 & A_3 & C_3 & \\ & & \ddots & \ddots & \ddots \\ & & & B_{N_i} & A_{N_i} \end{bmatrix}$$

Permute Matrix

$$\left[\begin{array}{ccccc|cccc} A_1 & & & & & C_1 & & & \\ & A_3 & & & & B_3 & C_3 & & \\ & & \ddots & & & & B_5 & \ddots & \\ & & & A_{N_i-2} & & & & \ddots & C_{N_i-2} \\ & & & & A_{N_i} & & & & B_{N_i} \\ \hline B_2 & C_2 & & & & A_2 & & & \\ & B_4 & C_4 & & & & A_4 & & \\ & & \ddots & \ddots & & & & \ddots & \\ & & & B_{N_i-1} & C_{N_i-1} & & & & A_{N_i-1} \end{array}\right]$$

**Odd**

**Even**

Eliminate Even Rows

$$\left[\begin{array}{cccc|cccc} A_1 & & & & C_1 & & & \\ & A_3 & & & B_3 & C_3 & & \\ & & \ddots & & & B_5 & \ddots & \\ & & & & & & \ddots & C_{N_i-2} \\ & & & A_{N_i} & & & & B_{N_i} \\ \hline & & & & A_1^{(i+1)} & C_1^{(i+1)} & & \\ & & 0 & & B_2^{(i+1)} & A_2^{(i+1)} & C_2^{(i+1)} & \\ & & & & & \ddots & \ddots & \ddots \\ & & & & & & B_{N_{i+1}}^{(i+1)} & A_{N_{i+1}}^{(i+1)} \end{array}\right]$$

**( Forms Schur complement)**

Repeat

# Multi-core MATLAB Tests: State of Art Comparison

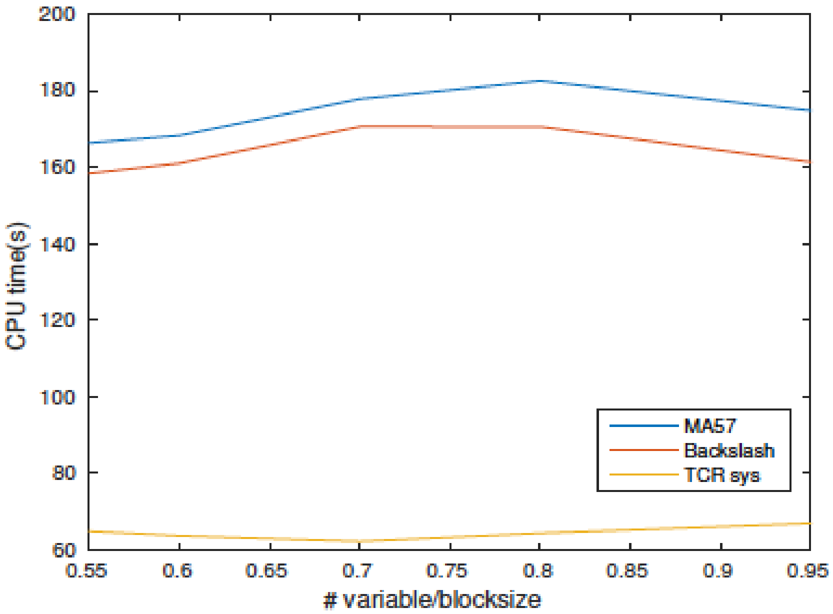



Figure 8: CPU time versus variable ratio

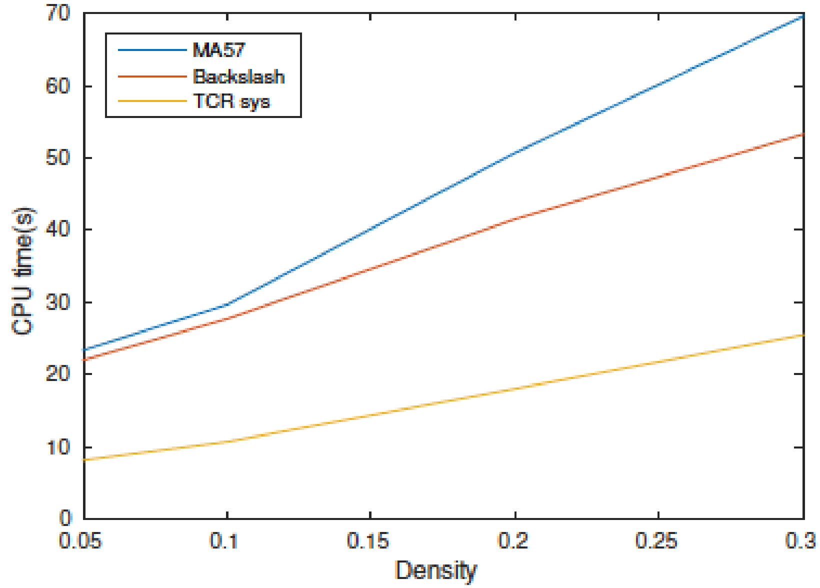



Figure 9: CPU time versus density

- CR vs. Backslash vs. Sparse HSL
- Amdahl's Law Supersedes Moore's Law
- Multiple cores compensate for stagnant clock times
- **NLP must embrace Parallel Decompositions**

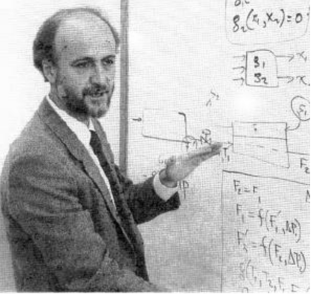
# 2040: Giga-scale Process Optimization

**Enabling Tools:**

- Structured NLPs with billions of variables
- Friendly, Powerful and Intelligent Optimization Modeling Environments
- Distributed Optimization Solvers with Exploitable Large-scale Structures
- Integrated with Advanced Parallel Computation Environments (Multi-core CPUs, GPUs…)

**Applications:**

- Dynamic Global Network Models
- Large, Smart Electric Grid Optimization
- Gas and Oil Pipeline Optimization
- Enterprise-Wide Dynamic, Real-time Optimization



# Optimization Strategies and Process Insight: Back to 1980

## Synthesis of Process Flowsheets: An Adventure in Heuristic Design or a Utopia of Mathematical Programming?

George Stephanopoulos
University of Minnesota, Minneapolis, MN 55455

ABSTRACT

The problem of synthesizing a process flowsheet is analyzed from different angles like: ways to formulate it, methods to generate the structural alternatives, strategies to search for the optimum, etc. Such a critical review will be concerned with all the major contributions to this problem to date. Their strengths and weaknesses will be pointed out, while the future trends will be placed in perspective. Furthermore, several areas for future research will be examined and the potential benefits will be evaluated. The interrelationship between synthesis and analysis is recognized as the cornerstone in formulating the new, demanding analytical questions and in furthering the work on the synthesis of process flowsheets. Examples of this interplay are discussed with respect to the synthesis of heat exchanger networks, heat integrated distillations, and the selection of the most promising chemical reaction paths.

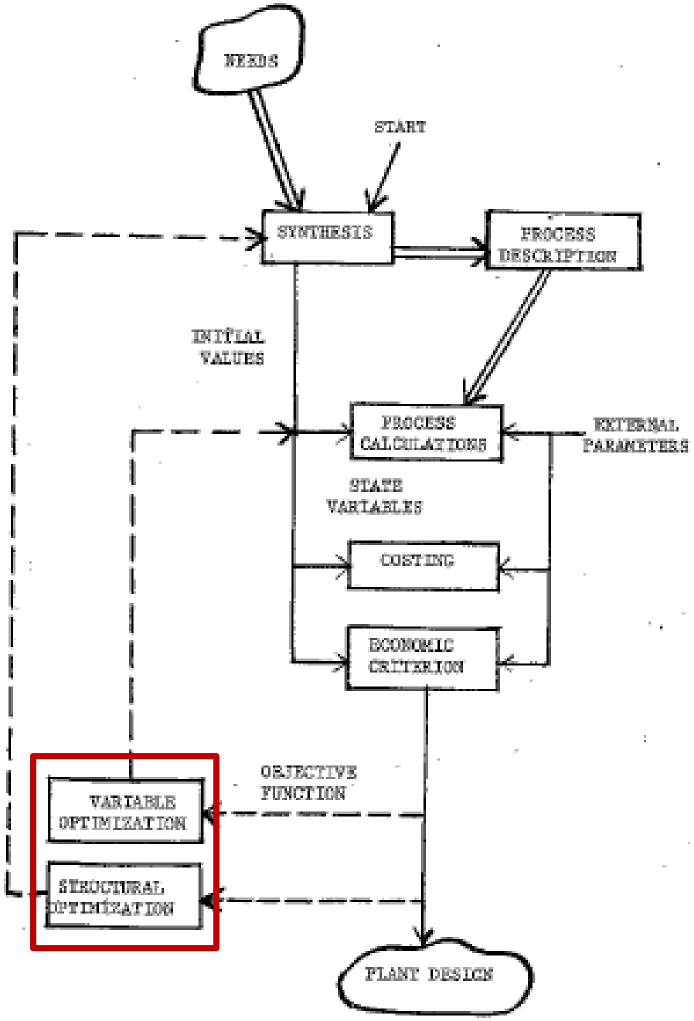
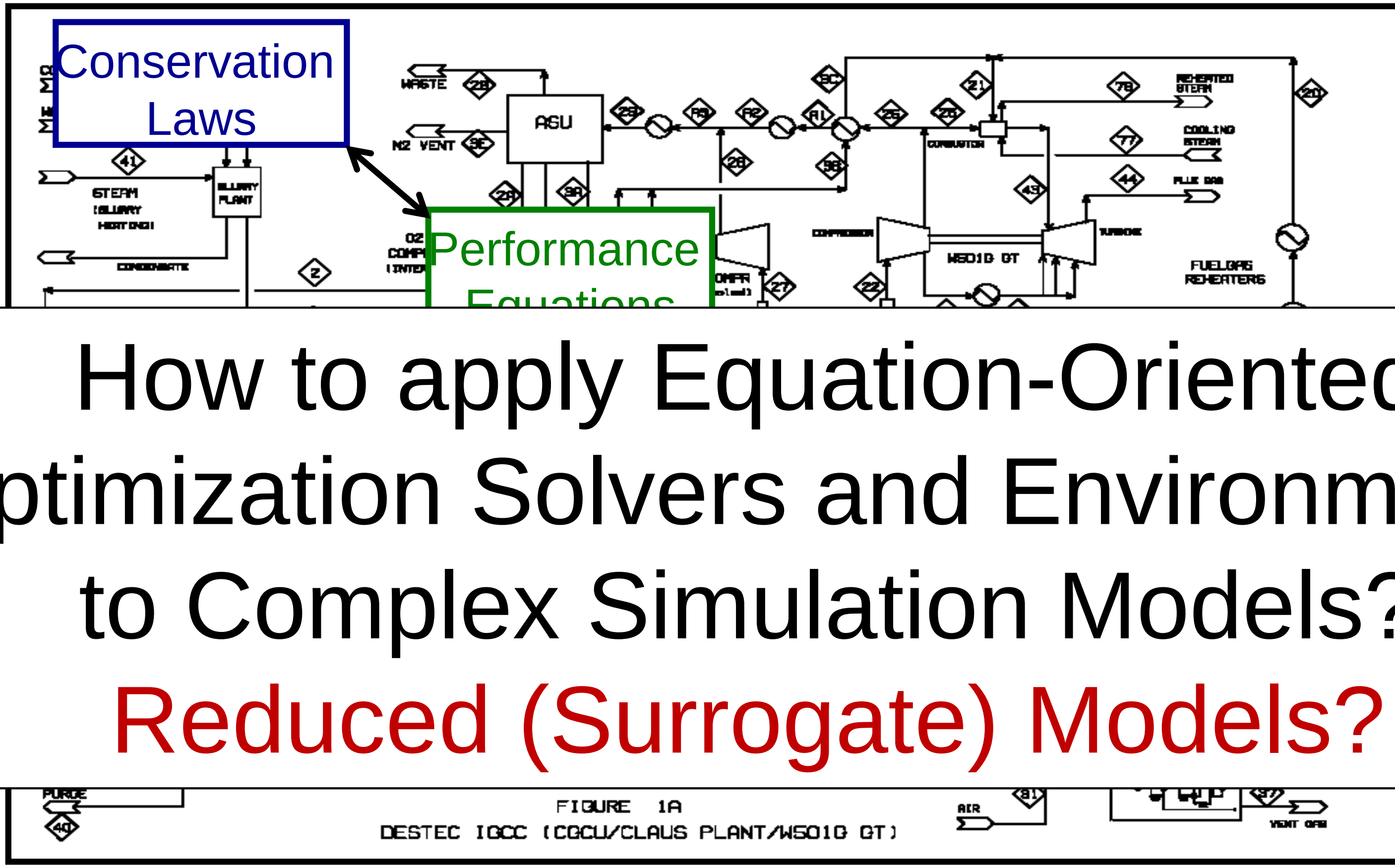



Figure 1. The structure of the design activities.

# From Nested to Equation-Oriented Optimization?




How to apply Equation-Oriented Optimization Solvers and Environments to Complex Simulation Models?

Reduced (Surrogate) Models?

<u>Model Hierarchies</u>

Conservation Laws: Often linear, straightforward to satisfy

Physical properties: Ideal → Specialized Nonideal

Separation Models: Shortcut → MESH, mass transfer

Reaction Elements: Stoichiometric → CFD, Multiphase

# Surrogate Models in Optimization?

- Some Detailed models may be too expensive for EO.
  - for routine simulation
  - integration with other subsystems (multi-scale)
  - for design and control
  - for optimization

- Physics-based Model Reduction
  - Limiting assumptions, spatial → lumped…
- Spectral Model Reduction
  - POD, SVD, Singular Perturbation
- Data-Driven Model Reduction
  - PCA, PLS, Neural Networks, Kriging, …
- Best model reduction strategies?
- How can they be used for optimization?

# Surrogates for Optimization?

Consistency

- ODM and Reduced model (RM) must have differential input-output maps
- ODM and Reduced model (RM) must match (be feasible)
- ODM and RM must recognize same optimum point

  => satisfy same KKT conditions (gradient-based)

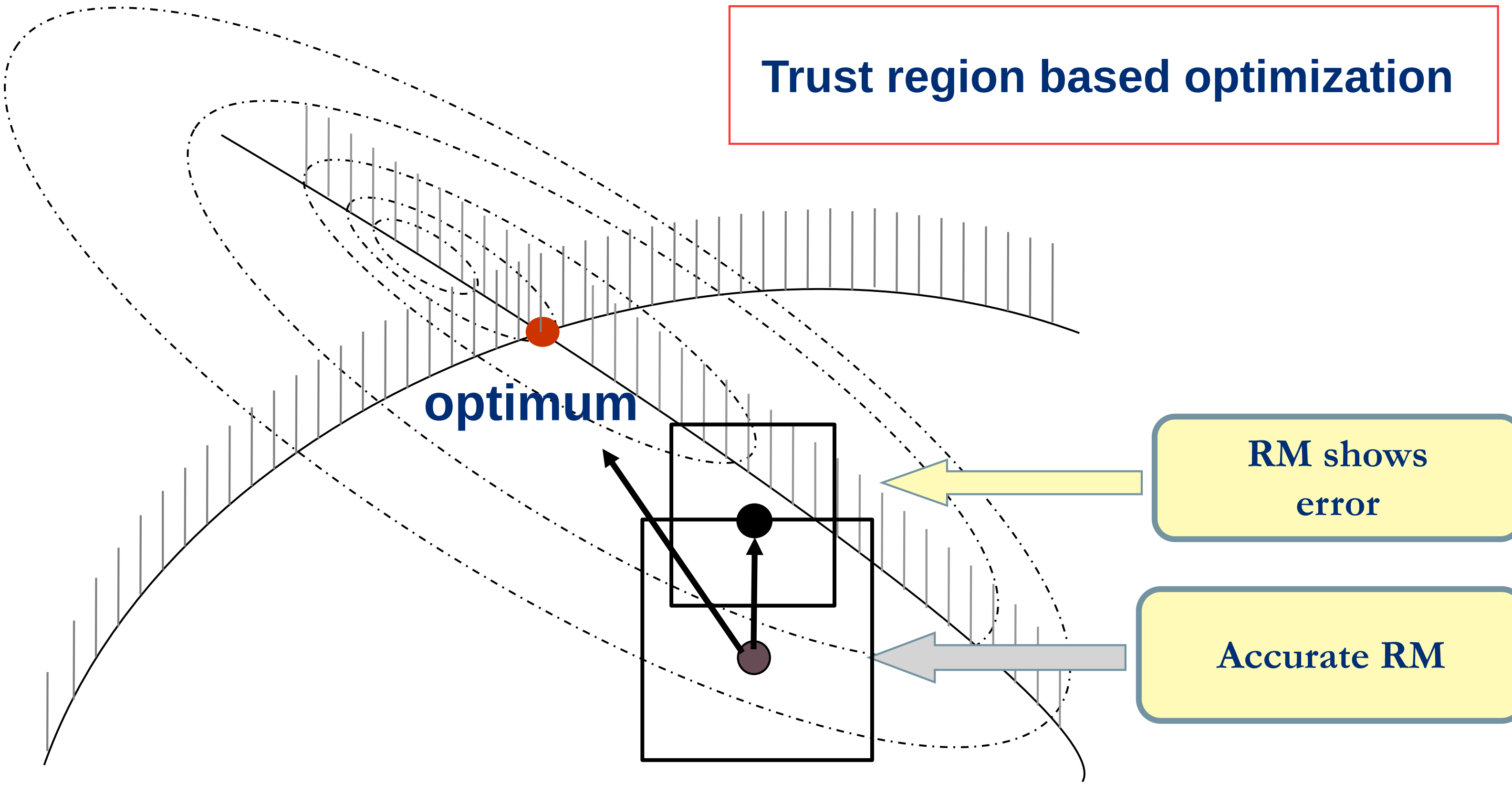
Stability

- Sequence of objective functions remains bounded
- Provide sufficient improvement toward ODM optimum

# Reduced Model Optimization Strategy

RM depends on ODM information at current parameter values

ODM gradients - often not available



# Toy Example for ROM-based Optimization
# Failure to Detect Solution (B., Grossmann, Westerberg, 1985)

(ODM) Min $y^2 + x^2$

s.t. $y - (x^3+x^2+1) = 0$

(ROM) Min $y^2 + x^2$

s.t. $y - (x + \underline{\mathbf{b}}) = 0$

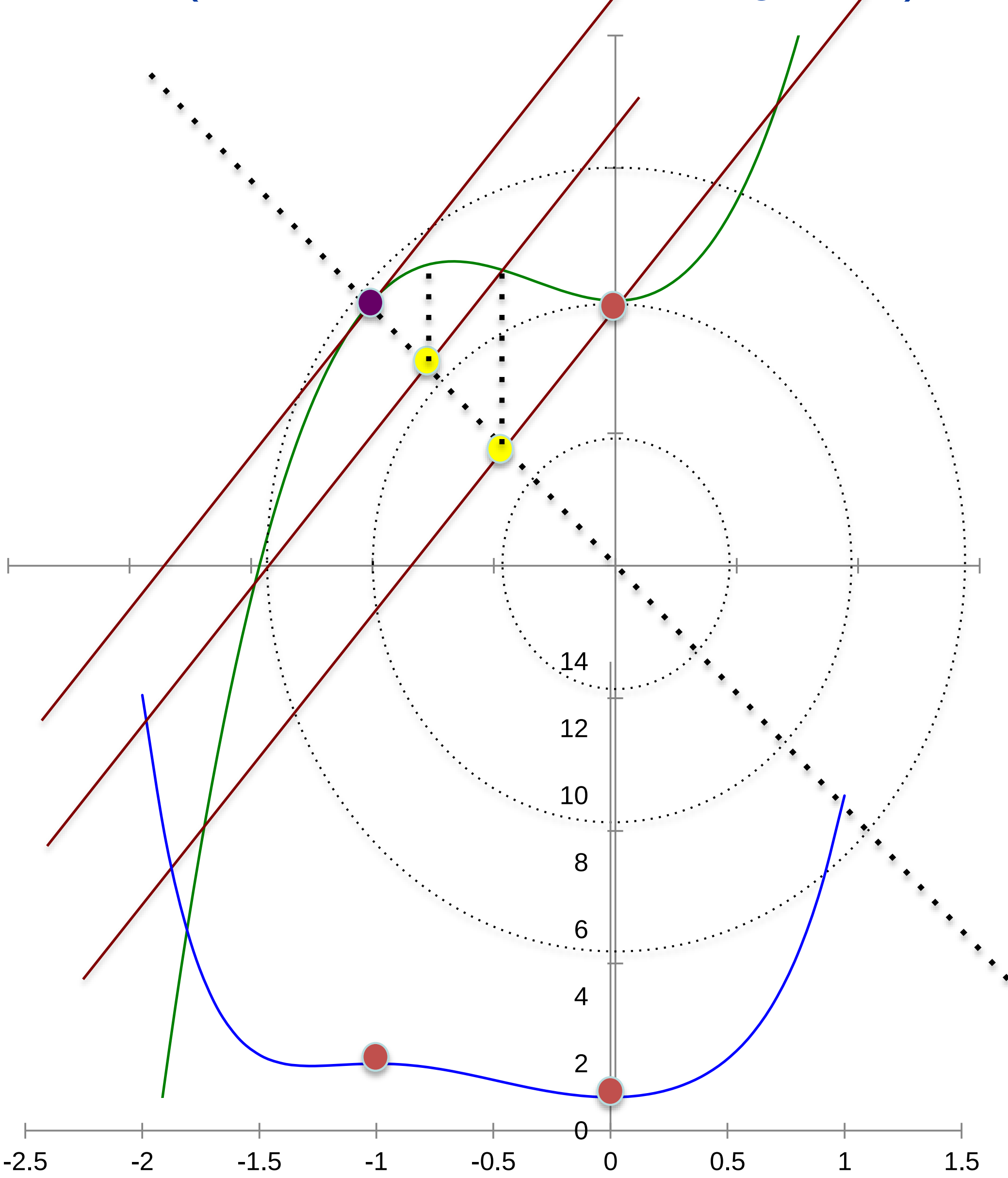
Two Local Minima:

$x = 0$, $y = 1$, $\Phi^* = 1$

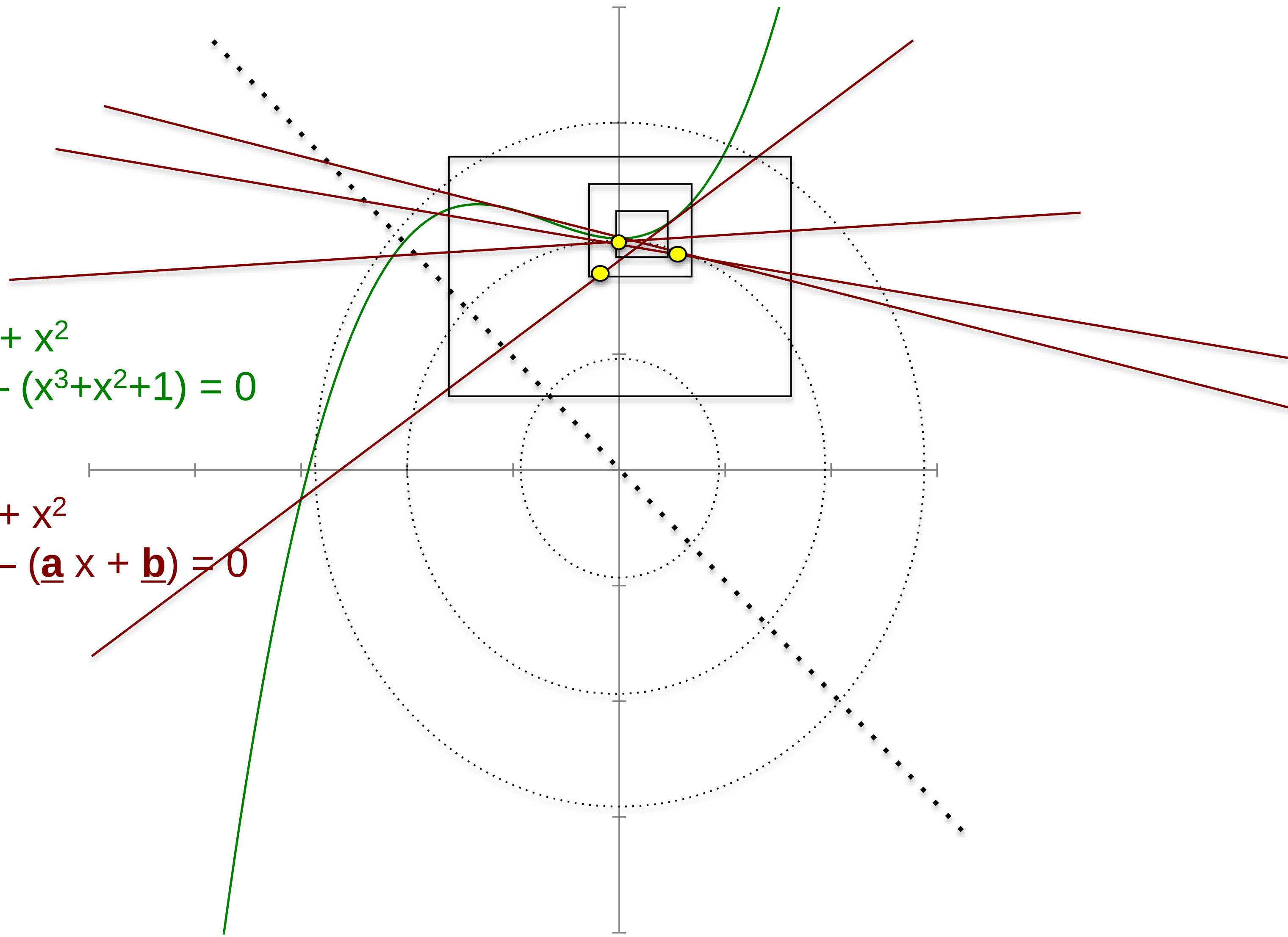
$x = -1.2785$, $y = 0.5448$, $\Phi^* = 1.9313$

***ROM-based optimum converges to local maximum!***

$x = -1$, $y = 1$, $\Phi^* = 2$



# Toy Problem with Trust Region Strategy



(ODM) Min $y^2 + x^2$

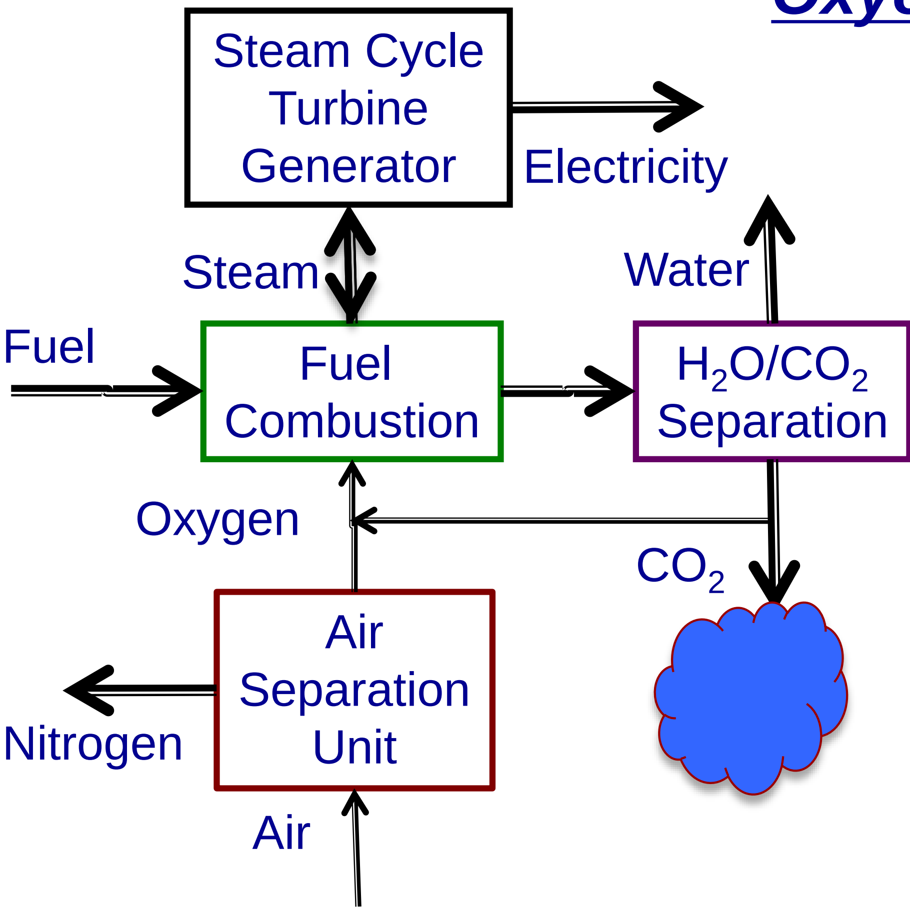
s.t. $y - (x^3+x^2+1) = 0$

(RM) Min $y^2 + x^2$

s.t. $y - (\underline{\mathbf{a}}\, x + \underline{\mathbf{b}}) = 0$

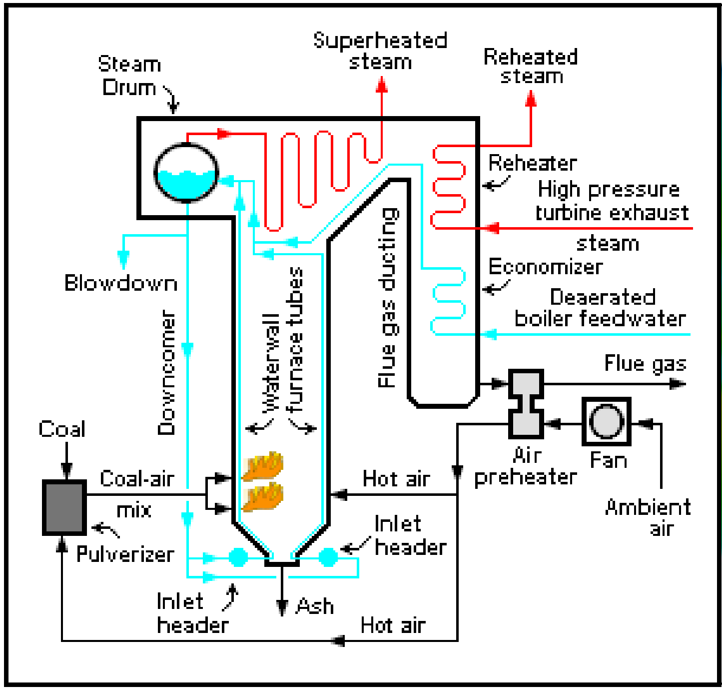
# Future Generation Power Plants: $CO_2$ Capture and Sequestration

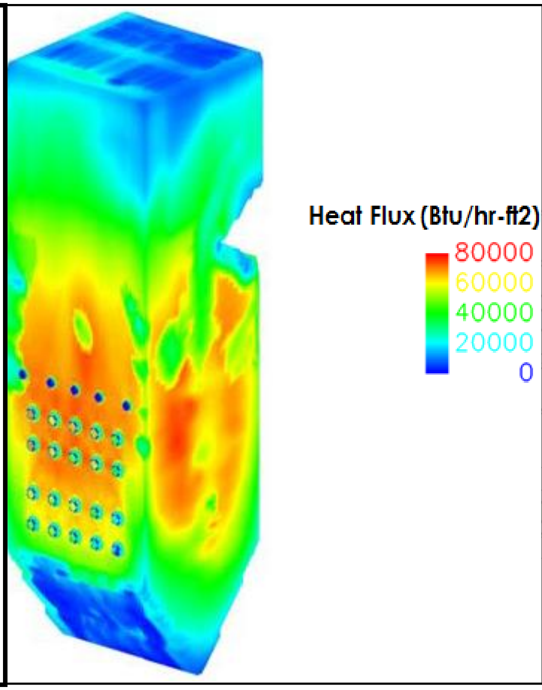
## ***Oxycombustion***

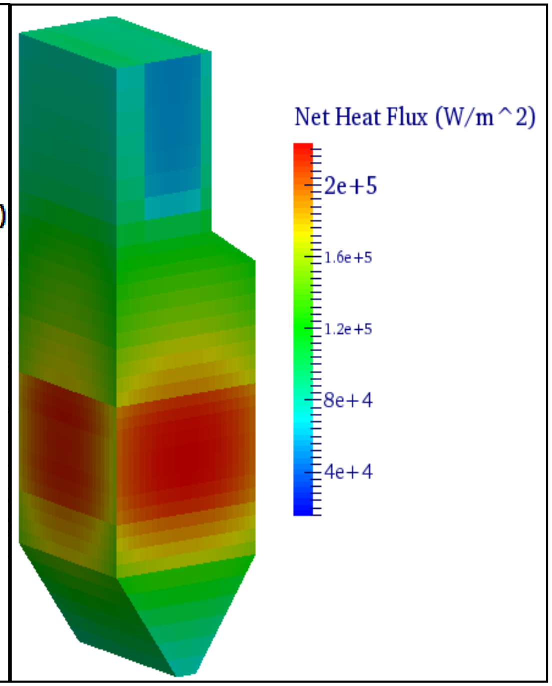


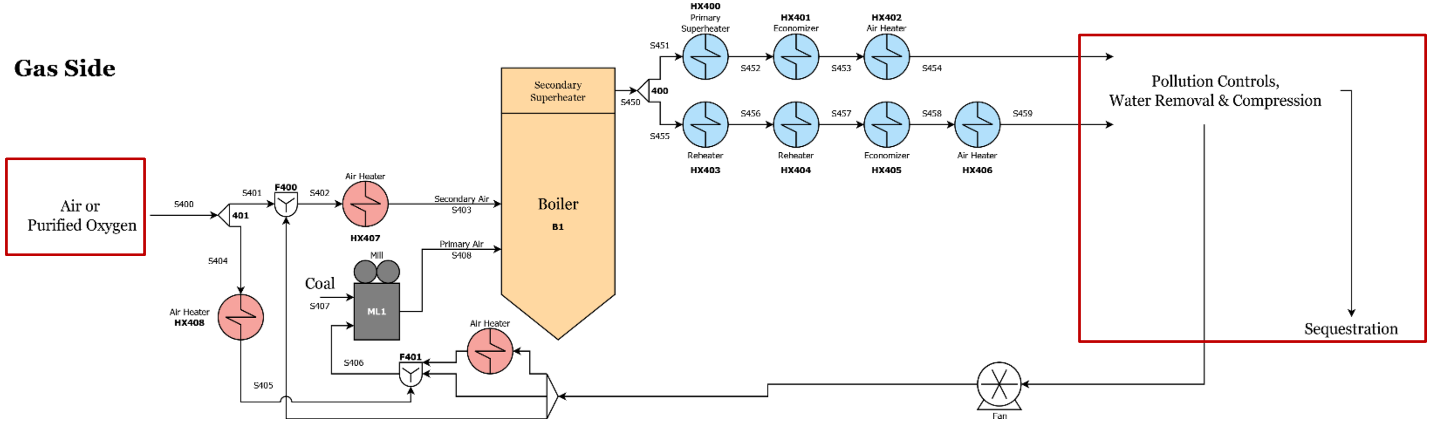

Schwarze Pumpe, 30MW Pilot (2008)
Feed: Lignite; Bituminous Coal
Brandenburg, Germany

# Integrated Combustion Models for Advanced Energy Systems



# Oxycombustion Optimization
## *(Dowling et al., 2015)*

*Max* **Thermal Efficiency**
s.t. Steam cycle connectivity
Heat exchanger model
Pump model
Fixed isentropic efficiency turbine model
Heat integration model
Correlation models for ASU and CPU
**3D Combustion PDE Model**
**Steam thermodynamics**

**Standard supercritical steam cycle**, double reheat

Using reduced models with trust region method ➔ rigorous optimum

Solved in GAMS 24.2.1 with CONOPT 3
Trust region algorithm in MATLAB R2013a

# *Effect of IRRCs on Power Plants*

| | Air-fired |
|---|---|
| Flue gas temperature (K) | 1600 |
| Steam exit temperature (K) | 835 |
| Steam exit pressure (bar) | 223 |
| Fuel rate, HHV (MW) | 1325.5 |
| ASU + CPU Power (MW) | N/A |
| Net Power (MWe) | **515.5** |
| Efficiency (HHV) | **38.9%** |

***5.7% penalty for oxy-fired configuration with CPU***

***4.4% penalty for oxy-fired with IRRCs with pumped $CO_2$***

# 2040: Multi-scale Optimization

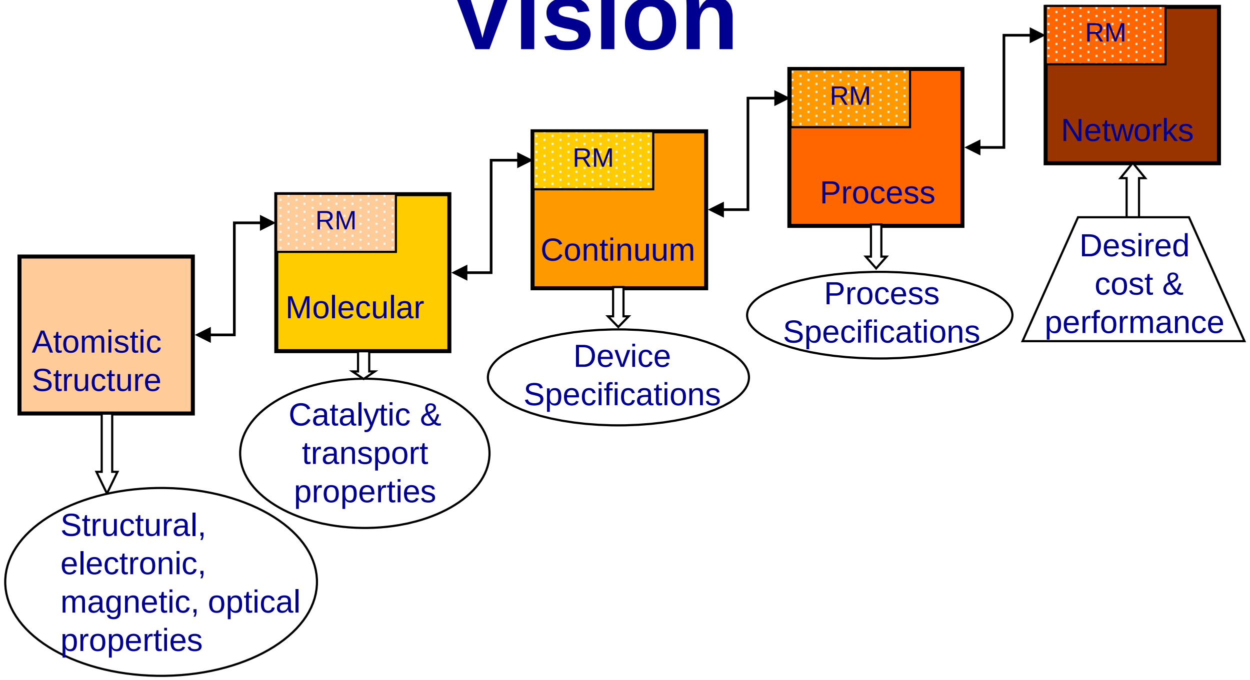
## Enabling Tools

- Leverage potential of Glass Box Optimization / Parallel Decompositions / Tailored Reduced Models
- Globally convergent trust region algorithms
- Large-scale, Tailored Reduced Modeling Platforms
- Globally Integrated Multi-scale Optimization

## Applications

- Heterogeneous models (PDAE/DAE/AE) – CFD + Process Flowsheets, Molecular Dynamics…
- Integrate process design / control / scheduling hierarchies
- Integrated optimal material, device, system and network design over orders of magnitude of time, length scales.

# Toward George's Multi-scale Vision




- Smooth Reduced Models are "glue" between scales
- **Enable fast large-scale, <u>convergent</u> optimization strategies**
- Some Recent Applications
  - Head-Disk Interfaces (Smith, Chung, Jhon, B., 2012)
  - Periodic Adsorption Processes (Agarwal, B., 2013)
  - Polymer Processing (Lang, Lin, B., 2014)
  - Oxycombustion Power Plants (Eason, B., 2016)
  - Integrated Power Plants (Zhu, Eason, B., 2017)

*To George: with deepest appreciation and gratitude for your wealth of research contributions.*

*Happy Birthday!*

*With best wishes for many more!*