CCSI
Carbon Capture Simulation Initiative

CAPD CENTER

Reduced Order Models for Oxycombustion Boiler Optimization

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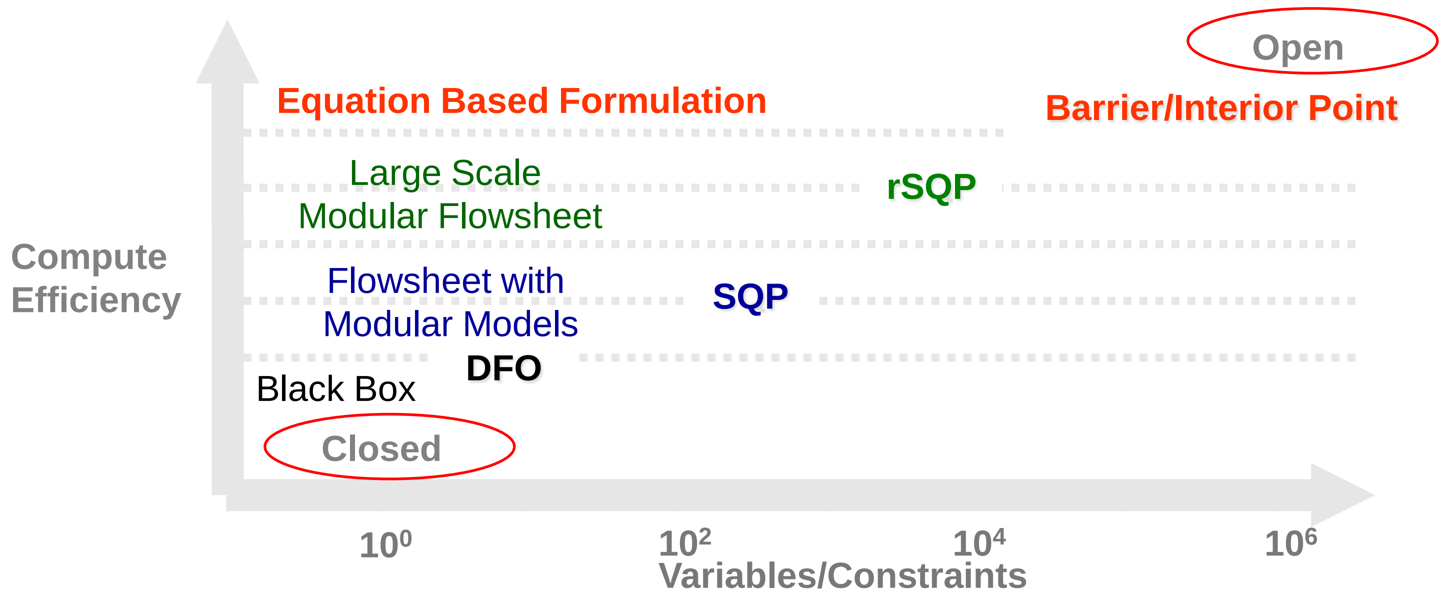
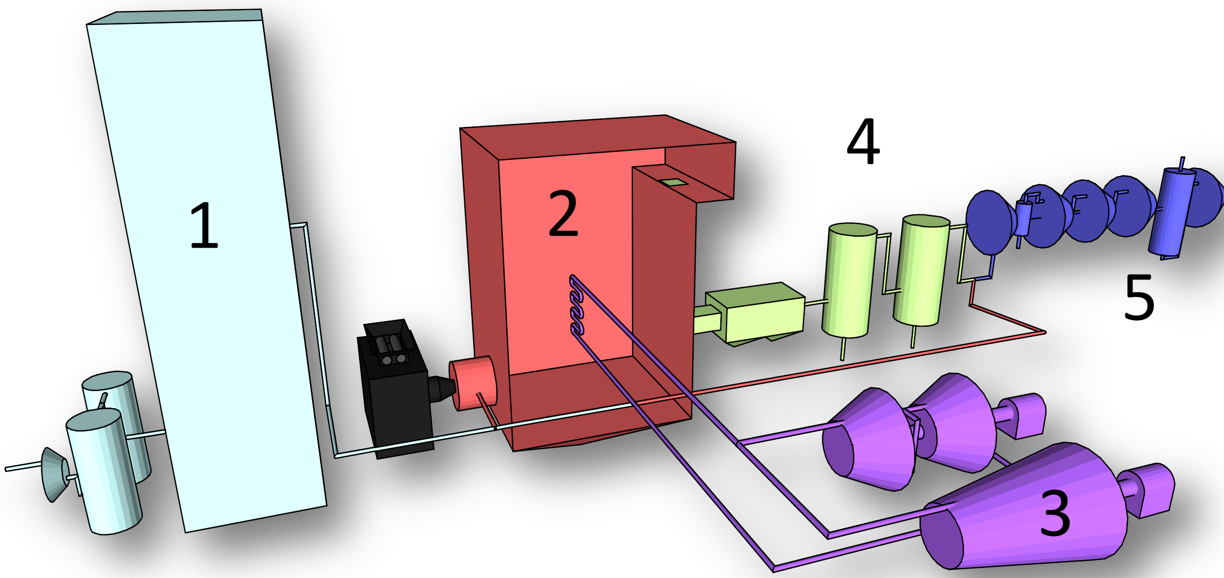
Project Objective

Develop an **equation oriented** framework to optimize a coal oxycombustion flowsheet.



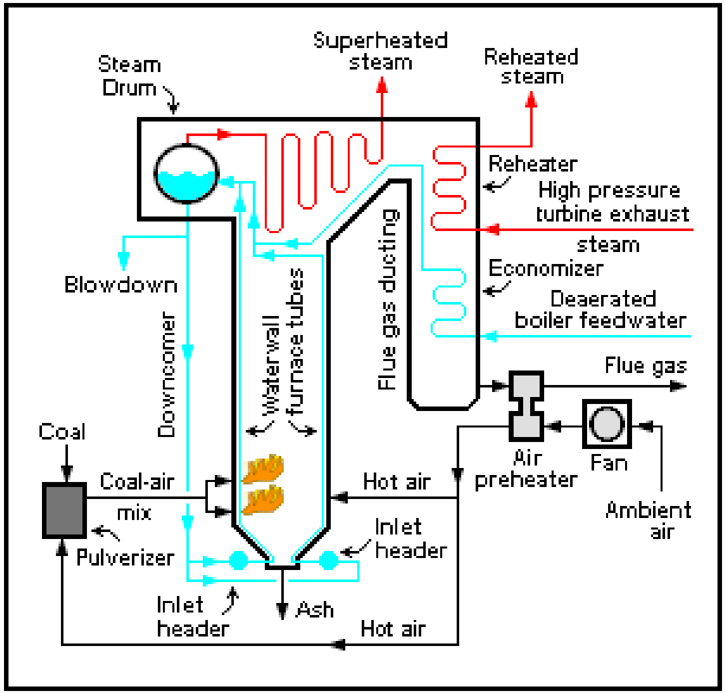
Oxycombustion Flowsheet



1. Air Separation Unit
2. Boiler
3. Steam Turbine
4. Pollution Controls
5. CO_2 Compression Train

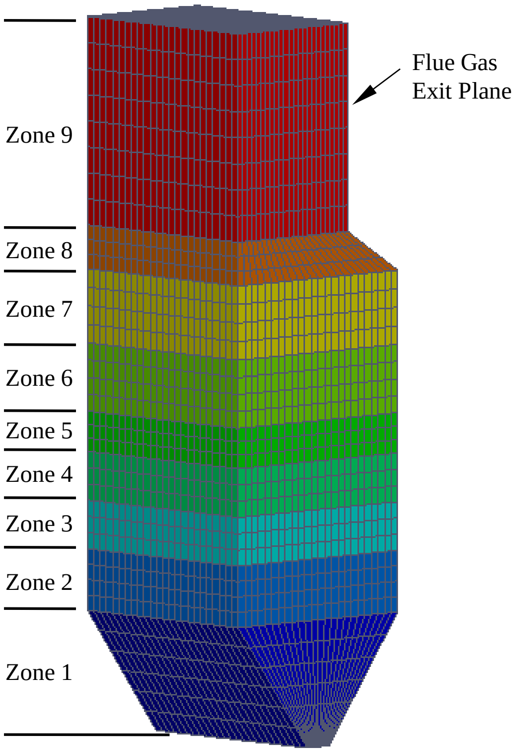
Boiler Design

- Economics of the power generation process depend strongly on optimized boiler performance
- Tight heat integration has been developed for traditional, air fired units
- Radiative heat transfer dominates
  - O_2 and CO_2 different properties than air
- Need detailed first principles model



Boiler Model

- Hybrid 1D reaction/3D radiation approach
- Reaction kinetics – considering particle size and composition
  - Boiler treated as vertical zones, each of which is a well mixed reactor
- Radiation – solved iteratively over a 3D mesh
  - 90% of heat transfer, convection is ignored in the radiative region
- Inlet stream properties → total heat transfer, outlet properties



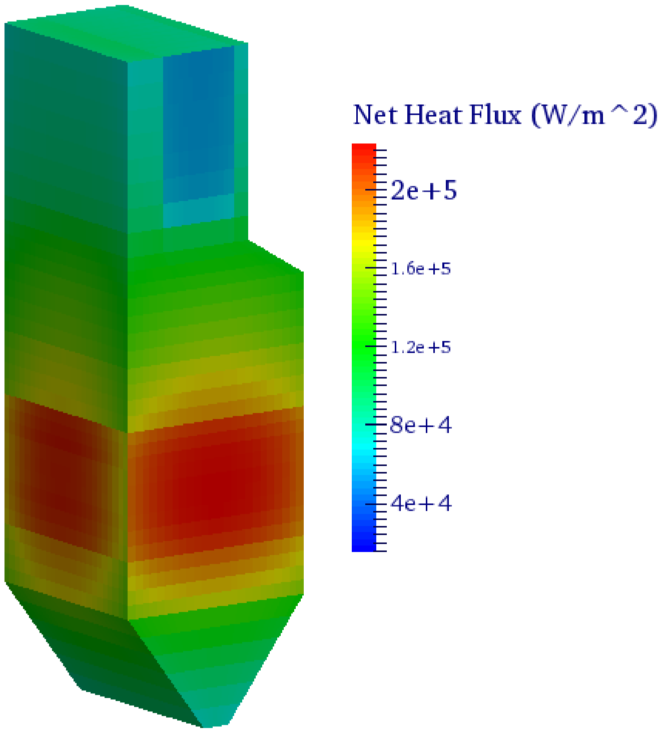
Model Validation

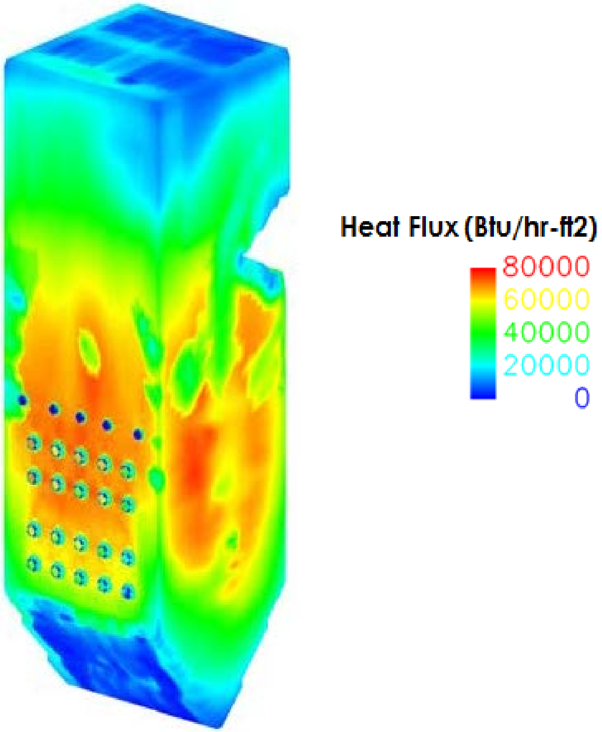
- Geometries and operating conditions of two existing utility boilers
  - PacificCorp's Hunter Unit 3

	Unit	Boiler Model	CFD Model	% error
Enclosure Wall	W	3.93×10^8	4.03×10^8	2.4%
Platen Superheater	W	9.89×10^7	1.09×10^8	9.2%

  - Trends in oxy vs. air-fired models match that of CFD simulations, e.g. higher burnout for oxy-fired boiler

Hybrid Model vs Full CFD Simulation





Reduced Order Models – Motivation

- Boiler model takes ~60 seconds to converge
- Iterative nature makes accurate derivatives difficult to obtain
- Construct simple algebraic representation (e.g. kriging), incorporate in equation oriented flowsheet
- Problem: How accurate should a ROM be to be useful for optimization? Can we find the optimum of the original detailed model?

Trust Region Framework - Introduction

- Allows us to carefully construct and update ROMs in a way that can guarantee convergence to a stationary point
- Consider the NLP:

$$\min f(x, y) \quad \text{s.t.} \;\; g(x, y) \leq 0, y = d(x)$$

- Using penalty functions to handle the constraints, restate the problem as an unconstrained objective:

$$\psi(x) = f(x) + \nu\varphi(g(x))$$

Trust Region Framework – Algorithm Outline

1) Given starting point x_0, construct ROM ψ^{R} around x_0
2) Solve trust region subproblem:

$$\min_{s} \psi^{R}(x_k + s), \quad \|x_k - s\| \leq \Delta_k$$

3) Evaluate original detailed model at new step $x_k + s$
4) Adjust trust region radius Δ_k
5) Go to 2)

Stopping Conditions

- Option 1: When gradient less than tol_g, enter criticality step
  - Systematically reduce TR around critical point until convergence or new improvement direction is found
- Option 2: ε-exact termination – given an estimate ε of the error of the ROM over the trust region
  - Stop if optimization terminates within trust region and $\varepsilon < tol_\varepsilon$

$$\|x^* - \bar{x}\| \leq (2\bar{\sigma})^{3/2}(\epsilon)^{1/2}/(\underline{\sigma})^2$$

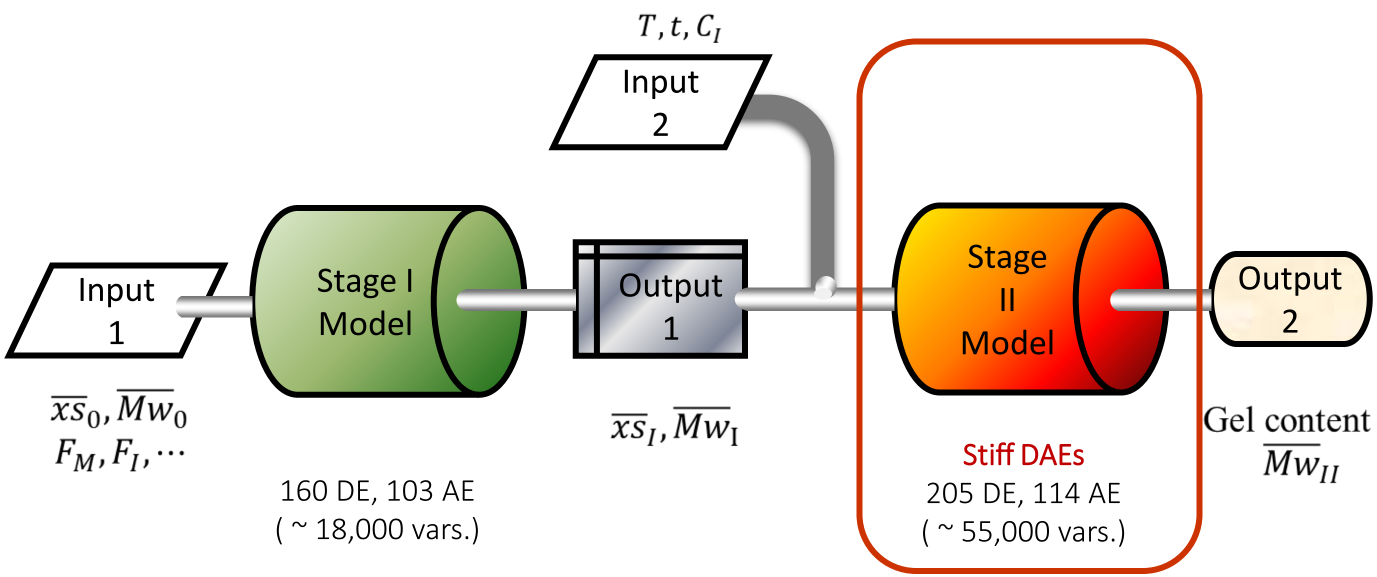
Conditions on Reduced Order Models

- The key to convergence is the fully linear property:

$$|f(x) - f^r(x)| \leq \kappa_f \Delta^2, \quad \|\nabla f(x) - \nabla f^r(x)\| \leq \kappa_g \Delta$$
$$\|g(x) - g^r(x)\| \leq \kappa_c \Delta^2, \quad \|\nabla g(x) - \nabla g^r(x)\| \leq \kappa_{gc} \Delta$$

- As trust region vanishes, function values and gradients approach original model
- Any type of ROM may be used satisfying this property

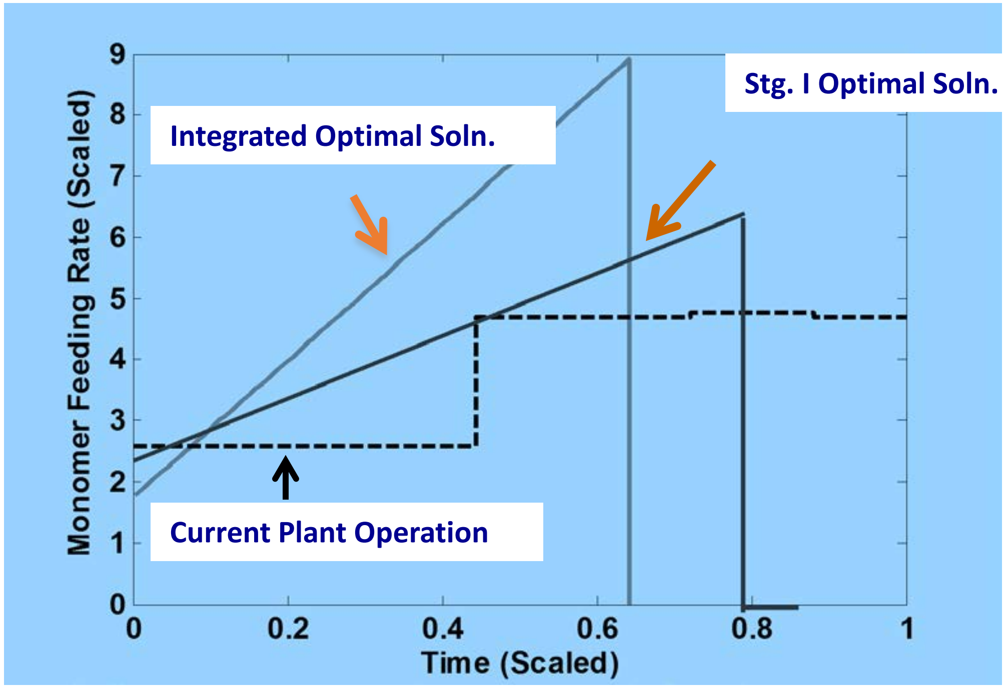
Optimization with Kriging Reduced Model



- Stage II has few degrees of freedom for optimization
- Easy to construct and validate an ε–exact Kriging approximation for Stage II model

Integrated Optimal Solution Comparison

Better solution is obtained with the integrated model



Improved computational efficiency over full 2-stage model

- 20% shorter batch time for integrated optimum
- Rigorous Optimum Verified

Conclusions

- Accurate representation of the boiler is essential for optimization of the oxy-combustion process
- Reduced order models allow optimization of flowsheets with complex black-box units
- Provably convergent trust region algorithms

Acknowledgements: David Miller, Jinliang Ma – National Energy Technology Laboratory

Alex Dowling, CMU

Kriging interpolation

- Given samples from Experimental design
- Choose linear basis of functions to fit with linear regression
- Exploit properties of Probability density function (assume white noise): Radial Basis Function (RBF), R(θ, x). (Note Gaussian has p = 2)
- Optimize regression with respect to θ
- Develop predictive model that combines linear regression model and RBF
- DACE MATLAB Toolbox (Lophaven et al., 2002)

Predictor:

$$Y = F(x)\beta + r(x)\gamma$$

$$\beta^* = (F^T R^{-1} F)^{-1} F^T R^{-1} Y$$

$$\sigma^2 = \frac{1}{m}(Y - F\beta^*)^T R^{-1}(Y - F\beta^*)$$

Correlation function

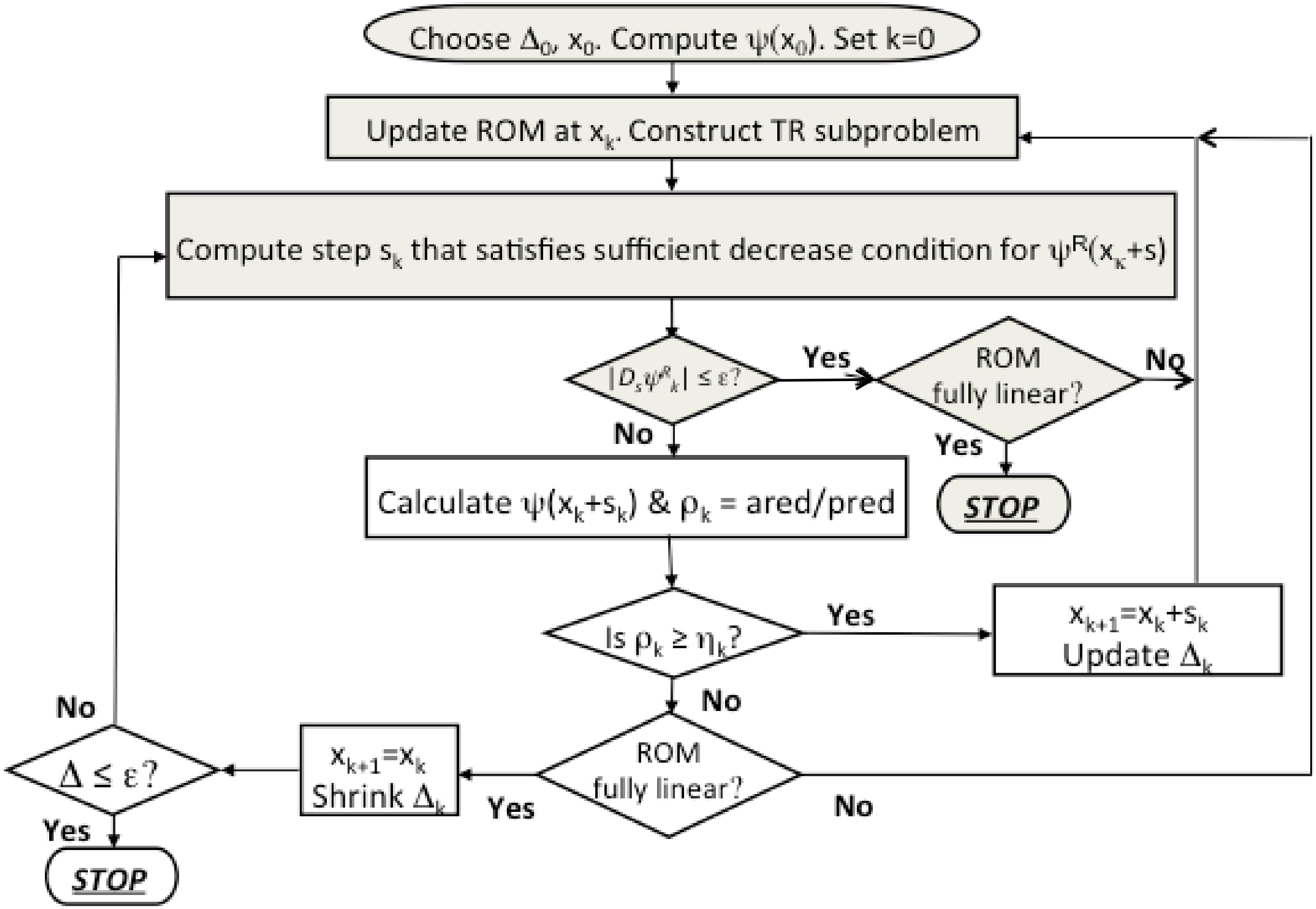
$$R(\theta, x_i, x_j) = \prod_{k=1}^{nd} R_k(\theta_k, x_i^k - x_j^k)$$

$$R_k = \exp(-\theta_k |x_i^k - x_j^k|^p)$$

θ_k: an indication of input correlation

(1) $\neq \theta^L$, $\neq \theta^U$
(2) Small ratio of $\max(\theta)/\min(\theta)$

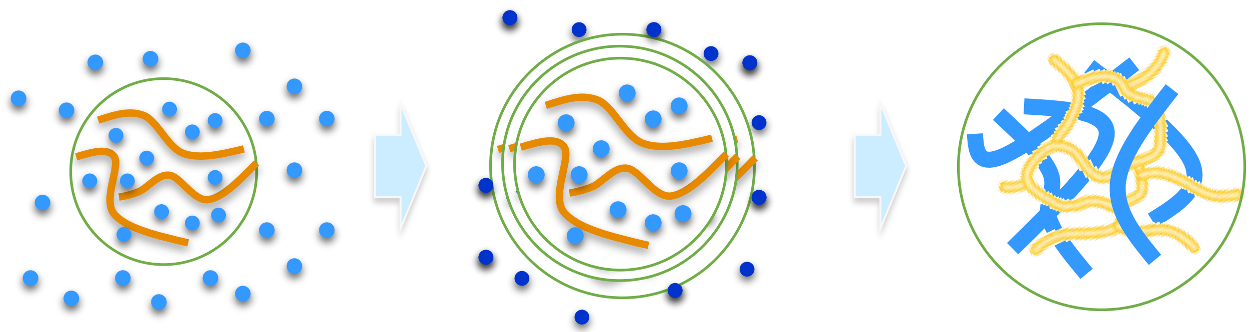
RM-based Trust Region Strategy without Gradients



Conn, A. R., Gould, N. I. M., and Toint, P. L., Trust Region Methods; SIAM (2000)
Conn, A. R., Scheinberg, K., and Vicente, L., Introduction to Derivative Free Optimization; SIAM (2010)

Case Study: Semi-Interpenetrating Polymer Network (SIPN)

0. Swelling | **I. Polymerization.** | **II. Crosslinking**



Particle Growth Model (make)

Semi-IPN Kinetic Model (bake)

- Monomer (B)
- Monomer / initiator
- Seed polymer (A)

Weijie Lin, PhD Thesis, Chemical Engineering, Carnegie Mellon Univ. , 2011

Integrated Optimization

- Include both models into optimization

New optimization problem formulation

$$
\begin{aligned}
\min_{v_c^I,\ v_c^{II}} \quad & t_I + t_{II} \\
s.t. \quad & \text{stage I model} \\
& \text{Stage II surrogate model:} \\
& \{\ \mathrm{Gel}_{\mathrm{end}} = S_1(v_c^{II}); \\
& \overline{Mw}_{end} = S_2(v_c^{II})\ \} \\
& Gel_{end} \geq Gel_{tar} \\
& \overline{Mw}_{end} \geq \overline{Mw}_{tar} \\
& v_I^L \leq v_c^I \leq v_I^U \\
& v_{II}^L \leq v_c^I \leq v_{II}^U
\end{aligned}
$$

→ Minimize overall reaction time

→ Subject to Rigorous Stage I model & Kriging Stage II model

→ Consider final property constraints

→ Control bounds