Reliable Modeling Using Interval Analysis: Chemical Engineering Applications

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Outline

- Motivation
- Problem-Solving Methodology
- Applications and Examples
  - Error-in-Variables Parameter Estimation
  - Phase Stability Analysis Using a Statistical Associating Fluid Theory (SAFT) Model
  - Density Functional Theory (DFT) Model of Phase Transitions in Nanoporous Materials
- Concluding Remarks

Motivation – Why Use Intervals?

- In process modeling, and in the modeling of complex physical phenomena, chemical engineers frequently need to solve nonlinear equation systems in which the variables are constrained physically within upper and lower bounds; that is, to solve:

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U$$

- These problems may:
  - Have multiple solutions
  - Have no solution
  - Be difficult to converge to any solution

- Interval methods provide the power to solve these problems with mathematical and computational certainty

Motivation (cont'd)

- There is also frequent interest in globally minimizing a nonlinear function subject to nonlinear equality and/or inequality constraints; that is, to solve (globally):

$$\min_{\mathbf{x}} \phi(\mathbf{x})$$

subject to

$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{g}(\mathbf{x}) \geq \mathbf{0}$$

$$\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U$$

- These problems may:
  - Have multiple local minima (in some cases, it may be desirable to find them all)
  - Have no solution (infeasible NLP)
  - Be difficult to converge to any local minima

- Interval methods provide the power to solve these problems with mathematical and computational certainty

Some Applications in Chemical Engineering

- Fluid phase stability and equilibrium
  - Activity coefficient models (Stadtherr *et al.*, 1995; Tessier *et al.*, 2000)
  - Cubic EOS (Hua *et al.*, 1996, 1998, 1999)

$\Longrightarrow$ SAFT EOS (Xu *et al.*, 2002)

- Combined reaction and phase equilibrium

- Location of azeotropes (Maier *et al.*, 1998, 1999, 2000)
  - Homogeneous
  - Heterogeneous
  - Reactive

- Location of mixture critical points (Stradi *et al.*, 2001)

Applications (cont'd)

- Solid-fluid equilibrium
  - Single solvent (Xu *et al.*, 2000, 2001)
  - Solvent and cosolvents (Xu *et al.*, 2002)

- Parameter estimation
  - Relative least squares (Gau and Stadtherr, 1999, 2000)

$\Longrightarrow$ Error-in-variables approach (Gau and Stadtherr, 2000, 2002) – Largest problem solved: 264 variables

$\Longrightarrow$ Density-functional-theory model of phase transitions in nanoporous materials (Maier *et al.*, 2001)

- General process modeling problems (Schnepper and Stadtherr, 1996)

Problem-Solving Methodology

Core methodology is Interval-Newton/Generalized Bisection (IN/GB):

Problem: Solve $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ for all roots in $\mathbf{X}^{(0)}$.

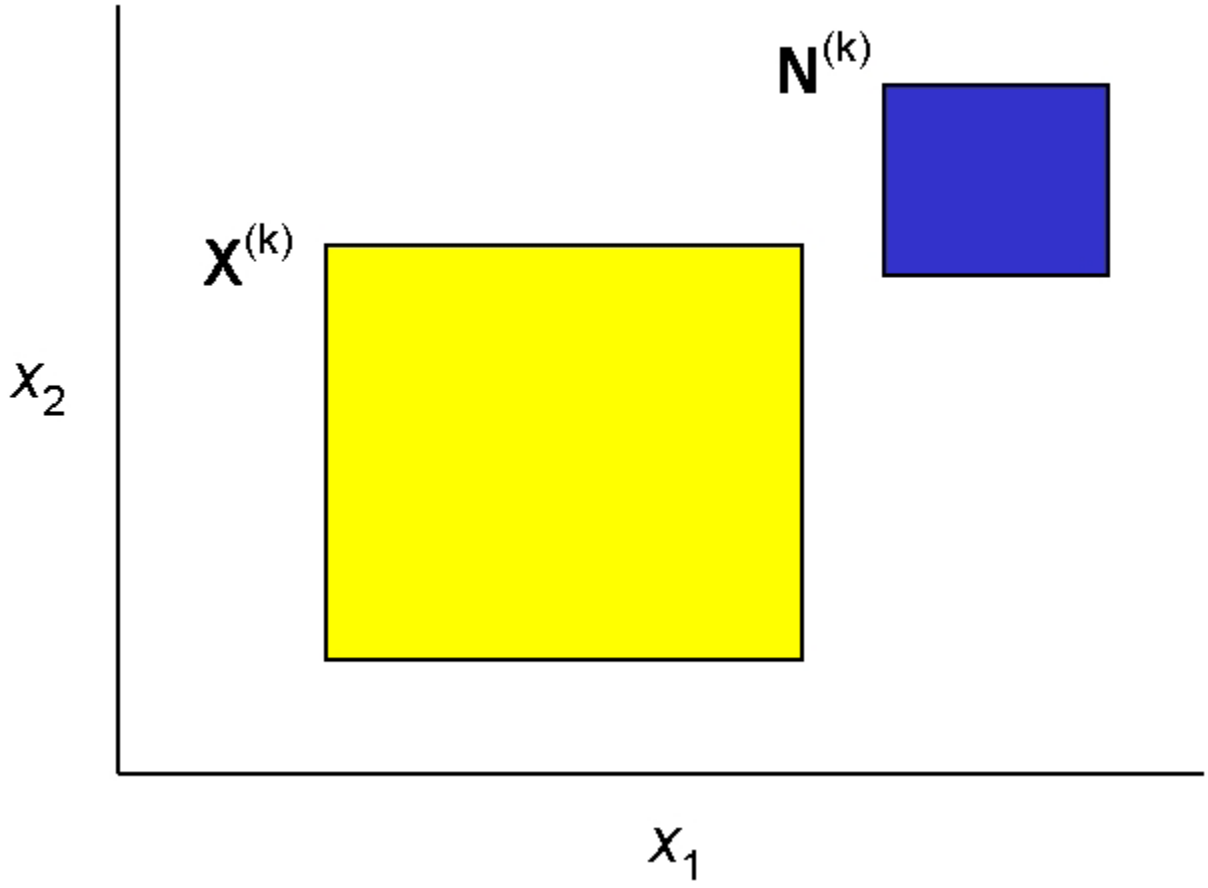
Basic iteration scheme — For a particular subinterval (box), $\mathbf{X}^{(k)}$, perform root inclusion test:

- (Range Test) Compute interval extension $\mathbf{F}(\mathbf{X}^{(k)})$.
  - If $0 \notin \mathbf{F}(\mathbf{X}^{(k)})$, delete the box.
- (Interval-Newton Test) Compute the $image$, $\mathbf{N}^{(k)}$, of the box by solving the linear interval equation system

$$Y^{(k)} F'(\mathbf{X}^{(k)})(\mathbf{N}^{(k)} - \mathbf{x}^{(k)}) = -Y^{(k)} \mathbf{f}(\mathbf{x}^{(k)})$$

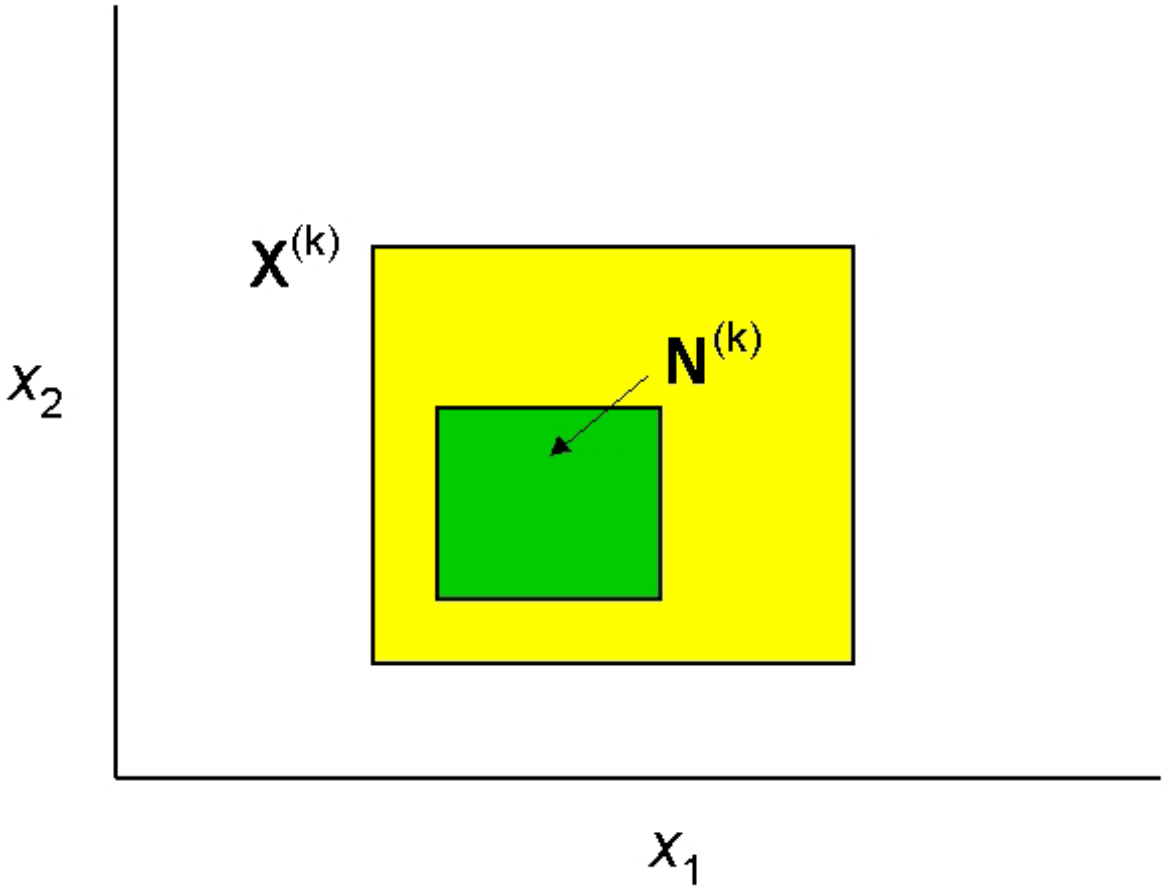
  - $\mathbf{x}^{(k)}$ is some point in $\mathbf{X}^{(k)}$.
  - $F'\left(\mathbf{X}^{(k)}\right)$ is an interval extension of the Jacobian of $\mathbf{f}(\mathbf{x})$ over the box $\mathbf{X}^{(k)}$.
  - $Y^{(k)}$ is a scalar preconditioning matrix.

Interval-Newton Method



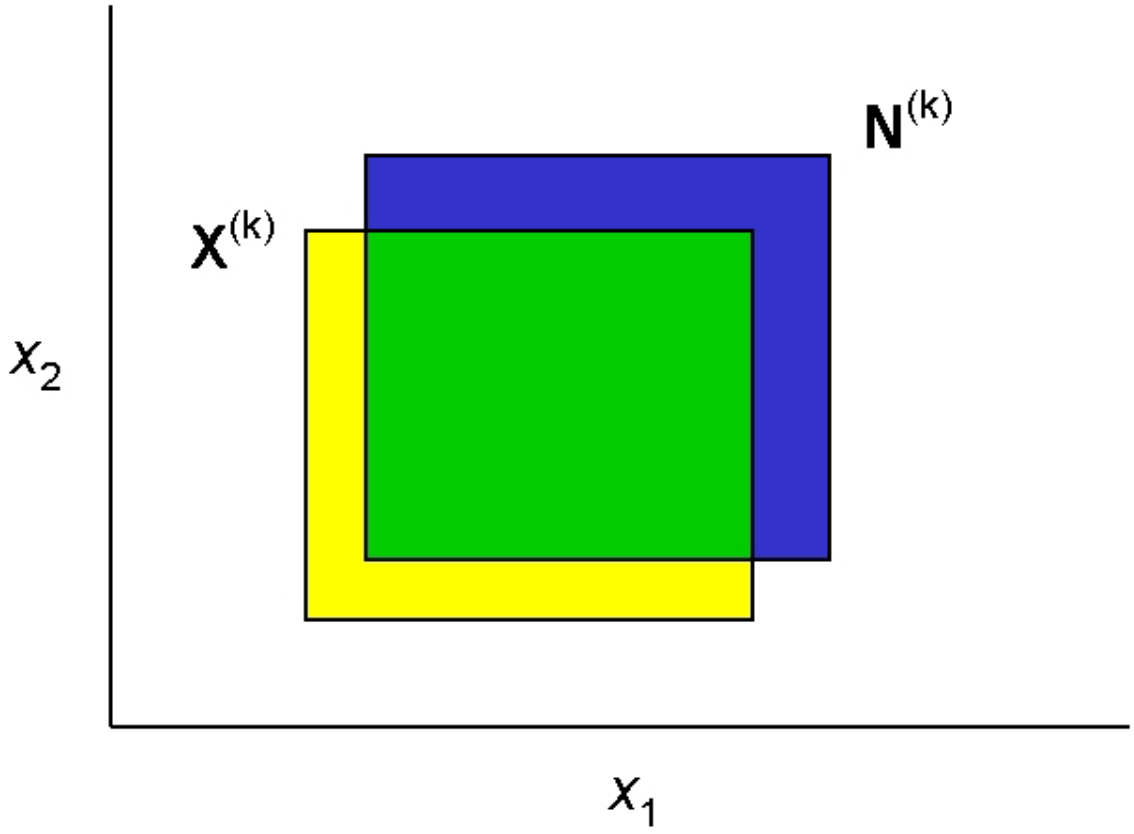
- There is no solution in $\mathbf{X}^{(k)}$.

Interval-Newton Method



- There is a $unique$ solution in $\mathbf{X}^{(k)}$.
- This solution is in $\mathbf{N}^{(k)}$.
- Additional interval-Newton steps will tightly enclose the solution with quadratic convergence.

Interval-Newton Method



- Any solutions in $\mathbf{X}^{(k)}$ are in $\mathbf{X}^{(k)} \cap \mathbf{N}^{(k)}$.

- If intersection is sufficiently small, repeat root inclusion test. Otherwise, bisect the intersection and apply root inclusion test to each resulting subinterval.

- This is a branch-and-prune scheme on a binary tree.

Methodology (Cont'd)

- This also can be applied to global optimization problems.
- For unconstrained problems, solve for stationary points.
- For constrained problems, solve for KKT points (or more generally for Fritz-John points).
- Add an additional pruning condition (Objective Range Test):
  - Compute interval extension of the objective function.
  - If its lower bound is greater than a known upper bound on the global minimum, prune this subinterval since it cannot contain the global minimum.
- This is a branch-and-bound scheme on a binary tree.

Methodology (Cont'd)

Enhancements to basic methodology:

- Hybrid of inverse-midpoint and pivoting preconditioner.
- Selection of $\mathbf{x}^{(k)}$: Do not always use the midpoint.
- Constraint propagation (problem specific).
- Tighten interval extensions using known function properties (problem specific).

Preconditioning Strategy

- The scalar preconditioning matrix $Y^{(k)}$ is often chosen to be an inverse-midpoint preconditioner: inverse of the midpoint of the interval Jacobian matrix, or inverse of the Jacobian matrix at midpoint of the interval.

- Preconditioners that are optimal in some sense have been proposed by Kearfott (1990,1996) based on LP strategies.

- A pivoting preconditioner (Kearfott $et\ al.$, 1991) has only one nonzero element (pivot) in each row $\mathbf{y}_i$ of $Y^{(k)}$.

- Hybrid strategy:
  - Select pivot in $\mathbf{y}_i$ to minimize the width of $N_i^{(k)} \cap X_i^{(k)}$.
  - Use this $\mathbf{y}_i$ if it reduces width of $N_i^{(k)} \cap X_i^{(k)}$ compared to use of $\mathbf{y}_i$ from inverse-midpoint preconditioner.

Background—EIV Parameter Estimation

- "Standard" approach
  - A distinction is made between dependent and independent variables.
  - It is assumed there is no measurement error in the independent variables.
  - Result is an estimate of the parameter vector.

- "Error-in-variables" (EIV) approach
  - Measurement error in all (dependent and independent) variables is taken into account.
  - Result is an estimate of the parameter vector, and of the "true" values of the measured variables.
  - Simultaneous parameter estimation and data reconciliation.

EIV Parameter Estimation (cont'd)

- Measurements $\mathbf{z}_i = (z_{i1}, ..., z_{in})^{\mathrm{T}}$ from $i = 1, \ldots, m$ experiments are available.

- Measurements are to be fit to a model (p equations) of the form $\mathbf{f}(\boldsymbol{\theta}, \mathbf{z}) = \mathbf{0}$, where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_q)^{\mathrm{T}}$ is an unknown parameter vector.

- There is a vector of measurement errors $\mathbf{e}_i = \tilde{\mathbf{z}}_i - \mathbf{z}_i$, $i = 1, \ldots, m$, that reflects the difference between the measured values $\mathbf{z}_i$ and the unknown "true" values $\tilde{\mathbf{z}}_i$.

- The standard deviation associated with the measurement of variable j is σ_j.

EIV Parameter Estimation (cont'd)

- Using a maximum likelihood estimation with usual assumptions, the EIV parameter estimation problem is

$$\min_{\boldsymbol{\theta}, \tilde{\mathbf{z}}_i} \sum_{i=1}^{m} \sum_{j=1}^{n} \frac{(\tilde{z}_{ij} - z_{ij})^2}{\sigma_j^2}$$

  subject to the model constraints

$$\mathbf{f}(\boldsymbol{\theta}, \tilde{\mathbf{z}}_i) = \mathbf{0}, \quad i = 1, \ldots, m.$$

- This is an $(nm + q)$-variable optimization problem.

- Since optimization is over both $\boldsymbol{\theta}$ and $\tilde{\mathbf{z}}_i$, $i = 1, \ldots, m$, this is likely to be a nonlinear optimization problem even for models that are linear in the parameters.

EIV Parameter Estimation (cont'd)

- If the p model equations can be used to solve algebraically for p of the n variables, then an unconstrained formulation can be used

$$\min_{\boldsymbol{\theta}, \tilde{\mathbf{v}}_i} \phi(\boldsymbol{\theta}, \tilde{\mathbf{v}}_i)$$

- $\tilde{\mathbf{v}}_i$, $i = 1, \ldots, m$, refers to the $n - p$ variables not eliminated using the model equations.

- $\phi(\boldsymbol{\theta}, \tilde{\mathbf{v}}_i)$ is the previous objective function after elimination of the p variables by substitution.

- Could solve by seeking stationary points: Solve $\mathbf{g}(\mathbf{y}) \equiv \nabla\phi(\mathbf{y}) = \mathbf{0}$, where $\mathbf{y} = (\boldsymbol{\theta}, \tilde{\mathbf{v}}_i)^{\mathrm{T}}$.

Solution Methods

- Various local methods have been used.
  - SQP (for constrained formulation)
  - Broyden (for unconstrained formulation)
  - Etc.

- Since most EIV optimization problems are nonlinear, and many may be nonconvex, local methods may not find the global optimum.

- Esposito and Floudas (1998) apply a powerful deterministic global optimization technique using branch-and-bound with convex underestimators.

Problem 1

- Estimation of Van Laar parameters from VLE data (Kim et al., 1990; Esposito and Floudas, 1998).

$$P = \gamma_1 x_1 p_1^0(T) + \gamma_2(1 - x_1)p_2^0(T)$$

$$y_1 = \frac{\gamma_1 x_1 p_1^0(T)}{\gamma_1 x_1 p_1^0(T) + \gamma_2(1 - x_1)p_2^0(T)}$$

where

$$p_1^0(T) = \exp\left[18.5875 - \frac{3626.55}{T - 34.29}\right]$$

$$p_2^0(T) = \exp\left[16.1764 - \frac{2927.17}{T - 50.22}\right]$$

and

$$\gamma_1 = \exp\left[\frac{A}{RT}\left(1 + \frac{A}{B}\frac{x_1}{1 - x_1}\right)^{-2}\right]$$

$$\gamma_2 = \exp\left[\frac{B}{RT}\left(1 + \frac{B}{A}\frac{1 - x_1}{x_1}\right)^{-2}\right] .$$

- There are five data points and four measured variables with two parameters to be determined.

Problem 1 (cont'd)

- Unconstrained formulation is a 12-variable optimization problem.
- Same search space used as in Esposito and Floudas ($\pm 3\sigma$ for the data variables).
- Global optimum found using IN/GB with hybrid preconditioner in 807.9 seconds on Sun Ultra 2/1300 workstation (SPECfp95 = 15.5).
- Same as result found by Esposito and Floudas in 1625 seconds on HP 9000/C160 workstation (SPECfp95 = 16.3).
- Using inverse-midpoint preconditioner, solution time is $>$ 2 CPU days (Sun Ultra 2/1300).

Problem 2

- Estimation of parameters in CSTR model (Kim et al., 1990; Esposito and Floudas, 1998).

- Reaction is $\mathrm{A} \xrightarrow{\mathrm{k_1}} \mathrm{B}$.

$$\frac{1}{\tau}(A_0 - A) - k_1 A = 0$$

$$\frac{-B}{\tau} + k_1 A = 0$$

$$\frac{1}{\tau}(T_0 - T) + \frac{-\Delta H_{\mathrm{r}}}{\rho C_{\mathrm{p}}}(k_1 A) = 0$$

where

$$k_1 = c_1 \exp\left(\frac{-Q_1}{RT}\right)$$

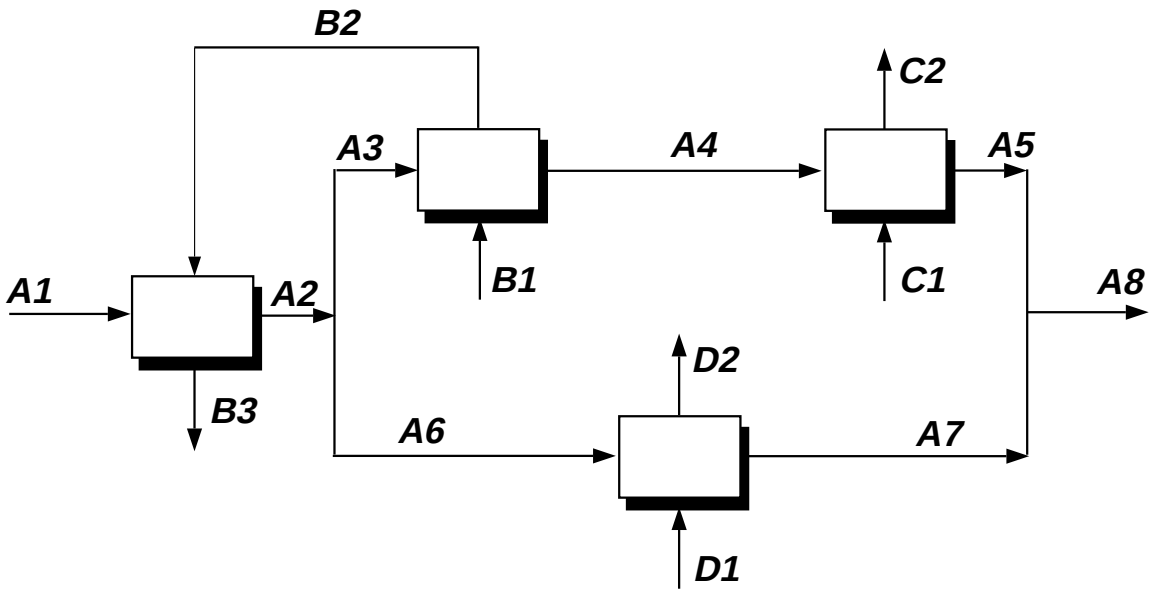
- There are ten data points and five measured variables with two parameters to be determined.

Problem 2 (cont'd)

- Unconstrained formulation is a 22-variable optimization problem.
- Same search space used as in Esposito and Floudas ($\pm 3\sigma$ for the data variables).
- Global optimum found using IN/GB with hybrid preconditioner in 28.8 seconds on Sun Ultra 2/1300 workstation (SPECfp95 = 15.5).
- Same as result found by Esposito and Floudas in 282.2 seconds on HP 9000/C160 workstation (SPECfp95 = 16.3).
- Using inverse-midpoint preconditioner, solution time is $>$ 2 CPU days (Sun Ultra 2/1300).

Problem 3

- Estimation of parameters in heat exchanger network (Biegler and Tjoa, 1993).
- Network of four exchangers.
- Estimate rating parameter $(UA)_i$ for each exchanger.
- There are 20 data points with 19 measured variables (flowrates and temperatures).



Problem 3 (cont'd)

- Six variables can be eliminated using material and energy balance constraints.

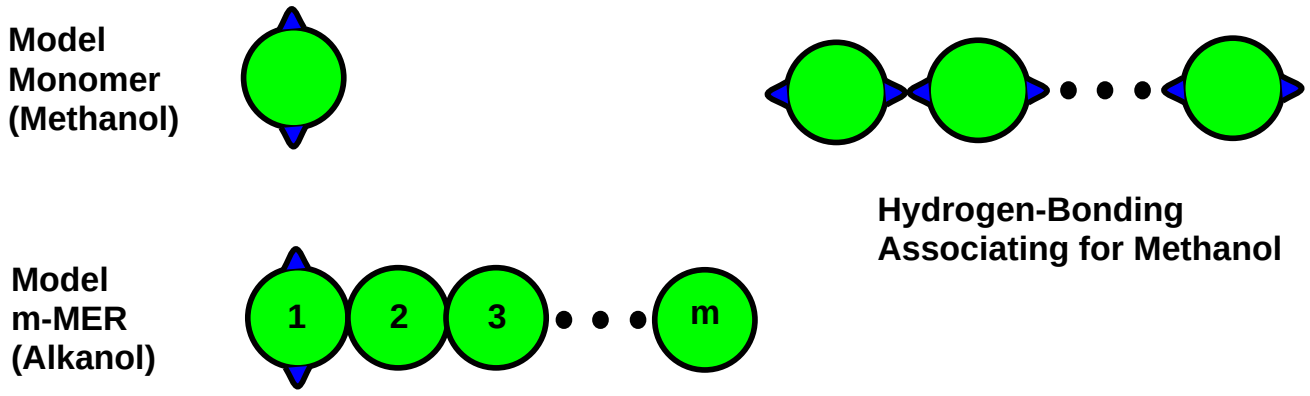
- Unconstrained formulation is a 264-variable optimization problem.

- Initial interval for parameters $(UA)_i \in [1, 10]$.

- Global optimum found using interval method in 2157.5 seconds on Sun Ultra 2/1300 workstation.

$$(UA)_1 = 4.84$$
$$(UA)_2 = 4.00$$
$$(UA)_3 = 6.81$$
$$(UA)_4 = 5.35$$

Background—SAFT Models



In statistical associating fluid theory (SAFT), a molecule is modeled as a chain of tangentially connected hard spheres, which may associate (weakly bond) with each other at specified "association sites".

SAFT (cont'd)

- The equation of state (EOS) model can be expressed in terms of residual Helmholtz energy a^{res} as a function of composition (mole fraction) vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ and mixture density ϱ.

- The expression for $a^{\mathrm{res}}(\mathbf{x}, \varrho)$ is very complicated.

- Alternatively, the EOS can be expressed in terms of the Helmholtz energy density $\tilde{a}$ as a function of the component density vector $\boldsymbol{\rho} = (\rho_1, \rho_2, \ldots, \rho_n)^{\mathrm{T}}$.

$$\tilde{a}(\boldsymbol{\rho}) = \varrho a^{\mathrm{res}}(\mathbf{x}, \varrho) + RT \sum_i \rho_i \ln[\rho_i RT]$$

- Problem of interest: Use the SAFT EOS model to perform phase stability analysis.

Phase Stability Analysis

- Will a mixture (feed) at a given T, P, and composition $\mathbf{x_0}$ split into multiple phases?

- A key subproblem in determination of phase equilibrium, and thus in the design and analysis of separation operations.

- Tangent plane analysis: A mixture is not stable if the $\tilde{a}$ vs. $\boldsymbol{\rho}$ surface ever falls below a plane tangent to the surface at the feed density $\boldsymbol{\rho}_0$.

- That is, if the tangent plane distance function

$$D(\boldsymbol{\rho}) = \tilde{a}(\boldsymbol{\rho}) - [\tilde{a}(\boldsymbol{\rho}_0) + \nabla\tilde{a}(\boldsymbol{\rho}_0) \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0)]$$

  is negative for any composition $\boldsymbol{\rho}$, the mixture is not stable.

- To determine if D is ever negative, determine its global minimum.

Phase Stability Analysis (cont'd)

Solution Procedure—Part 1

Given T, P and $\mathbf{x}_0$, find the feed tangent point $\boldsymbol{\rho}_0$. To do this:

- Solve

$$P - \varrho^2 \left(\frac{\partial a^{\mathrm{res}}(\mathbf{x}, \varrho)}{\partial \varrho} \right)_{\mathbf{x},T} - \varrho RT = 0$$

  for all ϱ roots (there may be many).

- Choose the ϱ root corresponding to the smallest value of the Gibbs energy $g = (\tilde{a} + P)/\varrho$. Then $\boldsymbol{\rho}_0 = \varrho \mathbf{x_0}$.

Phase Stability Analysis (cont'd)

Solution Procedure—Part 2

Determine the global minimum of tangent plane distance D. To do this:

- Determine stationary points of D by solving

$$\nabla \tilde{a}(\boldsymbol{\rho}) - \nabla \tilde{a}(\boldsymbol{\rho}_0) = \mathbf{0}$$

  for all $\boldsymbol{\rho}$ roots (there may be many).

- If D is nonnegative at all stationary points, the mixture is stable.

Problem 4

Mixtures of n-heptane and 1-propanol at $T = 333$ K and $P = 0.35$ bar.

Feed Composition $(x_{1,0}, x_{2,0})$	Roots ϱ (mol/L) in Part 1	Roots (ρ_1, ρ_2) (mol/L) in Part 2	D/RT value	Total CPU time (seconds)†
$(0.975,$ $0.025)$	$(6.84^*;\ 0.90;$ $0.013)$	$(6.667, 0.171)$ $(2.768, 0.069)$ $(0.010, 0.002)$	0.0 0.005 0.58×10^{-6}	143.3
$(0.875,$ $0.125)$	$(0.0128^*;\ 7.169;$ $0.968)$	$(0.011, 0.002)$ $(2.708, 0.049)$ $(6.736, 0.112)$	0.0 0.004 -0.597×10^{-3}	289.1
$(0.45,$ $0.55)$	$(0.0128^*;\ 1.173;$ $9.175)$	$(0.006, 0.007)$ $(2.706, 0.726)$ $(1.511, 10.12)$	0.0 0.006 -0.176×10^{-3}	386.5
$(0.10,$ $0.90)$	$(11.92^*;\ 0.0128;$ $1.250)$	$(1.192, 10.72)$ $(2.667, 0.960)$ $(0.005, 0.007)$	0.0 0.006 0.896×10^{-6}	189.2

* feed density root corresponding to lowest Gibbs energy for feed mixture

† CPU time on Sun Ultra 10/440 workstation

Background—Density Functional Theory

- Popular tool for modeling adsorption and other physical phenomena.
- Basic idea: Model system free energy and entropy as functionals of the density distribution $\rho(r)$.
- Lattice (discrete density distribution) or nonlattice models can be used.
- Determine equilibrium density profile by solving appropriate minimization problem, generally by numerical solution of a nonlinear equation system for stationary points in the optimization problem.
- This equation system may have multiple roots, especially in regions of phase transitions and hysteresis.
- For reliable study of phase behavior using DFT, a solution technique is needed that can reliably find all roots of a nonlinear equation system.

Solution Methods

- Local methods with multiple initial guesses
  - Broyden (e.g., Neimark and Ravikovitch, 1998)
  - Successive substitution (e.g., Lastoskie *et al.*, 1993)
  - No guarantee that all solutions are found.

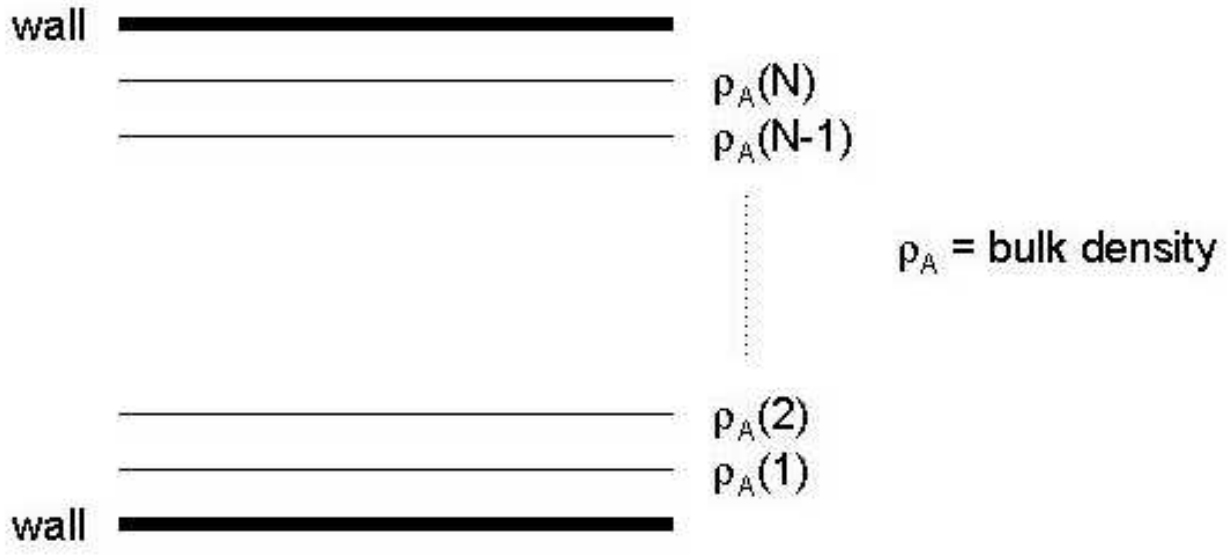
- Path tracking approach (Aranovich and Donohue, 1998, 1999)
  - No guarantee that all solutions are found.

- We propose using an interval-Newton/generalized-bisection (IN/GB) approach.
  - Mathematical and computational guarantee that all solutions are found.

Example – DFT Model of Adsorption in Nanoscale Pores

- Lattice model of binary system (A and B): Aranovich and Donohue (1999).

- Single component system is special case of B = holes.



$\rho_A(i) =$ fraction of lattice sites in layer i occupied by A
$\rho_B(i) = 1 - \rho_A(i)$

DFT Model (cont'd)

- The equilibrium density profile is a solution of

$$\ln \frac{\rho_A(i)(1-\rho_A)}{[1-\rho_A(i)]\rho_A} - \{z_1[\rho_A(i+1)-\rho_A]$$
$$+z_2[\rho_A(i)-\rho_A]+z_1[\rho_A(i-1)-\rho_A]\}\Delta/kT$$
$$=0, \quad 2 \le i \le N-1$$

$$\ln \frac{\rho_A(1)(1-\rho_A)}{[1-\rho_A(1)]\rho_A} - \{z_2[\rho_A(1)-\rho_A]$$
$$+z_1[\rho_A(2)-\rho_A]+z_1\rho_A\}\Delta/kT$$
$$-z_1(\epsilon_{AB}-\epsilon_{BB})/kT+(\epsilon_{AS}-\epsilon_{BS})/kT=0$$

$$\rho_A(1)=\rho_A(N)$$

where z_1 and z_2 are lattice coordination numbers, $\Delta = 2\epsilon_{AB} - \epsilon_{AA} - \epsilon_{BB}$, and ρ_A is a given bulk mole fraction of A.

Example Problems

- Single component systems of $N = 2$ to $N = 20$ layers (1 to 10 variables) were considered (same as solved by Aranovich and Donohue, 1999).

- For each system, the equation system was solved for the density profile (layer concentrations) $\rho_A(i), \quad i = 1, \ldots, N$ for many values of the bulk concentration ρ_A.

- An initial interval of [0,1] was used for each variable $\rho_A(i)$.

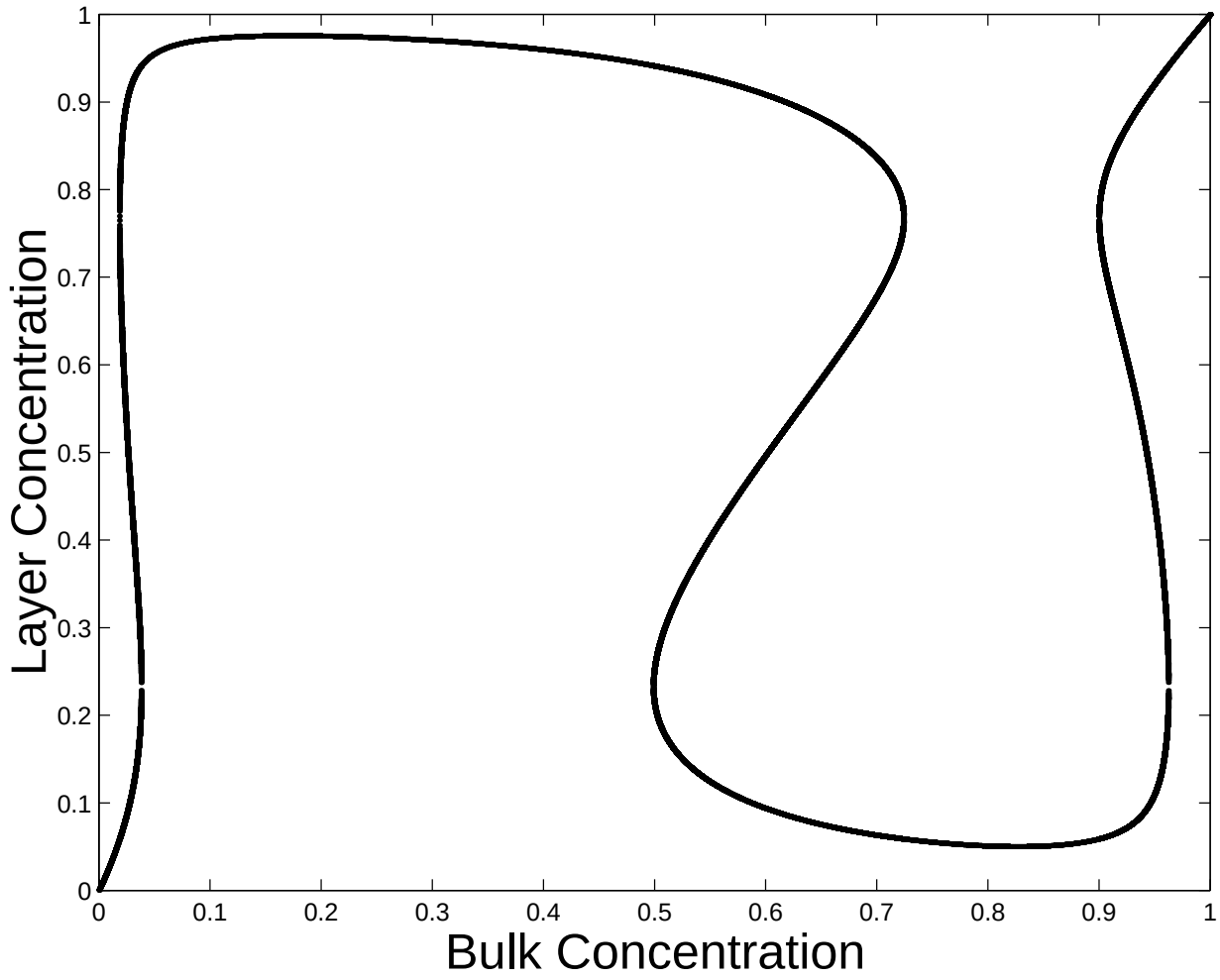
- Hybrid preconditioning approach (Gau and Stadtherr, 2002) used to solve interval Newton equation.

- All computations were done using a Sun Ultra 10/440 workstation.

Problem 5

$N = 2$

$z_1 = 1,\ z_2 = 3,\ \epsilon_{AA}/kT = -1.4,\ \epsilon_{AS}/kT = -1.0$

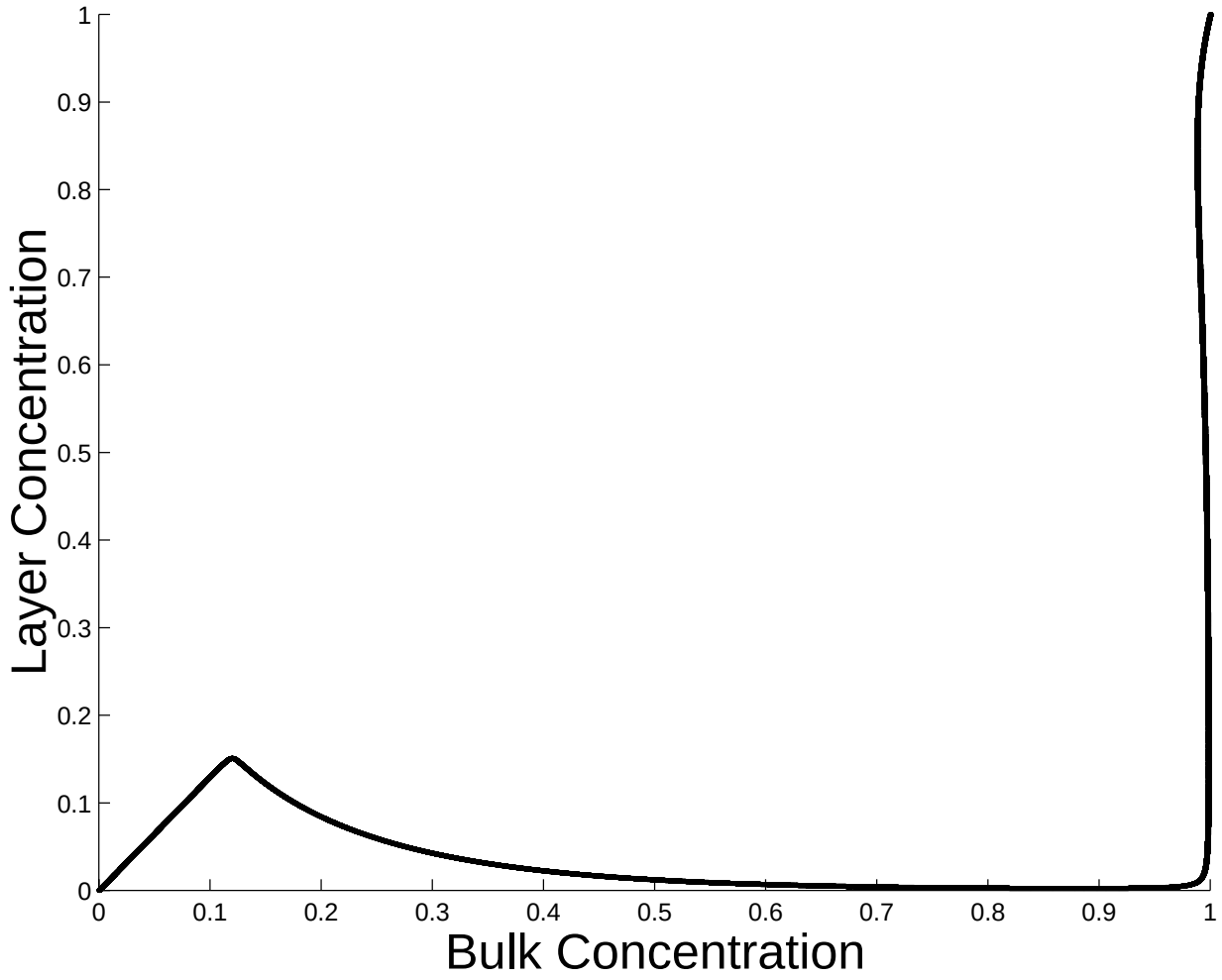


Problem 6

$N = 2$

$z_1 = 1,\ z_2 = 3,\ \epsilon_{AA}/kT = -1.9,\ \epsilon_{AS}/kT = -.258$

Result using path tracking method of Aranovich and Donohue (1998).

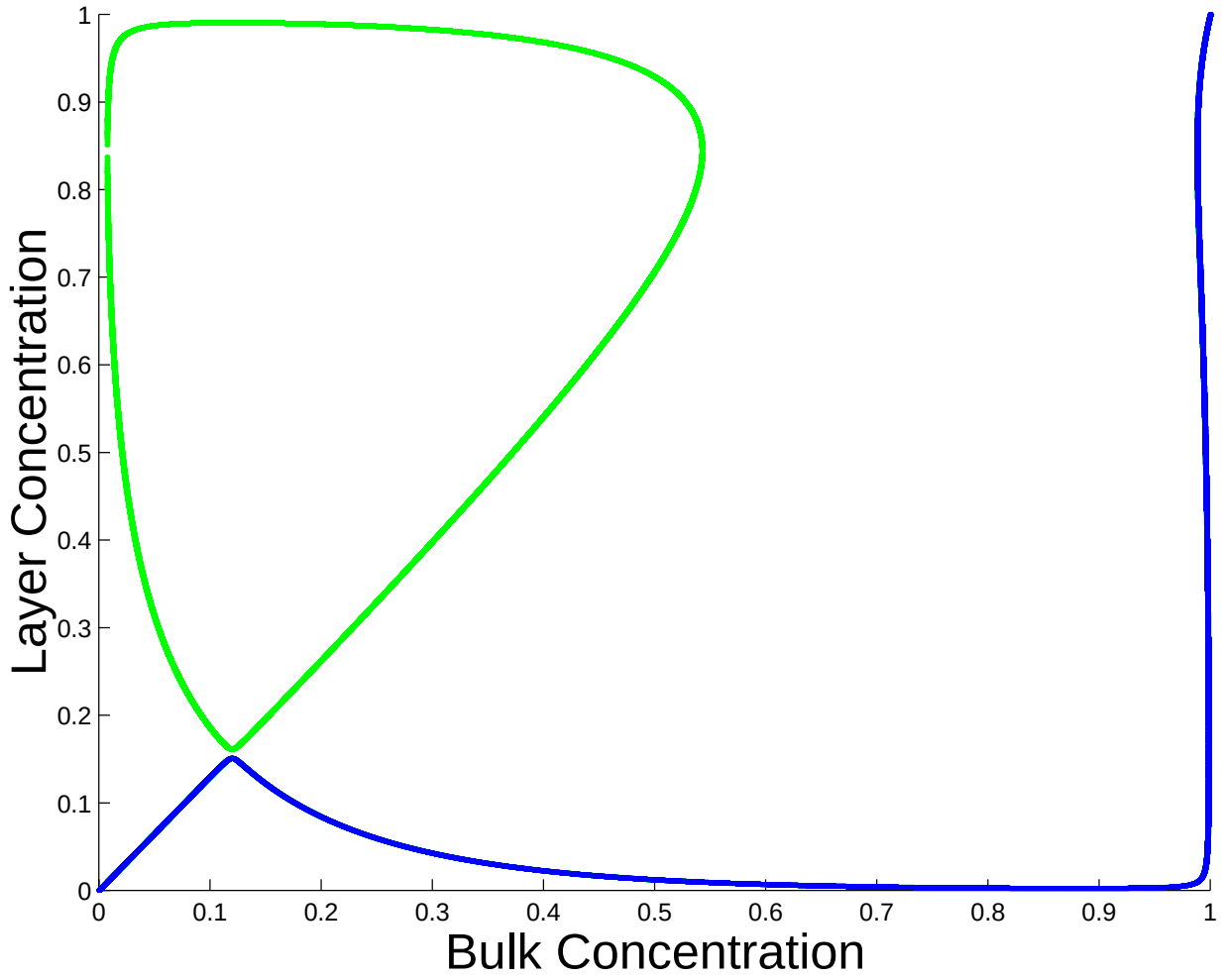


Problem 6 (cont'd)

$N = 2$

$z_1 = 1,\ z_2 = 3,\ \epsilon_{AA}/kT = -1.9,\ \epsilon_{AS}/kT = -.258$

Result using IN/GB approach.



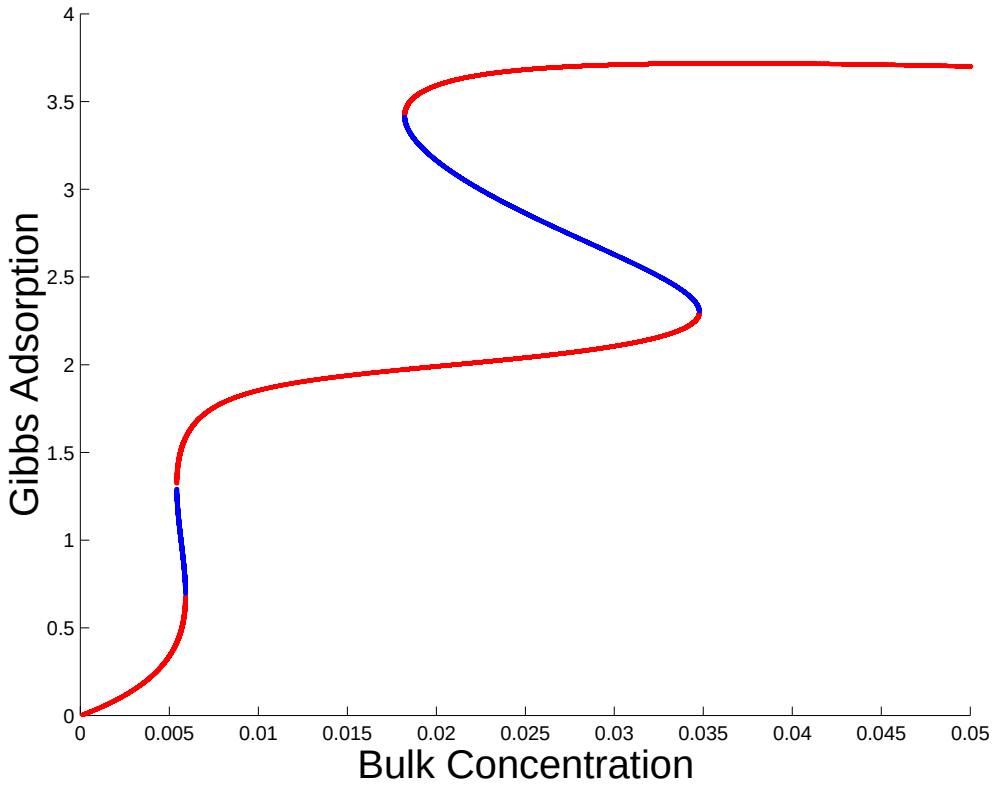
Problem 7

$N = 4$

$z_1 = 1,\ z_2 = 4,\ \epsilon_{AA}/kT = -1.1,\ \epsilon_{AS}/kT = -3.0$

Plot of Gibbs adsorption $\Gamma = \sum_{1=1}^{N} [\rho_A(i) - \rho_A]$

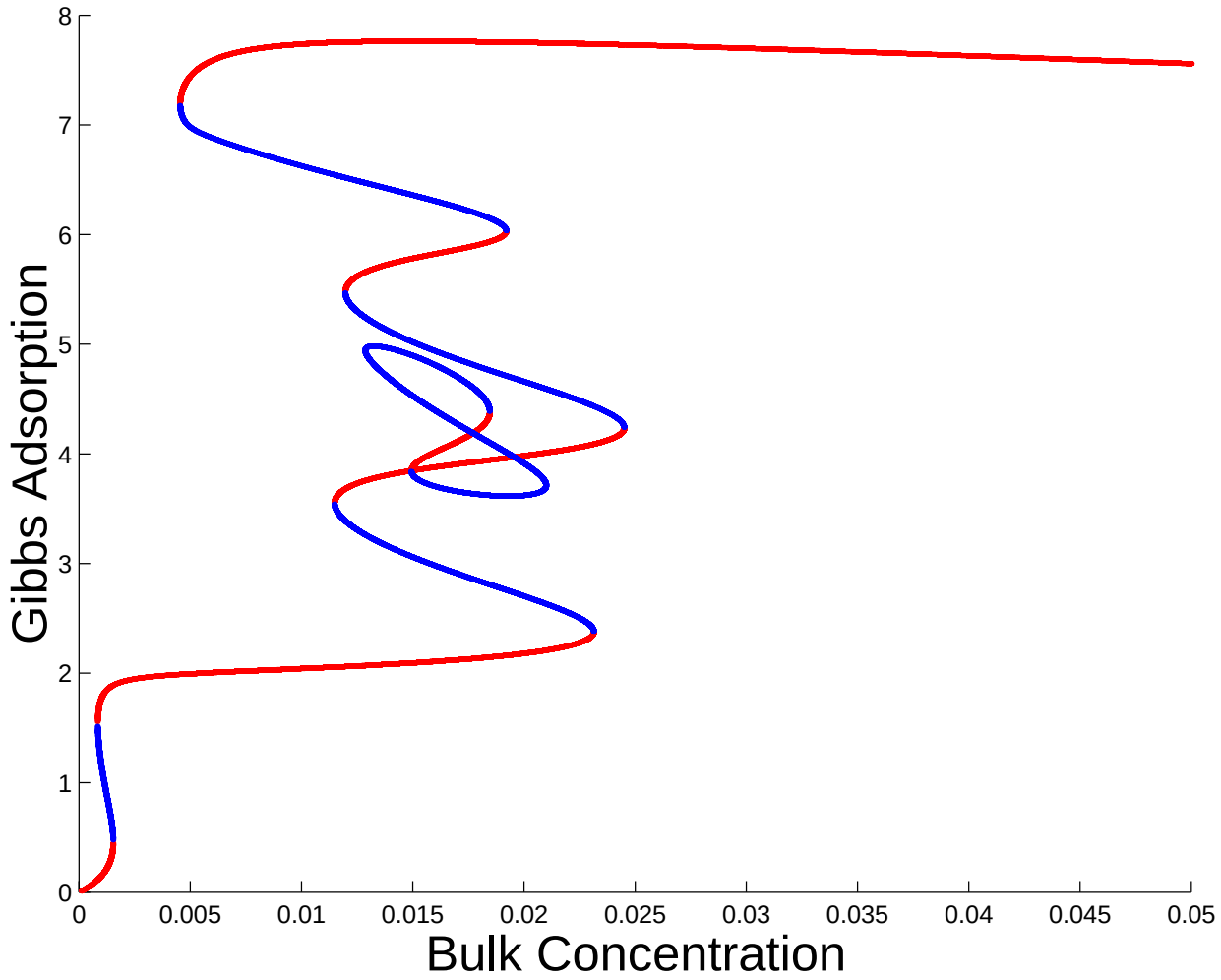
Red $\rightarrow$ local (or global) minimum in optimization problem (stable or metastable state).



Problem 8

$N = 8$

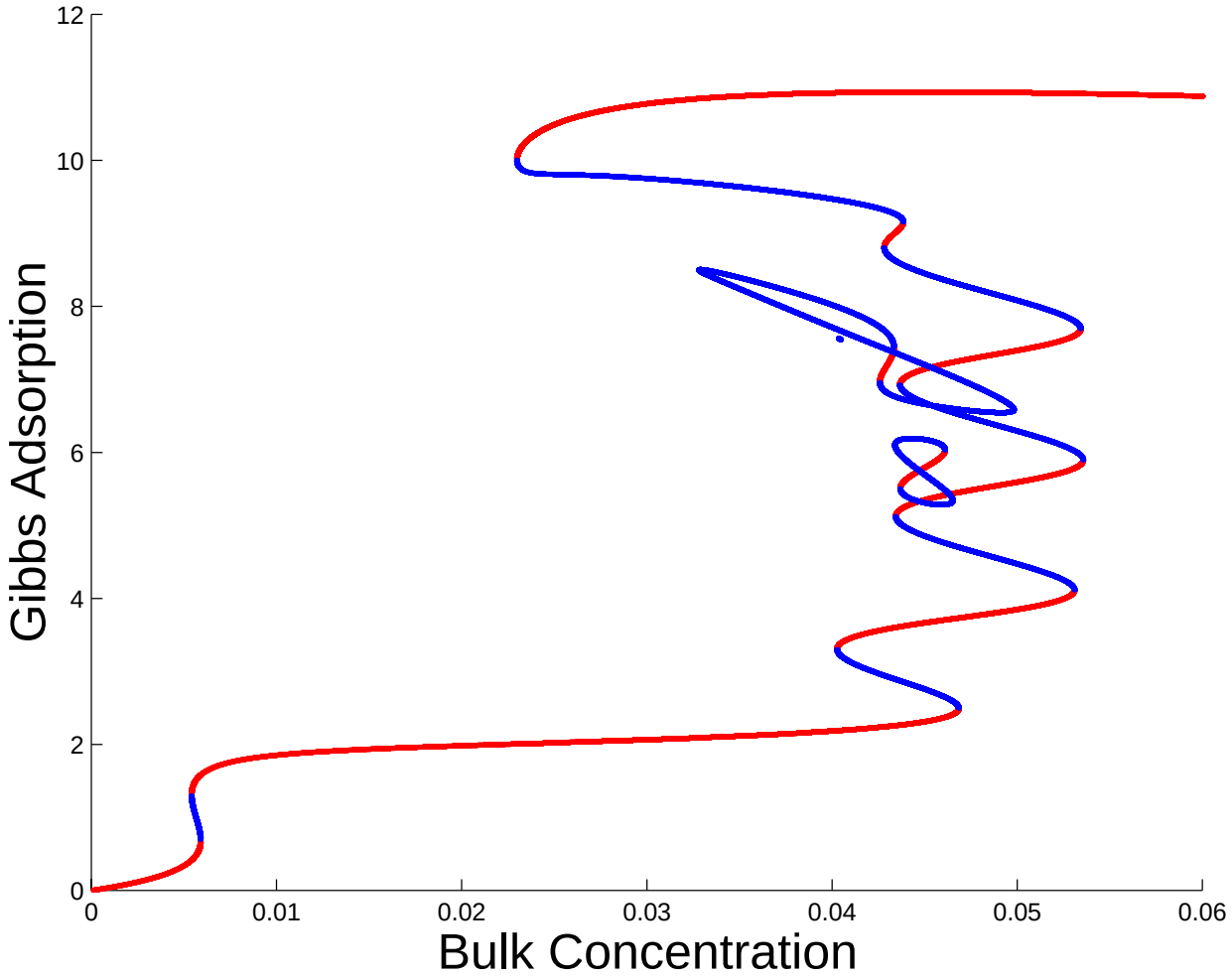
$z_1 = 1,\ z_2 = 4,\ \epsilon_{AA}/kT = -1.4,\ \epsilon_{AS}/kT = -4.0$



Problem 9

$N = 12$

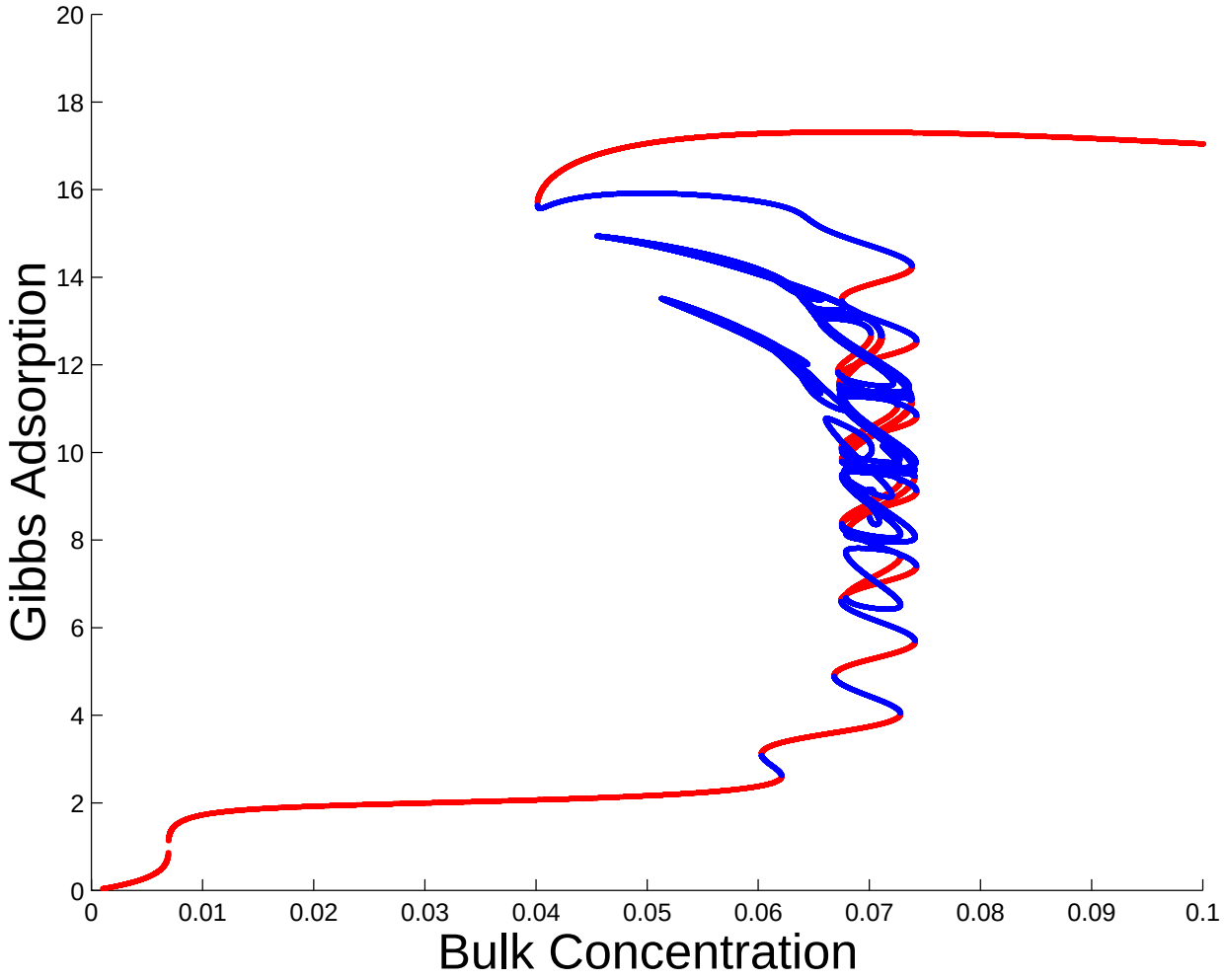
$z_1 = 1,\ z_2 = 4,\ \epsilon_{AA}/kT = -1.1,\ \epsilon_{AS}/kT = -3.0$



Problem 10

$N = 20$

$z_1 = 1,\ z_2 = 4,\ \epsilon_{AA}/kT = -1.0,\ \epsilon_{AS}/kT = -3.0$



Computational Performance

Layers (N)	Variables ($N/2$)	Average Solution Time (ms)
2	1	1
4	2	2
6	3	3
8	4	6
12	6	19
20	10	316

- Average solution time is the average CPU time required to obtain all solutions of the nonlinear equation system for a particular given value of the bulk concentration.

- Times are on a Sun Ultra 10/440 workstation.

Some Other Types of Chemical Engineering Applications

- Dealing with uncertainties (interval-valued parameters)
- Identifying feasible (or safe) operating regions or product spans given ranges of process inputs or ranges of equipment designs
- Operations research problems (e.g., planning, scheduling, etc.)

Concluding Remarks

- Interval analysis is a powerful general-purpose and model-independent approach for solving a variety of process modeling problems, providing a mathematical and computational guarantee of reliability.

- Guaranteed reliability of interval methods comes at the expense of a significant CPU requirement. Thus, there is a choice between fast local methods that are not completely reliable, or a slower method that is guaranteed to give the correct answer.

- The modeler must make a decision concerning how important it is to get the correct answer.

- Continuing advances in computing hardware and software will make this approach even more attractive.
  - Compiler support for interval arithmetic (Sun Microsystems)
  - Parallel computing (Gau and Stadtherr, 2002)

Concluding Remarks (cont'd)

- With effective load management strategies, parallel branch-and-bound (BB) and branch-and-prune (BP) problems can be solved (using interval methods or other approaches) very efficiently using MPI on a networked cluster of workstations (Gau and Stadtherr, 2000).
  - Good scalability
  - Exploit potential for superlinear speedup in BB

- Parallel computing technology can be used not only to solve problems faster, but to solve problems more reliably.

- Reliability issues are often overlooked:

  Are we just getting the wrong answers faster?

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