Reliable Modeling and Optimization for Chemical Engineering Applications: Interval Analysis Approach

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Outline

- Motivation – Reliability in Computing
- Problem Solving Methodology
- Applications in Chemical Engineering
  - Overview
  - Parameter estimation in modeling of vapor-liquid equilibrium (VLE)
  - Nonlinear dynamics – ecological modeling
  - Molecular modeling – transition state analysis
- Concluding Remarks
Motivation

- Many applications in chemical engineering deal with nonlinear models of complex physical phenomena, on scales from macroscopic to molecular.

- A common problem is the need to solve a nonlinear equation system in which the variables are constrained physically within upper and lower bounds; that is, to solve:

  \[ f(x) = 0 \]
  \[ x^L \leq x \leq x^U \]

- These problems may:
  - Have multiple solutions – Have all been found?
  - Have no solution – Can this be verified?
  - Be difficult to converge to any solution using standard methods.
Motivation (Cont’d)

● Another common problem is the need to globally minimize a nonlinear function, subject to nonlinear equality and/or inequality constraints:

$$\min_x \phi(x)$$

subject to

$$h(x) = 0$$

$$g(x) \geq 0$$

$$x^L \leq x \leq x^U$$

● These problems may:
  – Have multiple local minima – Has the global minimum been found?
  – Require finding all local minima or stationary points – Have all been found?
  – Have no solution (infeasible NLP) – Can this be verified?
  – Be difficult to converge to any local minima using standard methods
One approach for dealing with these issues is interval analysis.

Interval analysis can:

- Provide the tools needed to solve modeling and optimization problems with complete certainty.
- Provide problem-solving reliability not available when using standard local methods.
- Deal automatically with rounding error, thus providing both mathematical and computational guarantees.
Interval Methodology

- Core methodology is Interval Newton/Generalized Bisection (IN/GB)
  - Given a system of equations to solve, an initial interval (bounds on all variables), and a solution tolerance:
  - IN/GB can find (enclose) with mathematical and computational certainty either all solutions or determine that no solutions exist
  - IN/GB can also be extended and employed as a deterministic approach for global optimization problems
- A general purpose approach; in general requires no simplifying assumptions or problem reformulations
- No strong assumptions about functions need to be made
Interval Methodology (Cont’d)

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

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

- (Range Test) Compute the interval extension $F(X^{(k)})$ of $f(x)$ (this provides bounds on the range of $f(x)$ for $x \in X^{(k)}$
  - If $0 \notin F(X^{(k)})$, delete the box. Otherwise,

- (Interval Newton Test) Compute the image, $N^{(k)}$, of the box by solving the linear interval equation system

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

- $\tilde{x}^{(k)}$ is some point in $X^{(k)}$
- $F'(X^{(k)})$ is an interval extension of the Jacobian of $f(x)$ over the box $X^{(k)}$
Interval Methodology (Cont’d)

- There is no solution in $X^{(k)}$
There is a *unique* solution in $X^{(k)}$

- This solution is in $N^{(k)}$

- Additional interval-Newton steps will tightly enclose the solution with quadratic convergence
Any solutions in $X^{(k)}$ are in intersection of $X^{(k)}$ and $N^{(k)}$

- 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
Interval Methodology (Cont’d)

• Can be extended to **global optimization** problems

• For unconstrained problems, solve for **stationary points** \( \nabla \phi = 0 \)

• For constrained problems, solve for **KKT** or **Fritz-John points**

• Add an additional pruning condition (objective range test):
  – Compute interval extension of objective function
  – If its lower bound is greater than a known upper bound on the global minimum, prune this subinterval

• This combines IN/GB with a branch-and-bound scheme on a binary tree
Interval Methodology (Cont’d)

Enhancements to basic methodology:

- Hybrid preconditioning strategy (HP) for solving interval-Newton equation (Gau and Stadtherr, 2002)

- Strategy (RP) for selection of the real point \( \tilde{x}^{(k)} \) in the interval-Newton equation (Gau and Stadtherr, 2002)

- Use of linear programming techniques to solve interval-Newton equation — LISS/LP (Lin and Stadtherr, 2003, 2004)
  
  - Exact bounds on \( N^{(k)} \) (within roundout)

- Constraint propagation (problem specific)

- Tighten interval extensions using known function properties (problem specific)
Example

- Trefethen (2002) Challenge Problem #4 — Find the Global Minimum

\[ f(x, y) = \exp(\sin(50x)) + \sin(60 \exp(y)) + \sin(70 \sin(x)) + \sin(\sin(80y)) - \sin(10(x + y)) + (x^2 + y^2)/4; \quad x \in [-1, 1]; \quad y \in [-1, 1] \]
Example (Cont’d)

- Global minimum is easily found using interval approach

\[ x \in [-0.02440307969437517, -0.02440307969437516] \]
\[ y \in [0.2106124271553557, 0.2106124271553558] \]
\[ f \in [-3.306868647475245, -3.306868647475232] \]

- CPU time (LISS/LP): 0.16 seconds on SUN Blade 1000 model 1600 workstation
Another Example

• Find the global minimum of the function (Siirola et al., 2002):

\[
f(x) = 100 \prod_{i=1}^{N} \sum_{j=1}^{5} \left( \frac{j^5}{4425} \cos(j + jx_i) \right) + \frac{1}{N} \sum_{i=1}^{N} (x_i - x_{0,i})^2
\]

where \(x_{0,i} = 3\), \(x_i \in [x_{0,i} - 20, x_{0,i} + 20]\), \(i = 1, ..., N\).

• For \(N = 6\), there are \(\approx 10^{10}\) local optima.

• Results:

<table>
<thead>
<tr>
<th>(N)</th>
<th>(x_i^*)</th>
<th>(x_{j\neq i}^*)</th>
<th>Global Minimum</th>
<th>CPU time (s)</th>
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<td>413.61</td>
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<td>-87.2413242244</td>
<td>4566.42</td>
</tr>
</tbody>
</table>

CPU times on Dell workstation – 1.7 GHz Xeon running Linux
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)
  - SAFT EOS (Xu et al., 2002)
- **Combined reaction and phase equilibrium** (Burgos et al., 2004)
- **Location of azeotropes: Homogeneous, Heterogeneous, Reactive** (Maier et al., 1998, 1999, 2000)
- **Location of mixture critical points** (Stradi et al., 2001)
- **Solid-fluid equilibrium**
  - Single solvent (Xu et al., 2000, 2001)
  - Solvent and cosolvents (Scurto et al., 2003)
Applications (cont’d)

- **General process modeling problems** (Schnepper and stadtherr, 1996)

- **Parameter estimation**
  - Relative least squares (Gau and Stadtherr, 1999, 2000)
    - Error-in-variables approach (Gau and Stadtherr, 2000, 2002)

- **Nonlinear dynamics**
  - Equilibrium states and bifurcations in ecological models (Gwaltney et al., 2004)

- **Molecular Modeling**
  - Density-functional-theory model of phase transitions in nanoporous materials (Maier et al., 2001)
  - Transition state analysis (Lin and Stadtherr, 2004)
    - Molecular conformations (Lin and Stadtherr, 2004)
Example – Parameter Estimation in VLE Modeling

• Goal: Determine parameter values $\theta$ in activity coefficient models (e.g., Wilson, van Laar, NRTL, UNIQUAC):

$$\gamma_{\mu i,\text{calc}} = f_i(x_\mu, \theta)$$

• Use a relative least squares objective; thus, seek the minimum of:

$$\phi(\theta) = \sum_{i=1}^{n} \sum_{\mu=1}^{p} \left[ \frac{\gamma_{\mu i,\text{calc}}(\theta) - \gamma_{\mu i,\text{exp}}}{\gamma_{\mu i,\text{exp}}} \right]^2$$

• Experimental values $\gamma_{\mu i,\text{exp}}$ of the activity coefficients are obtained from VLE measurements at compositions $x_\mu, \mu = 1, \ldots, p$

• This problem has been solved for many models, systems, and data sets in the DECHEMA VLE Data Collection (Gmehling et al., 1977-1990)
Parameter Estimation in VLE Modeling

- One binary system studied was benzene (1) and hexafluorobenzene (2)
- Ten problems, each a different data set from the DECHEMA VLE Data Collection were considered
- The model used was the Wilson equation

\[
\begin{align*}
\ln \gamma_1 &= -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left[ \frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right] \\
\ln \gamma_2 &= -\ln(x_2 + \Lambda_{21} x_1) - x_1 \left[ \frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2} \right]
\end{align*}
\]

- This has binary interaction parameters

\[
\begin{align*}
\Lambda_{12} &= (v_2/v_1) \exp(-\theta_1/RT) \\
\Lambda_{21} &= (v_1/v_2) \exp(-\theta_2/RT)
\end{align*}
\]

where \(v_1\) and \(v_2\) are pure component molar volumes

- The energy parameters \(\theta_1\) and \(\theta_2\) must be estimated
Results

- Each problem was solved using the IN/GB approach to determine the globally optimal values of the $\theta_1$ and $\theta_2$ parameters.
- For each problem, the number of local minima in $\phi(\theta)$ was also determined (branch and bound steps were turned off).
- Table 1 compares parameter estimation results for $\theta_1$ and $\theta_2$ with those given in the DECHEMA Collection – New globally optimal parameter values are found in five cases.
- CPU times on Sun Ultra 2/1300.
Table 1: IN/GB results vs. DECHEMA values

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Data points</th>
<th>$T$ (°C)</th>
<th>DECHEMA</th>
<th>IN/GB</th>
<th>No. of Minima</th>
<th>CPU time(s)</th>
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<tr>
<td></td>
<td></td>
<td></td>
<td>$\theta_1$</td>
<td>$\theta_2$</td>
<td>$\phi(\theta)$</td>
<td>$\theta_1$</td>
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<td>0.0382</td>
<td>-468</td>
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<td>2*</td>
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<td>40</td>
<td>405</td>
<td>-405</td>
<td>0.0327</td>
<td>-459</td>
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<td>-374</td>
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<td>-449</td>
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<td>-342</td>
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<td>-424</td>
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<td>10</td>
<td>60</td>
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<td>0.0047</td>
<td>-439</td>
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<tr>
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<td>70</td>
<td>-424</td>
<td>1035</td>
<td>0.0032</td>
<td>-425</td>
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</table>

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Data points</th>
<th>$P$ (mmHg)</th>
<th>DECHEMA</th>
<th>IN/GB</th>
<th>No. of Minima</th>
<th>CPU time(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\theta_1$</td>
<td>$\theta_2$</td>
<td>$\phi(\theta)$</td>
<td>$\theta_1$</td>
<td>$\theta_2$</td>
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<tr>
<td>7*</td>
<td>17</td>
<td>300</td>
<td>344</td>
<td>-347</td>
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<td>-405</td>
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<td>17</td>
<td>760</td>
<td>-407</td>
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<td>760</td>
<td>-333</td>
<td>702</td>
<td>0.0146</td>
<td>-335</td>
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</table>

*New globally optimal parameters found
Discussion

- Does the use of the globally optimal parameters make a significant difference when the Wilson model is used to predict vapor-liquid equilibrium (VLE)?

- A common test of the predictive power of a model for VLE is its ability to predict azeotropes.

- Experimentally this system has two homogeneous azeotropes.

- Table 2 shows comparison of homogeneous azeotrope prediction when the locally optimal DECHEMA parameters are used, and when the global optimal parameters are used.
Table 2: Homogeneous azeotrope prediction

<table>
<thead>
<tr>
<th>Data Set</th>
<th>$T(°C)$ or P (mmHg)</th>
<th>DECHEMA</th>
<th>IN/GB</th>
</tr>
</thead>
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<tr>
<td></td>
<td></td>
<td>$x_1$</td>
<td>$x_2$</td>
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<tr>
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</tr>
<tr>
<td>3</td>
<td>50</td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>50</td>
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<td></td>
</tr>
<tr>
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</tr>
<tr>
<td>7</td>
<td>$P=300$</td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Based on DECHEMA results, one would conclude Wilson is a poor model for this system. But actually Wilson is a reasonable model if the parameter estimation problem is solved correctly.
Example – Nonlinear Dynamics

- Nonlinear dynamic systems are of frequent interest in engineering and science

\[ \dot{x} = \frac{dx}{dt} = f(x, p); \quad x = \text{state variables}; \quad p = \text{parameters} \]

- Common problems include computing
  - Equilibrium states (\( \dot{x} = 0 \))
  - Bifurcations of equilibria
  - Limit cycles
  - Bifurcations of cycles

- Of specific interest are food chain/web models
  - Use to predict impact on ecosystems of introducing new materials (ionic liquids) into the environment
Ionic Liquids

- Ionic liquids (ILs) are salts that are liquid at or near room temperature
- Many attractive properties
  - No measurable vapor pressure – ILs do not evaporate
  - Many potential applications, including replacement of volatile organic compounds (VOCs) currently used as industrial solvents
  - Eliminates a major source of air pollution
- Could enter the environment via aqueous waste streams
  - Very little environmental toxicity information available
  - Single species toxicity information is not sufficient to predict ecosystem impacts
- Need for ecological risk assessment – Modeling can play an important role
Finding Equilibrium States and Bifurcations

- Equilibrium states: Solve equilibrium conditions for $x$

$$\dot{x} = \frac{dx}{dt} = f(x) = 0$$

- Bifurcations of equilibria: Solve augmented equilibrium conditions for $x$ and parameter(s) of interest

- Augmenting conditions (in terms of Jacobian matrix $J = df/dx$)
  - Fold and transcritical bifurcations: $\det(J(x, \alpha)) = 0$
  - Hopf bifurcation: $\det(2J(x, \alpha) \otimes I) = 0$
  - Fold-fold or fold-Hopf bifurcations: $\det(J(x, \alpha, \beta)) = 0$ and $\det(2J(x, \alpha, \beta) \otimes I) = 0$
Finding Equilibrium States and Bifurcations (cont’d)

- These equation systems commonly have multiple solutions
- Typically these systems are solved using a continuation-based strategy (e.g., Kuznetsov, 1991; AUTO software)
  - Initialization dependent
  - No guarantee of locating all solution branches
- Interval mathematics provides a method that is
  - Initialization independent
  - Capable of locating all solution branches with certainty
- As a relatively simple test problem (Gwaltney et al., 2004), consider a tritrophic food chain with logistic prey and hyperbolic predator and superpredator response functions (Rosenzweig-MacArthur model)
Rosenzweig-MacArthur model

In terms of prey(1), predator(2) and superpredator(3) biomasses \( x_1, x_2 \) and \( x_3 \), the model is given by

\[
\frac{dx_1}{dt} = x_1 \left[ r \left(1 - \frac{x_1}{K}\right) - \frac{a_2 x_2}{b_2 + x_1}\right]
\]

\[
\frac{dx_2}{dt} = x_2 \left[e_2 \frac{a_2 x_1}{b_2 + x_1} - \frac{a_3 x_3}{b_3 + x_2} - d_2\right]
\]

\[
\frac{dx_3}{dt} = x_3 \left[e_3 \frac{a_3 x_2}{b_3 + x_2} - d_3\right]
\]

Here \( r \) is the prey growth rate constant, \( K \) is the prey carrying capacity of the ecosystem, the \( d_i \) are death rate constants, the \( a_i \) represent maximum predation rates, the \( b_i \) are half-saturation constants, and the \( e_i \) are predation efficiencies.
Results – Rosenzweig-MacArthur Model

Example of a solution-branch diagram (equilibrium states vs. one parameter with other parameters fixed) – here $x_1$, $x_2$ and $x_3$ vs. $d_2$
Results – Rosenzweig-MacArthur Model

Example of a bifurcation diagram (parameter value at which bifurcation occurs vs. another parameter – here $r$ vs. $K$ with other parameters fixed)

TE = Transcritical of equilibrium; FE = Fold of equilibrium; H = Hopf; $H_p$ = Planar Hopf; FH = Fold-Hopf
Results – Canale’s Chemostat Model

This is a more complex model (4 state variables). This is the computed $D$ vs. $x_n$ bifurcation diagram.

TE = Transcritical of equilibrium; FE = Fold of equilibrium; H = Hopf; $H_p$ = Planar Hopf; FH = Fold-Hopf
Example – Transition State Analysis

- Transition state analysis is widely used in engineering and science to study the kinetics of various phenomena, e.g.,
  - Chemical reactions
  - Adsorption/desorption to/from surfaces
  - Diffusion through a porous media (e.g., zeolites)

- The key step is identifying stationary points on the potential energy surface $V$ that characterizes the intermolecular and intramolecular interactions governing the system

- Motion in the system then is assumed to proceed as a series of hops from one local minimum to another, passing through a saddle point (transition state)

- Need a method that is guaranteed to find all stationary points of $V$
Transition State Analysis (cont’d)

- One example problem – diffusion of xenon in silicalite (June et al., 1991; Lin and Stadtherr, 2004)

- Use truncated Lennard-Jones 6-12 potential

\[
V = \sum_{i=1}^{N} V_i
\]

\[
V_i = \begin{cases} 
\frac{a}{r_{i}^{12}} - \frac{b}{r_{i}^{6}} & r_i < r_{\text{cut}} \\
0 & r_i \geq r_{\text{cut}}
\end{cases}
\]

\[
r_i^2 = (x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2
\]

where \((x, y, z)\) are the Cartesian coordinates of the xenon, and \((x_i, y_i, z_i), i = 1, \ldots, N\) are the Cartesian coordinates of the \(N = 192\) oxygen atoms in a unit cell of the silicalite lattice

- Problem is to solve \(\nabla V(x, y, z) = 0\) for all stationary points \((x, y, z)\)
Results using interval-Newton methodology (LISS_LP)

<table>
<thead>
<tr>
<th>No.</th>
<th>Type</th>
<th>Energy (kcal/mol)</th>
<th>x(Å)</th>
<th>y(Å)</th>
<th>z(Å)</th>
<th>Connects</th>
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<td>14*</td>
<td>2nd order</td>
<td>-4.1404</td>
<td>0.5883</td>
<td>4.8777</td>
<td>8.0138</td>
<td>(4,5),(4,4')</td>
</tr>
<tr>
<td>15</td>
<td>2nd order</td>
<td>-4.1027</td>
<td>9.1881</td>
<td>4.1629</td>
<td>11.8720</td>
<td>(2,3),(4,5)</td>
</tr>
</tbody>
</table>

* Not found by June et al. (1991)
Concluding Remarks

- Interval analysis provides a powerful general purpose and model independent approach for solving a wide variety of modeling and optimization problems, giving a mathematical and computational guarantee of reliability.

- Guaranteed reliability of interval methods comes at the expense of CPU time. 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
Concluding Remarks (cont’d)

• With effective load management strategies, interval methods can be implemented very efficiently using MPI on a networked cluster of workstations (Gau and Stadtherr, 2002).
  – Good scalability
  – Exploit potential for superlinear speedup in optimization

• 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?