A Fast Continuation Method for the Ornstein-Zernike Equations

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Joint work with
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November 2, 2004
Supported by NSF, ARO.
Outline

- The Ornstein-Zernike (OZ) Equations
- Fast solvers for compact fixed point problems
  Application to OZ + uniqueness problems
- Path following: introduction
  Nonlinear solvers
  Pseudo-arclength continuation
- Multilevel method.
- Results
OZ Equations: O-Z, 1914

Used to calculate probability distributions of atoms in fluid states. Unknowns are $h, c \in C[0, L]$.

- $h$: radial pair correlation function, observable
- $c$: direct correlation function, defined by IE

**Integral Equation:**

$$h(r) - c(r) - \rho(h \ast c)(r)$$

where

$$(h \ast c)(r) = \int_{R^3} c(\|r - r'\|) h(\|r'\|) dr'.$$
Algebraic Closure Constraint

\[ \exp(-\beta U(r) + h(r) - c(r)) - h(r) - 1 = 0. \]

where \( u \) is the Lennard-Jones potential.

\[ U(r) = 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right). \]
Parameters

Data are parameters

- $\rho$: number density, sometimes unknown
- $\beta = 1/(\text{absolute temperature} \times \text{Boltzmann’s constant})$
- $\varepsilon$: well depth of the potential
- $\sigma$: determines size of the particles
Discretization

- Uniform grid on $[0, L]$
- Trapezoid rule for integration
- Discrete Hankel transform for evaluation of integrals

\[
\mathcal{H}(h)(k) = 4\pi \int_0^\infty \frac{\sin(kr)}{kr} h(r) r^2 dr
\]

and

\[
h \ast c = \mathcal{H}^{-1}(\hat{h} \hat{c}).
\]

- Fast evaluation via FFT
Solution: $\rho = 0.2, \sigma = 2; \varepsilon = 0.1; \beta = 10; L = 9$
Reduction to single equation

Let $g = h - c$, then the closure constraint expresses $c$ as a function of $g$.

$$c(r) = c(g(r)) = \exp(-\beta U(r) + g(r)) - g(r) - 1.$$  

The integral equation is

$$h - \rho c * h = c.$$  

Take Hankel transforms

$$\hat{h} - \rho \hat{h} \hat{c} = \hat{c},$$  

and obtain $\hat{h} = \hat{c} / (1 - \rho \hat{c})$.  

$g \rightarrow c \rightarrow h$ leads to...

\[ h = h(c(g)) = c(g) + \mathcal{K}(g). \]

Subtract $c$ and obtain a fixed point problem for $g$.

\[ g = h(c(g)) - c(g) = \mathcal{K}(g). \]

$\mathcal{K}$ is a nonlinear integral operator with compact Fréchet derivative.
Alternative: reduce to single equation in $c$

- $c \rightarrow h(c)$ via solution of integral equation
- $h(c) - c = G(c)$, $G$ compact
- $K(c) = \exp(-\beta U - G(c)) - G(c) - 1$

Compact fixed point problem:

$$c = K(c)$$
More General OZ Equations

Unknowns $h, c, \rho, \in C[0, L]$

\[
h(r) = \exp(-\beta U(r) + h(r) - c(r)) - 1
\]

\[
h(r) = c(r) + \int_0^r c(r - r') \rho(r') h(r') \, dr'
\]

\[
\rho(r) = A_1 \exp\left(-\beta U(r) + \int_0^r \rho(r - r') c(r') \, dr'\right).
\]

Also matrix-valued unknowns.
Compact Fixed Point Problems

We’re worried about problems like

\[ F(u) = u - \mathcal{K}(u) = 0, \text{ on a Banach space } X, \]

where

- \( \mathcal{K} \in C^1_{LIP}(X). \)
- \( \mathcal{K}' \in \text{Com}(X). \)
- Compactness will lead to fast solvers.
How to exploit compactness

- Discretization
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  • Almost every reasonable scheme works, but
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- Newton-Krylov, Newton-MG nonlinear solvers work with no surprises (most of the time).
World’s Easiest Example

Linear Fredholm equation:

\[(I - K)u(x) = u(x) - \int_{0}^{1} k(x, y)u(y) \, dy = f(x),\]

\(f \in X = C[0, 1], \, k \in C([0, 1] \times [0, 1])\)

Approximating space: \(V_h = \text{span} \{\phi_i\}\)

\(P_h\) is a projection onto \(V_h\), and we seek \(u^h \in V_h\).

\[u^h(x) - K_hu^h(x) = u^h(x) - \int_{0}^{1} k_h(x, y)u^h(y) \, dy = P_hf(x)\]

where, \(k_h(x, y) = \sum_{i,j=1}^{N_h} k(x_i, x_j) \phi_i(x) \phi_j(y)\)
Properties of Discretization

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- Lots of flexibility in $P_h$
  Strong convergence to $I$ is all you need.
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- Lots of flexibility in $P_h$
  Strong convergence to $I$ is all you need.
- If $I - K$ is nonsingular, then

\[ u^h = (I - K_h)^{-1} P_h f \rightarrow (I - K)^{-1} f \]

Solve finite dimensional system for nodal values.
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Solve finite dimensional system for nodal values.

- Other choices of $K_h$ are possible
  Standard quadrature rule + fine-to-coarse by averaging
Nystrom interpolation

- Solve $\tilde{u}^h - K_h \tilde{u}^h = f$ rather than $u^h - K_h u^h = P_h f$.
- Multiply by $P_h$ and use $K_h = K_h P_h = P_h K_h$ to get

\[(P_h \tilde{u}) - P_h K_h (P_h \tilde{u}) = P_h f.\]

Finite dimensional system.
Solve for $u^h = P_h \tilde{u}^h$.

- $\tilde{u}^h = f + K_h u^h$
Performance of GMRES

Avoid the $O(N_h^3)$ cost of a direct solver, and compute

$$u^h = (I - K_h)^{-1} P_h f = \sum_{i=1}^{N_h} u_i^h \phi_i \in V_h.$$ 

with GMRES.

- Continuous problem: superlinear convergence
- Discrete problem: mesh independent performance
- Cost: One $K_h v$ evaluation/linear iteration
  Think $N_h \log N_h$ work if done slickly.

Nested iteration (aka grid sequencing) is a good idea.
Since $K_h \to K$ in the operator norm,

- $(I - K_H) (h << H)$ might be a good preconditioner for GMRES
Multilevel Method; K 95

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- Richardson iteration is a better idea thanks to LOW STORAGE.

$$u \leftarrow u - (I - K_H)^{-1} ((I - K_h)u - P_h f)$$
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$$u \leftarrow u - (I - K_H)^{-1}((I - K_h)u - P_hf)$$

- $H$ suff small implies
  - Krylovs independent of $H$.
  - One iteration/level suffices.
Nonlinear Problems

Generalization to the nonlinear case is easy,

\[ u \leftarrow u - (I - \mathcal{H}_H(u^H))^{-1} F_h(u) \]

if you’re careful about the fine-to-coarse transfer. If coarse mesh suff fine,

- Krylov/Newton independent of \( H \)
- one Newton/level suffices.
Nested Iteration: Bottom up; K 95

\[ h = H, \ i = 0 \]
Solve \( F_H(u^H) = 0 \) to high accuracy.
\[ u \leftarrow u^H \]
\textbf{for} \( i = 1, \ldots m \) \textbf{do}
\[ h \leftarrow h/2 \]
\[ u \leftarrow u - (I - \mathcal{K}_H^I(u^H))^{-1}F_h(u) \]
\textbf{end for}

- All the linear solver work is on the coarse mesh.
- Only two grids \( H \) and \( h \) active at any time.
- Cost of solve to truncation error:
  \(< 3 \) fine mesh evals, depending on cost of \( \mathcal{K}_h \)
Iteration statistics for three nested iterations

- Multilevel, Newton-GMRES, Picard
- Formulation in $c$:
  \[ c \rightarrow h(c) \] via integral equation
  \[ c = \mathcal{K}(c) \] via constraint
- Tabulate:
  \[ i^f_G \] = fine mesh GMRES/Newton (average)
  \[ i^c_G \] = coarse GMRES/Newton (average)
  incoming nonlinear residual $R_h$ ($R_{2h} \approx 4R_h$)
### Iteration Statistics: $h = 1/(N-1)$

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<th>$i^f_G$</th>
<th>$R_\delta$</th>
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Mission Accomplished?

- We found two solutions;
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- One can get one or the other by
  - varying the initial iterate,
  - varying the initial grid, or
  - varying the details of the algorithm,
- which motivates a parametric \((\sigma, \varepsilon, \rho \ldots)\) study of the OZ equations.
Path Following

\[ F : X \times [a,b], \text{ } F \text{ smooth, } X \text{ a Banach space.} \]

Objective: Solve \( F(u, \lambda) = 0 \) for \( \lambda \in [a, b] \)

Obvious approach:

Set \( \lambda = a \), solve \( F(u, \lambda) = 0 \) with Newton-(MG, GMRES, \ldots) to obtain \( u_0 = u(\lambda) \).

while \( \lambda < b \) do

Set \( \lambda = \lambda + d\lambda \).

Solve \( F(u, \lambda) = 0 \) with \( u_0 \) as the initial iterate.

\( u_0 \leftarrow u(\lambda) \)

end while

The implicit function theorem says: You will not find two solutions with identical parameter values this way.
What’s the problem?

- Multiple solutions, hysteresis
- No solutions
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A fix: Pseudo-arclength continuation.
Set \( x = (u, \lambda) \) and solve \( G(x, s) = 0 \), where, for example

\[
G(x, s) = \begin{pmatrix}
F \\
N
\end{pmatrix} = \begin{pmatrix}
F(u(s), \lambda(s)) \\
\dot{u}^T(u - u_0) + \dot{\lambda}^T(\lambda - \lambda_0) - (s - s_0)
\end{pmatrix}.
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$s$ is an artificial “arclength” parameter. $u_0$ and $\lambda_0$ are from the previous step. $\dot{u} \approx du/ds$ and $\dot{\lambda} \approx d\lambda/ds$,

(say by differences using $s_0$ and $s_{-1}$).
Simple Folds

We follow solution paths \( \{x(s)\} \).
Assume that \( F \) is smooth and

- \( G_x \) is nonsingular (not always true)
  So implicit function theorem holds in \( s \).

We are assuming that there is no true bifurcation and that the singularity in \( \lambda \) is at worst simple fold.

\[
\dim(\text{Null}(F_u)) = 1, \quad F_\lambda \neq \text{Ran}(F_u)
\]
Set $\lambda = a$, $s = 0$ solve $F(u, \lambda) = 0$ with
Newton-(MG, GMRES, ...) to obtain $u_0$.

Estimate $ds, \dot{u}, \dot{\lambda}$.

while $s < s_{max}$ do

$s \leftarrow s + ds$.

Solve $G(x, s) = 0$ with $u_0$ as the initial iterate.

$x_0 \leftarrow x$ 

Update $ds, \dot{u}, \dot{\lambda}$.

end while
How should compactness help?

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  - Appropriate coarse grid data depend on $s$. 
Multilevel Approach

Pathfollowing on coarse mesh + nested iteration fails.

- \( F(u, \lambda) = u - \mathcal{K}(u, \lambda) \)
- \( \lambda(s) \) is sensitive to the mesh.
- Track path on fine mesh.
- Use coarse mesh problem to approximate \( \mathcal{K}u \)
  Apply GMRES to new problem.
Coarse mesh problem construction

For continuation in $\lambda$

- $x^h = x^h + dx$, Euler predictor on fine mesh.
- $u^H = I_h^H(u^h)$, $\lambda = \lambda^H = \lambda^h$.
- Build $K_H = I_H^H \mathcal{K}_u^H(u^H, \lambda) I_h^H$
- Norm convergent (K, 1995) if $I_h^H$ is done right degenerate kernel approximation
- Approximate Newton step by solving
  
  $$s - K_H s = -F_h(u^H, \lambda).$$

  Fine mesh residual and coarse mesh solve.
Continuation in $s$

Approximate $G_x$ by

$$G_{u,\lambda}^H(u, \lambda) \equiv 
\begin{pmatrix}
I - \partial \mathcal{K}^H(I_h^H u, \lambda)/\partial u & -\partial \mathcal{K}^H(I_h^H u, \lambda)/\partial \lambda \\
(I_h^H \dot{u})^T & \dot{\lambda}
\end{pmatrix}.$$ 

and apply GMRES.
Continuation in $s$

Approximate $G_x$ by

\[ G^H, h_{u, \lambda} (u, \lambda) \equiv \begin{pmatrix}
I - \partial \mathcal{K}^H (I_h^H u, \lambda) / \partial u
& - \partial \mathcal{K}^H (I_h^H u, \lambda) / \partial \lambda \\
(I_h^H \dot{u})^T
& \dot{\lambda}
\end{pmatrix}. \]

and apply GMRES.

- Operator-function product is now on coarse mesh.
- Works for “black-box” functions. Flexible choice of $\mathcal{K}^H$.
- Theory follows from older work, if you coarsen only in $\mathcal{K}$, not in $G$. 
Details

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- $ds$ must be controlled by watching for
  - deviation of Newton’s/(step in s) from target
  - curvature estimation
  - true bifurcation
- occasional testing for bifurcation
Numerical Results: Three Solution Paths

For each solution we continue in $\rho$, and plot three scalars:

- Excess number
  \[ \int r^2 h(r) \, dr \]
- Pressure
  \[ \int r^3 U'(r)(h(r) + 1) \, dr \]
- Compressibility
  \[ \int r^2 c(r) \, dr \]

as functions of $\rho$. 
Path through physical solution

Diagram showing the relationship between pressure, compressibility, and excess number.
Path through non-physical solution
Conclusions

- OZ integro-algebraic equations
  Elimination leads to compact fixed point problem
- Multilevel method for integral equations
- Solves OZ, but finds too many solutions
- Bottom-up nesting goes the wrong way for continuation
- Top down works; currently 30% faster than GMRES