# A Fast Continuation Method for the Ornstein-Zernike Equations

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Joint work with

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# 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:

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

where

$$(h * c)(r) = \int_{R^3} c(\|\mathbf{r} - \mathbf{r}'\|) h(\|\mathbf{r}'\|) d\mathbf{r}'.$$

# 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
- $\beta = 1/($absolute temperature $\times$ 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

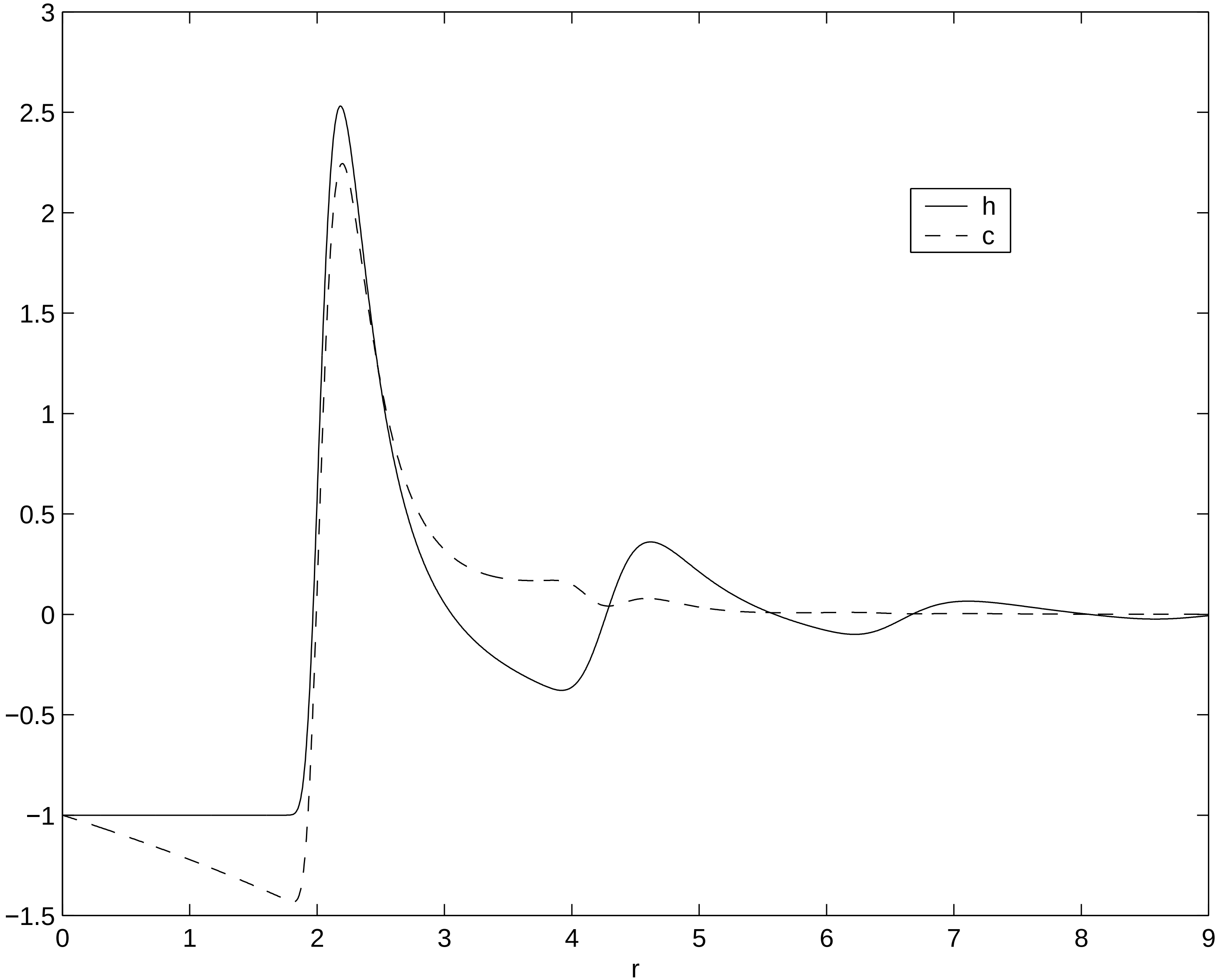
$$\mathscr{H}(h)(k) = 4\pi \int_0^\infty \frac{sin(kr)}{kr} h(r) r^2 dr$$

  and

$$h * c = \mathscr{H}^{-1}(\hat{h}\hat{c}).$$

- Fast evaluation via FFT

# **Solution:** $\rho = .2, \sigma = 2; \varepsilon = .1; \beta = 10; L = 9$



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

# $g \longrightarrow c \longrightarrow h$ leads to . . .

$$h = h(c(g)) = c(g) + \mathscr{K}(g).$$

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

$$g = h(c(g)) - c(g) = \mathscr{K}(g).$$

$\mathscr{K}$ is a nonlinear integral operator with compact Fréchet derivative.

# Alternative: reduce to single equation in $c$

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

Compact fixed point problem:

$$c = \mathscr{K}(c)$$

# More General OZ Equations

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

$$
\begin{aligned}
h(r) &= \exp\left(-\beta U(r) + h(r) - c(r)\right) - 1 \\
h(r) &= c(r) + \int_0^r c(r - r')\rho(r')h(r')\,dr' \\
\rho(r) &= A_1 \exp\left(-\beta U(r) + \int_0^r \rho(r - r')c(r')\,dr'\right).
\end{aligned}
$$

Also matrix-valued unknowns.

# Compact Fixed Point Problems

We're worried about problems like

$$F(u) = u - \mathscr{K}(u) = 0, \text{ on a Banach space } X,$$

where

- $\mathscr{K} \in C^1_{LIP}(X)$.
- $\mathscr{K}' \in Com(X)$.
- Compactness will lead to fast solvers.

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- Fast evaluation ($O(N \log(N))$) is common.
- 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: $V_h =$ span $\{\phi_i\}$
$P_h$ is a projection onto $V_h$, and we seek $u^h \in V_h$.

$$u^h(x) - K_h u^h(x) = u^h(x) - \int_0^1 k_h(x,y)u^h(y)\,dy = P_h f(x)$$

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

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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.

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

# Nonlinear Problems

Generalization to the nonlinear case is easy,

$$u \leftarrow u - (I - \mathscr{K}_H'(u^H))^{-1} F_h(u)$$

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

- Krylovs/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.
$u \leftarrow u^H$
**for** $i = 1, \ldots m$ **do**
  $h \leftarrow h/2$
  $u \leftarrow u - (I - \mathscr{K}_H'(u^H))^{-1} F_h(u)$
**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 $\mathscr{K}_h$

# Works great for OZ! K., Pettit 2004

Iteration statistics for three nested iterations

- Multilevel, Newton-GMRES, Picard
- Formulation in $c$:
  $c \rightarrow h(c)$ via integral equation
  $c = \mathscr{K}(c)$ via constraint
- Tabulate:
  $i_G^f$ = fine mesh GMRES/Newton (average)
  $i_G^c$ = coarse GMRES/Newton (average)
  incoming nonlinear residual $R_h$ ($R_{2h} \approx 4R_h$)

# Iteration Statistics: h = 1/(N-1)

| | Picard | | Newton-GMRES | | Multilevel | |
|---|---|---|---|---|---|---|
| $N$ | $R_\delta$ | $i_G^f$ | $R_\delta$ | $i_G^f$ | $R_\delta$ | $i_G^c$ |
| 65 | 3.5900e+00 | 650 | 3.5900e+00 | 85 | 3.5900e+00 | 85 |
| 129 | 1.3696e-01 | 11 | 1.3696e-01 | 4 | 1.3696e-01 | 8 |
| 257 | 2.0031e-02 | 3 | 2.9413e-02 | 5 | 4.1900e-02 | 7 |
| 513 | 4.8144e-03 | 9 | 6.9937e-03 | 5 | 9.4120e-03 | 7 |
| 1025 | 2.3568e-03 | 14 | 1.5400e-03 | 5 | 2.0205e-03 | 7 |
| 2049 | 3.6543e-04 | 15 | 3.5596e-04 | 7 | 4.6015e-04 | 8 |
| 4097 | 8.2396e-05 | 22 | 8.4570e-05 | 5 | 1.0831e-04 | 8 |
| 8193 | 2.2253e-05 | 38 | 2.0784e-05 | 7 | 2.6411e-05 | 8 |
| 16385 | 4.0075e-06 | 48 | 5.2729e-06 | 8 | 6.5042e-06 | 8 |
| 32769 | 9.7738e-07 | 32 | 1.2263e-06 | 5 | 1.6132e-06 | 8 |
| 65537 | 2.3869e-07 | 44 | 3.0647e-07 | 7 | 4.0169e-07 | 8 |

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  - varying the details of the algorithm,
- which motivates a parametric $(\sigma, \varepsilon, \rho \ldots)$ study of the OZ equations.

# Path Following

$F : X \times [a,b]$, $F$ smooth, $X$ 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, ...) 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?

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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.

$$\text{dim}(\text{Null}(F_u)) = 1, F_\lambda \neq \text{Ran}(F_u)$$

# Arclength Continuation Algorithm

Set $\lambda = a$, $s = 0$ solve $F(u, \lambda) = 0$ with Newton-(MG, GMRES, $\ldots$) 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**

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- Multilevel solvers
  - Easy to build. Compactness smooths for you.
  - Appropriate coarse grid data depend on $s$.

# Multilevel Approach

Pathfollowing on coarse mesh + nested iteration fails.

- $F(u,\lambda) = u - \mathscr{K}(u,\lambda)$
- $\lambda(s)$ is sensitive to the mesh.
- Track path on fine mesh.
- Use coarse mesh problem to approximate $\mathscr{K}^u$
  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 $K_H = I_H^h \mathscr{K}_u^H(u^H, \lambda) I_h^H$
- 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

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

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and apply GMRES.

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

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  - 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

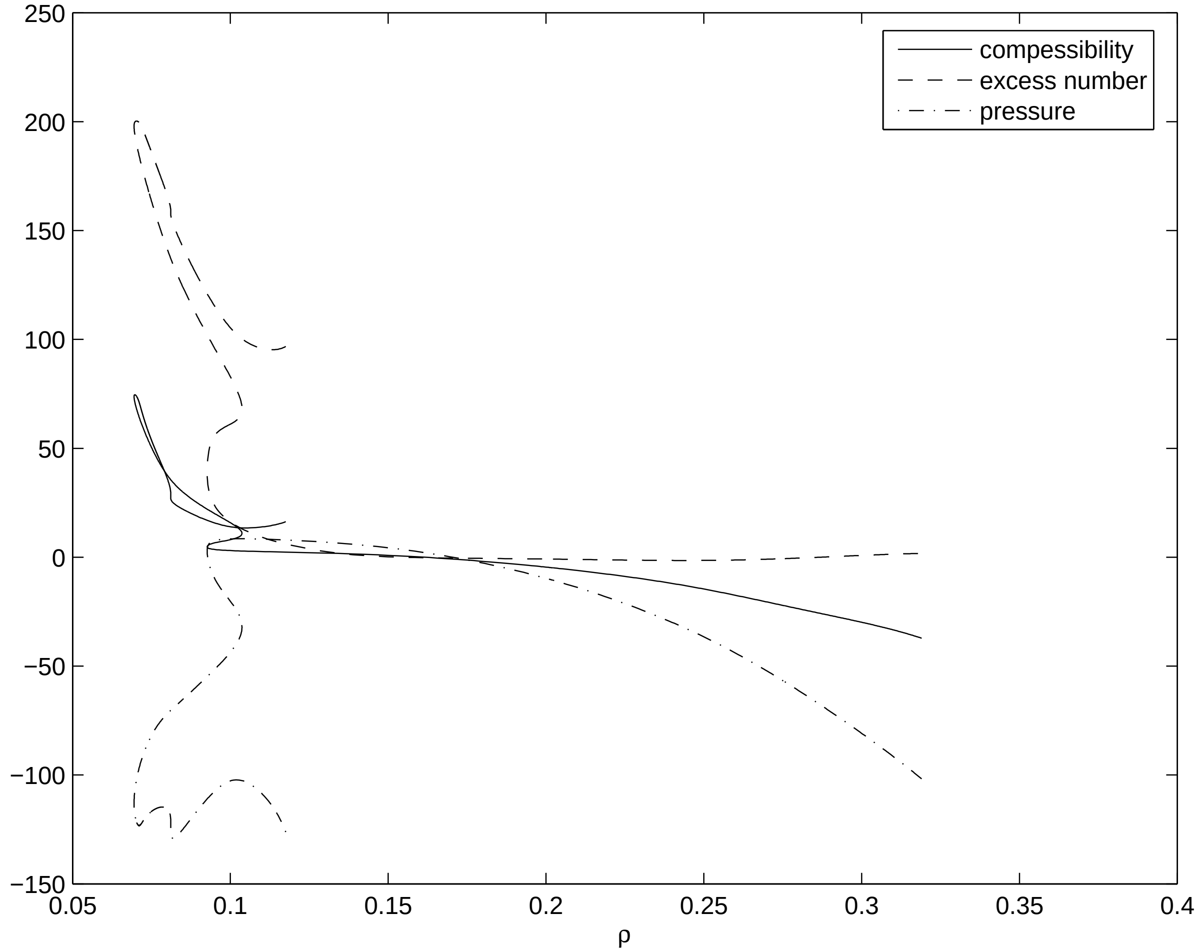
$$\int r^3 U'(r)(h(r)+1)\,dr$$

- Compressibility

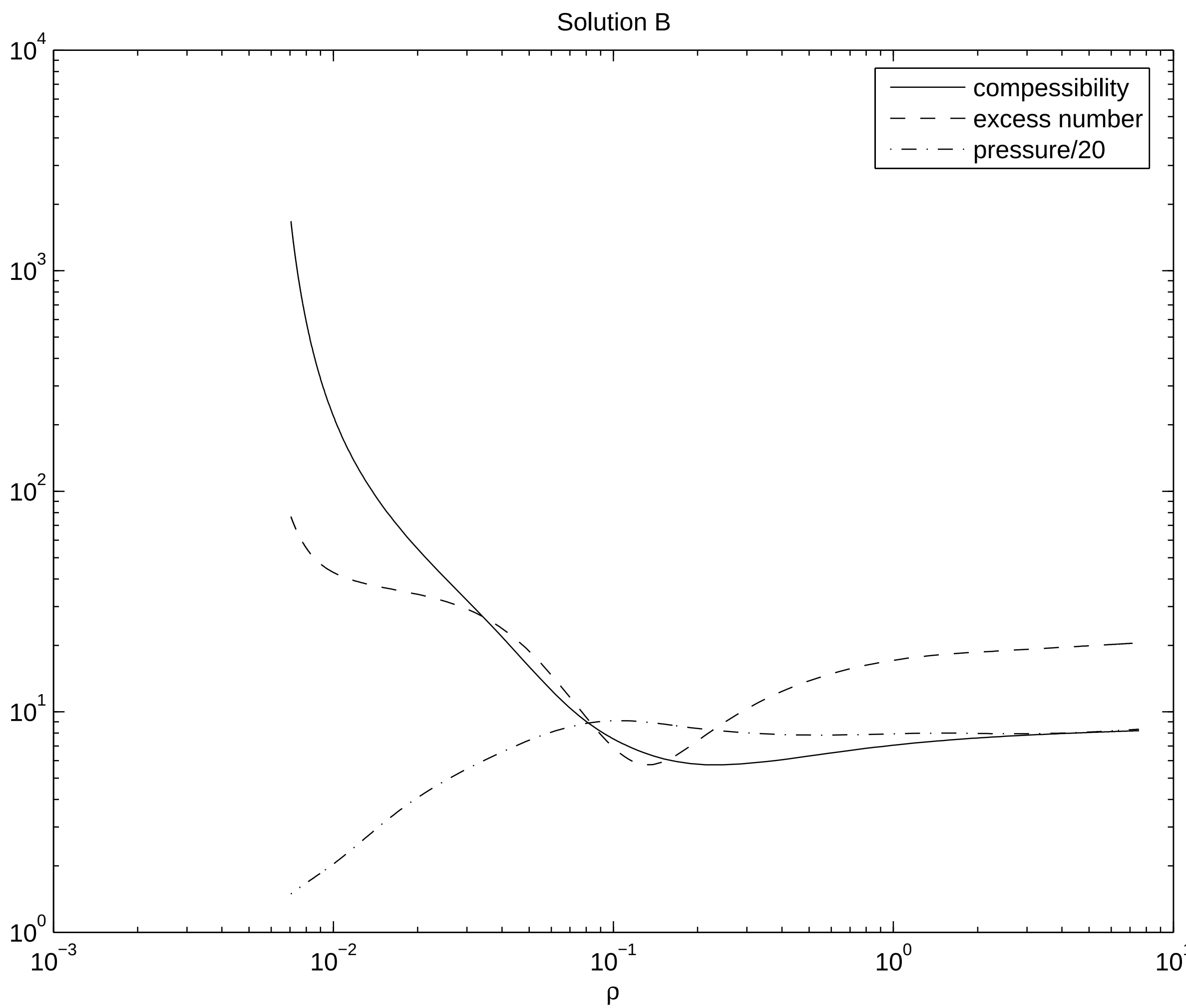
$$\int r^2 c(r)\,dr$$

as functions of $\rho$.

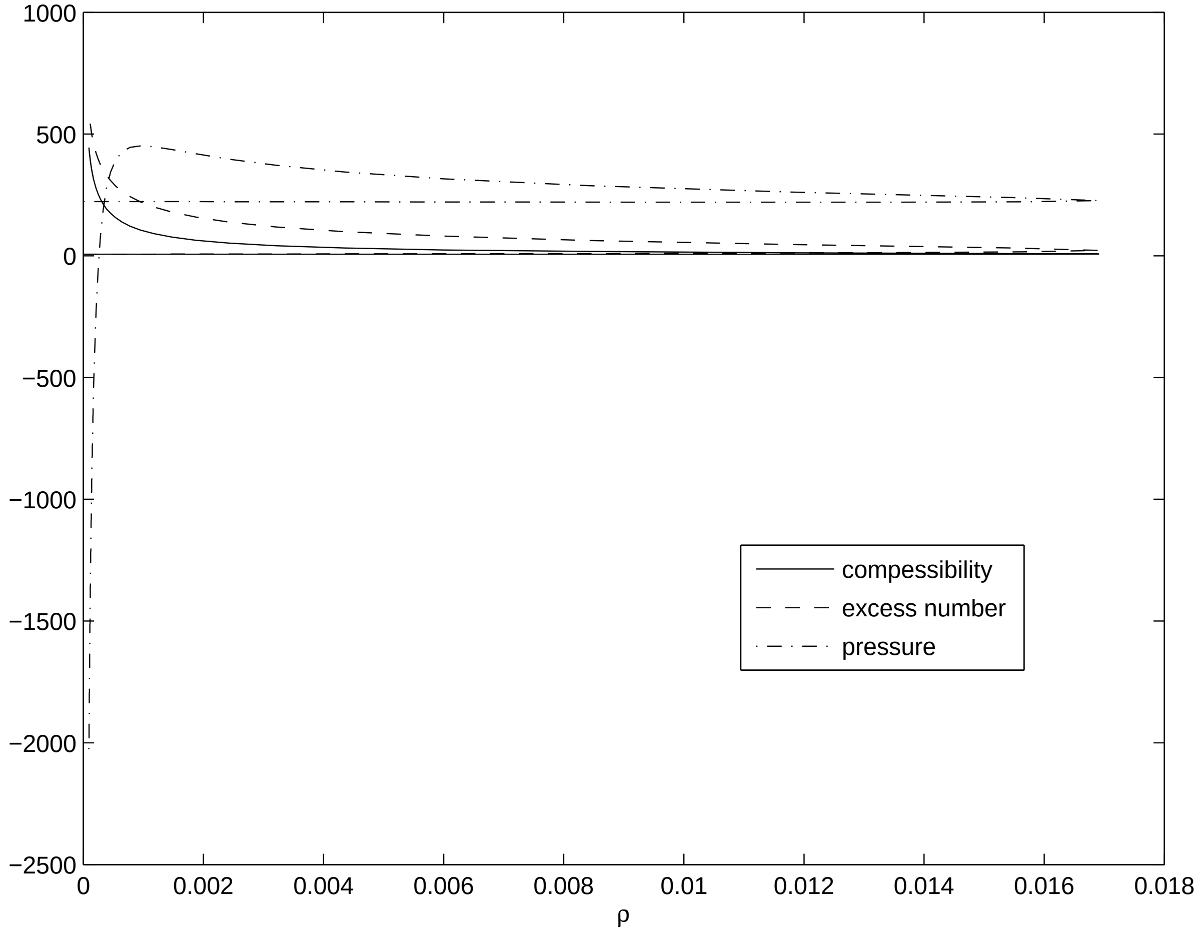
# Path through physical solution



# Path through non-physical solution



# Path through new 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