Continuation Algorithms for Parameter-Dependent Compact Fixed Point Problems

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Outline

- Fast introduction to compact fixed point problems
- Newton-GMRES and multilevel Newton-GMRES
- Path following: introduction
  Nonlinear solvers
  Pseudo-arclength continuation
- Three examples:
  - integral equation
    explicit integral operator
  - Wigner-Poisson Equation for RTDs
  - time-stepper for parabolic pde
    implicit integral operator
- Multilevel method.

Compact Fixed Point Problems

We're worried about problems like

$$F(u) = u - \mathscr{K}(u) = 0,$$

where

- F is Lipschitz continuously Frechét differentiable on a Banach space X.
- The "compact" part means that $\mathscr{K}'$ is a compact linear map on X.
- We want to exploit the compactness to design 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

$$(I-K)u(x) = u(x) - \int_0^1 k(x,y)u(y)\,dy = f(x),$$

$f \in C[0,1]$, $k \in C([0,1]\times[0,1])$
Discretization: $V_h =$ piecewise linears/piecewise constants

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

where,

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

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

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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

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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  - 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

$h = H$, $i = 0$
Solve $F_H(u^H) = 0$ to high accuracy.
$u \leftarrow u^H$
for $i = 1, \ldots m$ **do**
  $h \leftarrow h/2$
  $u \leftarrow u - (I - \mathscr{K}_H'(u^H))^{-1} F_h(u)$
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- Only two grids H and h active at any time.
- Cost of solve to truncation error:
  < 3 fine mesh evals, depending on cost of $\mathscr{K}_h$

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

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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 λ_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}).

Watch out for scaling!

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 λ is a simple fold.

Arclength Continuation Algorithm

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

Simple example: Chandreskhar H-Equation

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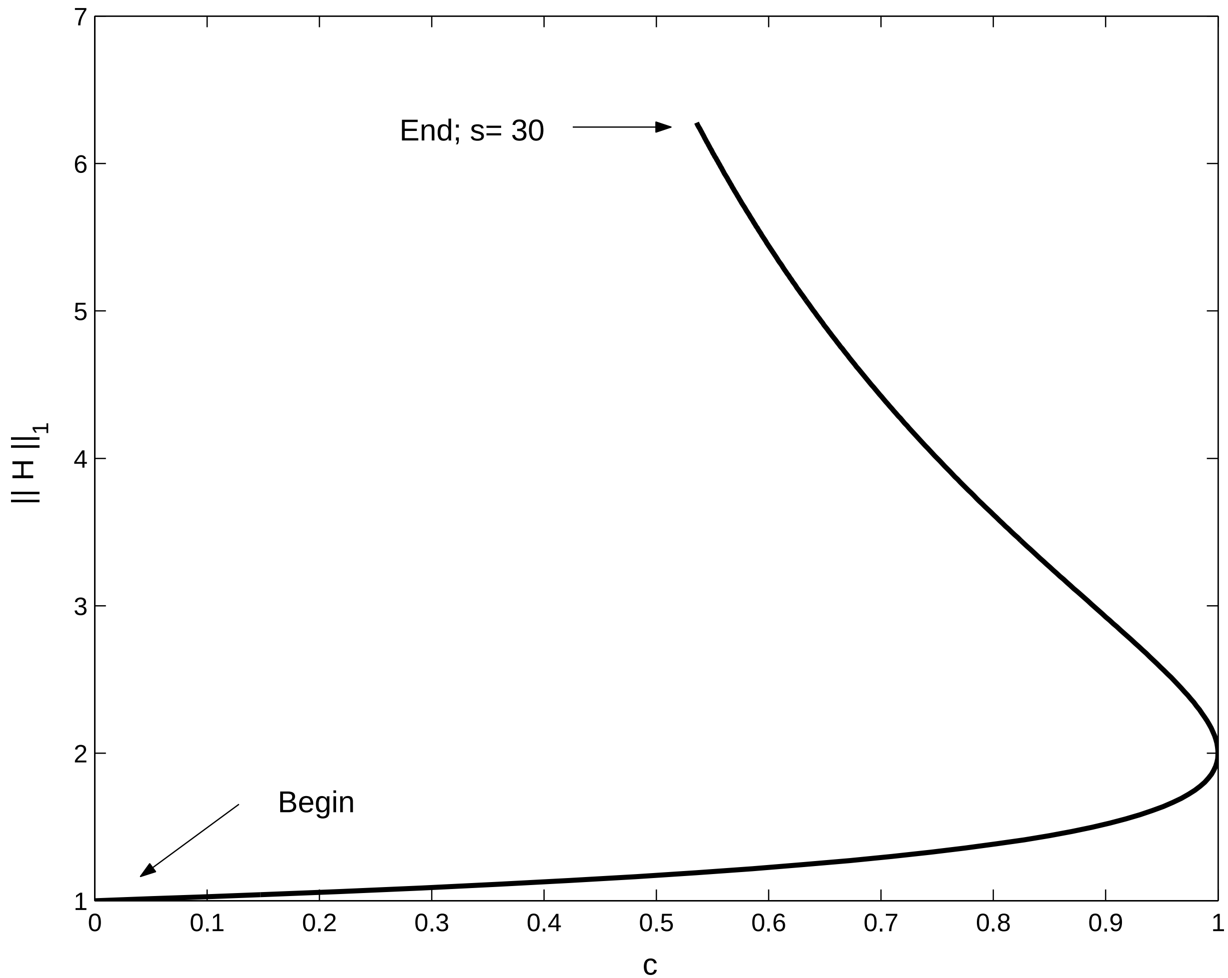
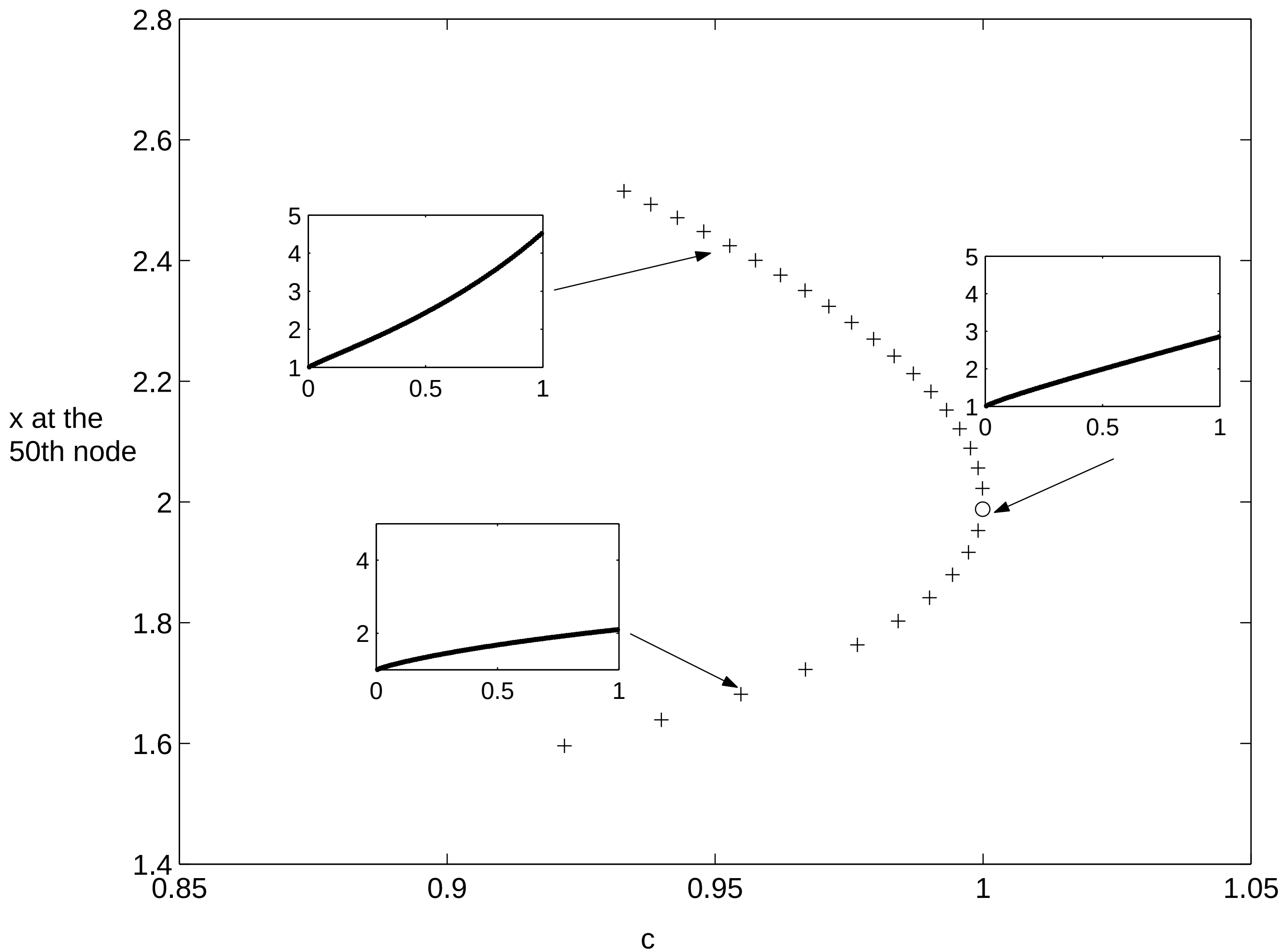
- Two solutions for $c \neq 0, 1$
  - Two continuous solutions for $0 < c < 1$.
  - Complex conjugate pairs for $c > 1$.
  - One continuous, one unbounded for $c < 0$.

$\|H\|_1$ vs c



H and the path



Wigner-Poisson Equation for $f(t,x,k)$

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$$V(f)(x,k) = \frac{1}{h}\int dk' f(x,k')\int dy[U(x+y)-U(x-y)]sin[2y(k-k')].$$

$$U(z) = u(z) + \Delta_c(z), \frac{d^2}{dx^2}u(x) = \frac{q^2}{\varepsilon}\left[N_d(x) - \int_{-\infty}^{\infty}\frac{dk}{2\pi}f(x,k)\right].$$

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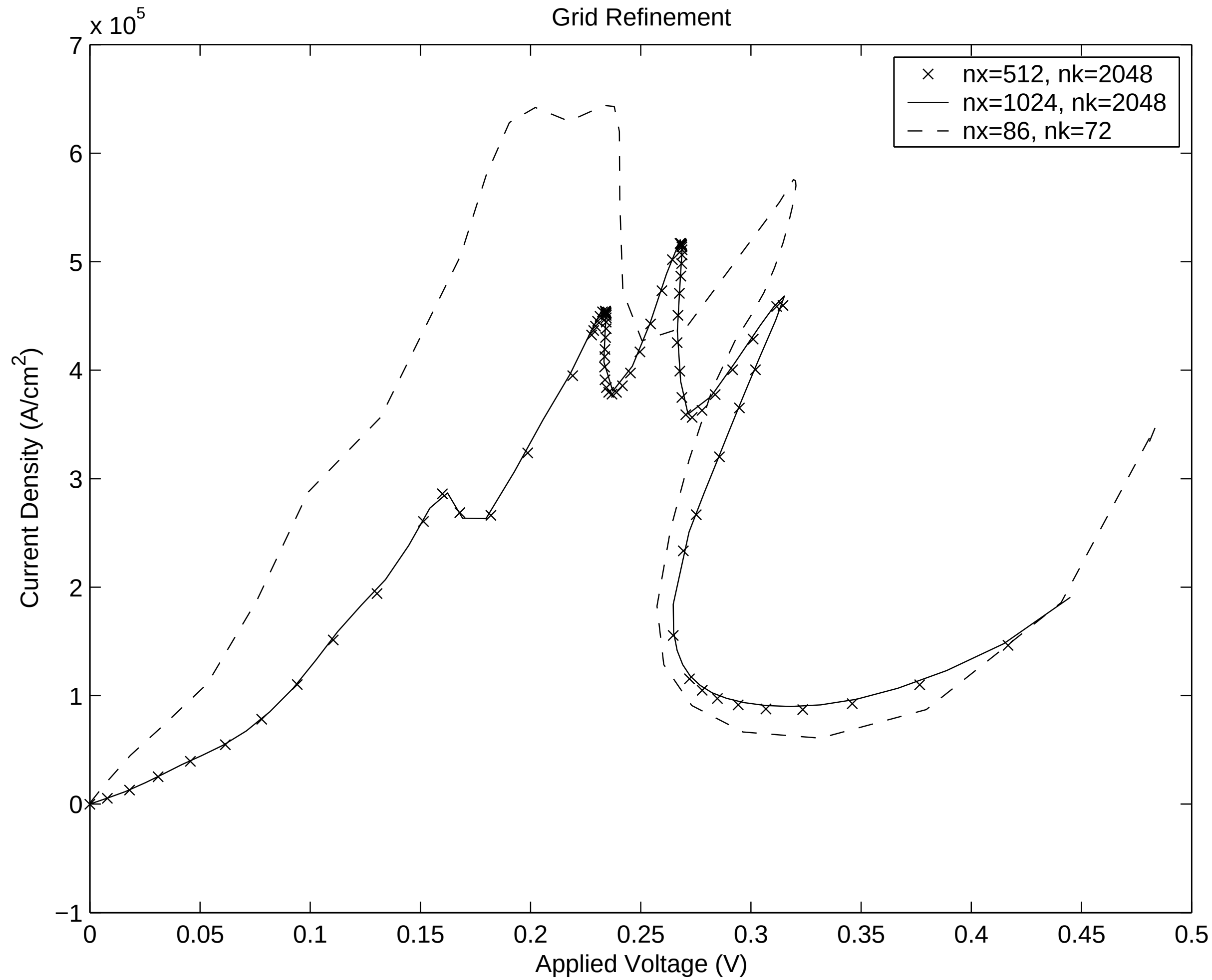
$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{1}{\tau}\left[\frac{f_0(x,k)}{\int dk\, f_0(x,k)}\int dk\, f(x,k) - f(x,k)\right].$$

Path following for Wigner Poisson Eq

- Use LOCA (Salinger-Phipps)
  NOX, AztecOO, Anasazi, Epetra
- Precondition with inverse of spatial differential operator
- Uniformly bounded, not quite compact
- Folds, hysteresis, Hopf bifurcation

Latest LOCA results



Time-stepper

Model Problem: Investigate steady-state solutions of the Chafee-Infante equation

$$u_t - \nu u_{xx} + u^3 - u = 0, x \in [0, \pi], u(0,t) = u(\pi,t) = 0,$$

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as functions of ν.
Method: Let $K(T,u,\nu)$ be the solution of the PDE at time T with initial data u. Solve

$$F(u,\nu) = u - K(T,u,\nu).$$

If $\nu > 0$, K is a smoother.
T becomes an algorithmic parameter.
More complex examples of this idea are in Schroff-Keller(93), Gear-Kevrekidis(03) ...

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  - Microscale simulations scales using non-DE methods
  - Large codes that are hard to modify and/or understand

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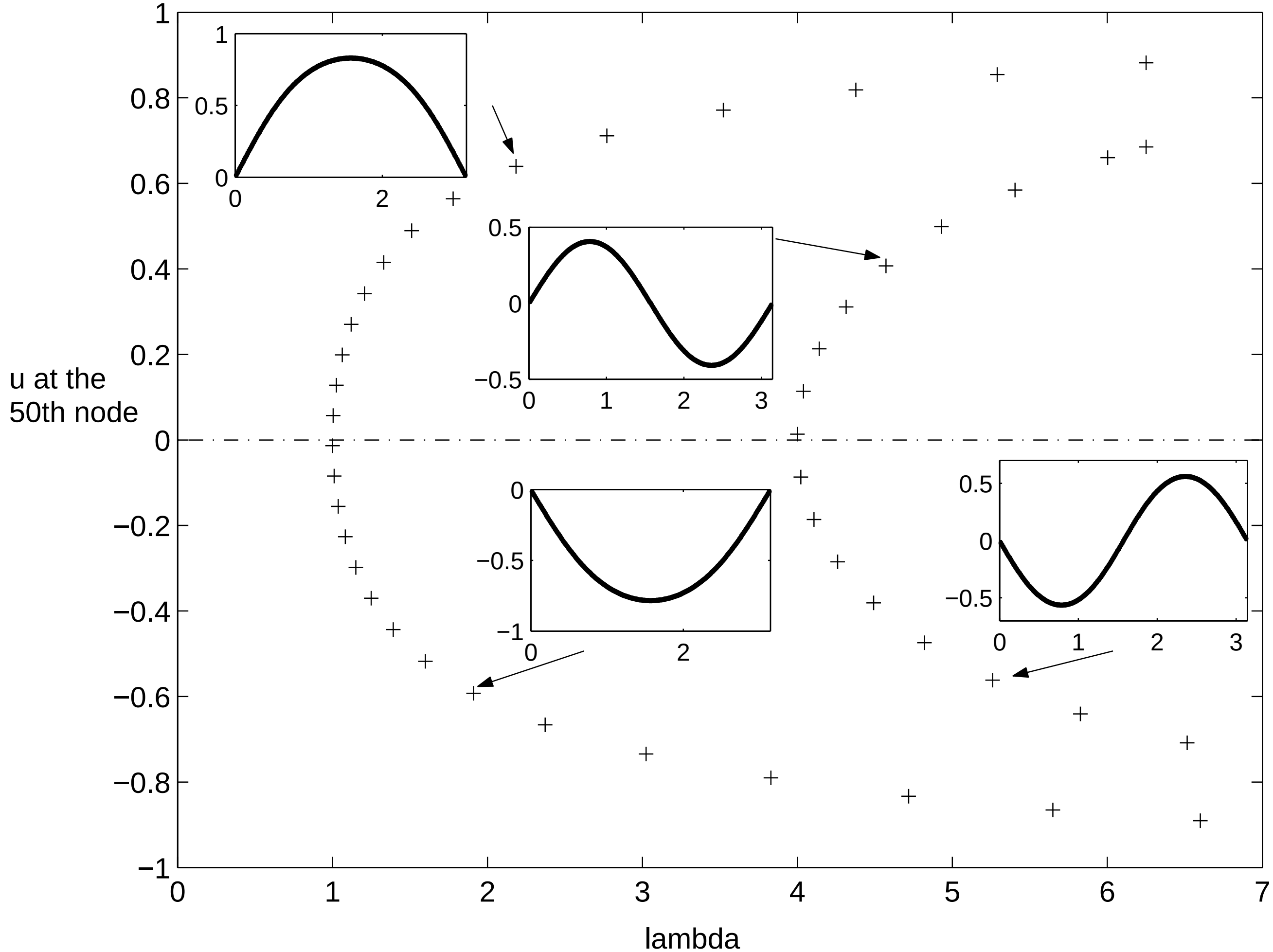

Branch Switching

These were not simple folds.

- Simple bifurcations (the forks) $\rightarrow$ sign change in determinant.
  How do you compute that determinant?
- Matrix-free detection $\rightarrow$
  - generalized eigenvalue problem $\rightarrow$
  - s^* and $w \neq 0$ such that $G_x(x(s^*))w = 0$
- At the bifurcation point s^*: choice of directions.
  $\dot{x}$ or the new direction $\pm w$.

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  - Appropriate coarse grid data depend on s.

Timesteppers and Compactness

Let D have dimension d

$$F_u(u,v) = I - K + E$$

where

- $K = P_D K P_D$, where P_D is a projection onto D
- $\|E\|$ is small, and
- we solve $F_u(u,v)s = -F(u,v)$ with GMRES.

Dimension of D will depend on T.
T should be selected with thought.

Convergence of GMRES

Let r_m be the mth GMRES residual.
Set

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we can apply standard GMRES theory to show

$$\|r_{m(d+1)}\| \leq \|p(F_u)^m r_0\| = O(\|E\|^m),$$

for all $m \geq 1$.

Inflated system

Same results for

$$G(x,s) = \begin{pmatrix} F \\ N \end{pmatrix} = \begin{pmatrix} F(u(s),\lambda(s)) \\ \dot{u}^T(u-u_0) + \dot{\lambda}^T(\lambda-\lambda_0) - (s-s_0) \end{pmatrix}.$$

with d replaced by $d+2$.
Meaning: cost of solve is independent of discretization,
unless d begins to increase with 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 λ

- $x^h = x^h + dx$, 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

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

and apply GMRES.

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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.

Conclusions

- Exploitation of compactness in path following
  - Simple folds
    - 6 coarse mesh Krylovs/Newton for H-equation
    - Multilevel Chafee-Infante results in progress
    - GMRES working for Wigner-Poisson Eq
  - Branching and Hopf in the works
    Wigner-Poisson results for Hopf almost there
- Scaling F vs N important as path grows