Pseudo-transient Continuation for Nonsmooth Nonlinear Equations

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Workshop on Solution Methods for Large Scale Nonlinear Problems

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NCSU Students/Postdocs

- PhD Students
  - Mike Tocci (1998, Mathworks)
  - Lea Jenkins (2000, Clemson)
  - Todd Coffey (2002, Sandia)
  - Katie Fowler (2003, Clarkson)
  - Jill Reese (200?, HA381)
- Postdoc: Chris Kees (HA 337)

Outline

- What is Ψtc ?
- Motivation
  - Unsaturated flow; nonsmooth constitutive laws (Tocci, Jenkins, Kavanagh, Kees, Howington, Farthing, Miller, K.)
  - CFD (Coffey, Keyes, McRae, McMullan, K.)
- Local convergence
  - What do you use for a Taylor expansion?
  - Quality of derivative approximation.
- Numerical example

What is Ψtc ?

- Find steady state solutions of

$$x' = F(x)$$

- Mimic temporal integration.
  Grow the time step in the terminal phase.
- Addresses failure mode of Newton-Armijo.
- Avoids non-physical results.

Newton-Armijo: the obvious thing

$$x_{n+1} = x_n + s \text{ where } s = \lambda d$$

and

$$\|F'(x_n)d + F(x_n)\| \le \eta_n \|F(x_n)\|.$$

You pick λ such that

$$\|F(x_n + \lambda d)\| \le (1 - \alpha\lambda)\|F(x_n)\|$$

where usually $\alpha = 10^{-4}$.

Newton-Armijo bottom line

If F is smooth and the computation of d and λ succeed, then either

- **BAD:** the iteration is unbounded, *i. e.* $\limsup \|x_n\| = \infty$,
- **BAD:** the derivatives tend to singularity, *i. e.* $\limsup \|F'(x_n)^{-1}\| = \infty$, or
- **GOOD:** the iteration converges to a solution x^* in the terminal phase, $\lambda = 1$, and

$$\|x_{n+1} - x^*\| = O(\|x_n - x^*\|\eta_n + \|x_n - x^*\|^2).$$

So what's the problem?

- Stagnation at singularity of F' really happens.
  - steady flow $\longrightarrow$ shocks in CFD
- Non-physical results
  - fires go out
  - negative concentrations
- Nonsmooth nonlinearities
  - are not uncommon: flux limiters, constitutive laws
  - globalization is harder
  - finite diff directional derivatives may be wrong

Ψtc is one way to fix it.

DAE Dynamics: semi-explicit

$x = (u, v)^T$ and

$$D \begin{pmatrix} u \\ v \end{pmatrix}' = -\begin{pmatrix} f(u,v) \\ g(u,v) \end{pmatrix} = -F(x), \quad x(0) = x_0,$$

where

$$D = \begin{pmatrix} D_{11} & 0 \\ 0 & 0 \end{pmatrix}, \text{ nonsingular .}$$

Differential variables u. Algebraic variables v.

Ψtc for smooth problems

$$x_{n+1} = x_n + s_n$$

where

$$\|(\delta_n^{-1} D + F'(x_n))s_n + F(x_n)\| \leq \eta_n \|F(x_n)\|$$

and (SER)

$$\delta_n = \max\left(\delta_{n-1}\frac{\|F(x_{n-1})\|}{\|F(x_n)\|}, \delta_{max}\right).$$

Theory for smooth problems

Joint with Todd Coffey, David Keyes

If

- $Dx' = -F(x)$; $x(0) = x_0$; $x^* = \lim_{t\to\infty} x(t)$.
- DAE has uniform index one (g_{vv} nonsingular near $x(t)$).
- x^* is stable steady state.
- δ_0 is sufficiently small.
- Update δ_n with SER.

Then $x_n \to x^*$ and local convergence is what you'd expect from inexact Newton.

That’s nice, but . . .

Not all nonlinearities are smooth.

- Slope limiters in CFD
- Non-differentiable constitutive laws.
  e. g. Groundwater flow in the unsaturated zone.
- Nonsmooth reaction models (see example).

Nonsmooth Calculus

Assume that F is Lipschitz continuous on R^N. Then F is differentiable almost everywhere.
The generalized Jacobian (Clarke) at x is

$$\partial F(x) = \text{co} \left\{ \lim_{x_j \to x; x_j \in D_F} F'(x_j) \right\}$$

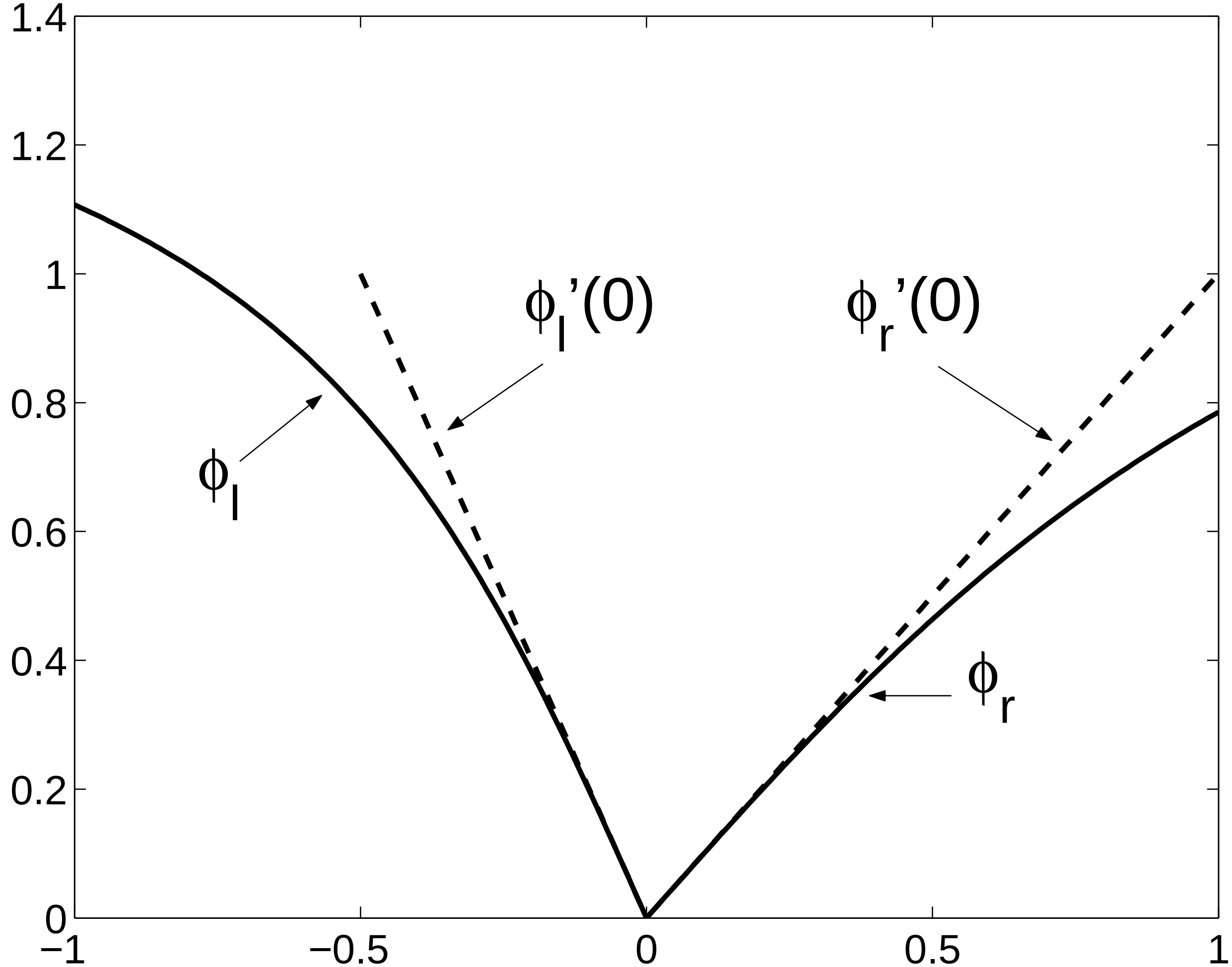
You'd like to replace Newton's method with

$$x_{n+1} = x_n - V_n^{-1} F(x_n)$$

where $V_n \in \partial F(x_n)$.
Does that work? How do you compute V_n?

Piecewise smooth function: $\phi = \phi_l + \phi_r$

$\partial\phi(0) = [\phi_l(0), \phi_r(0)]$, a **set**.



Difference approximations

Scalar functions

$$\partial_h \phi(x) = \frac{\phi(x+h) - \phi(x)}{h}$$

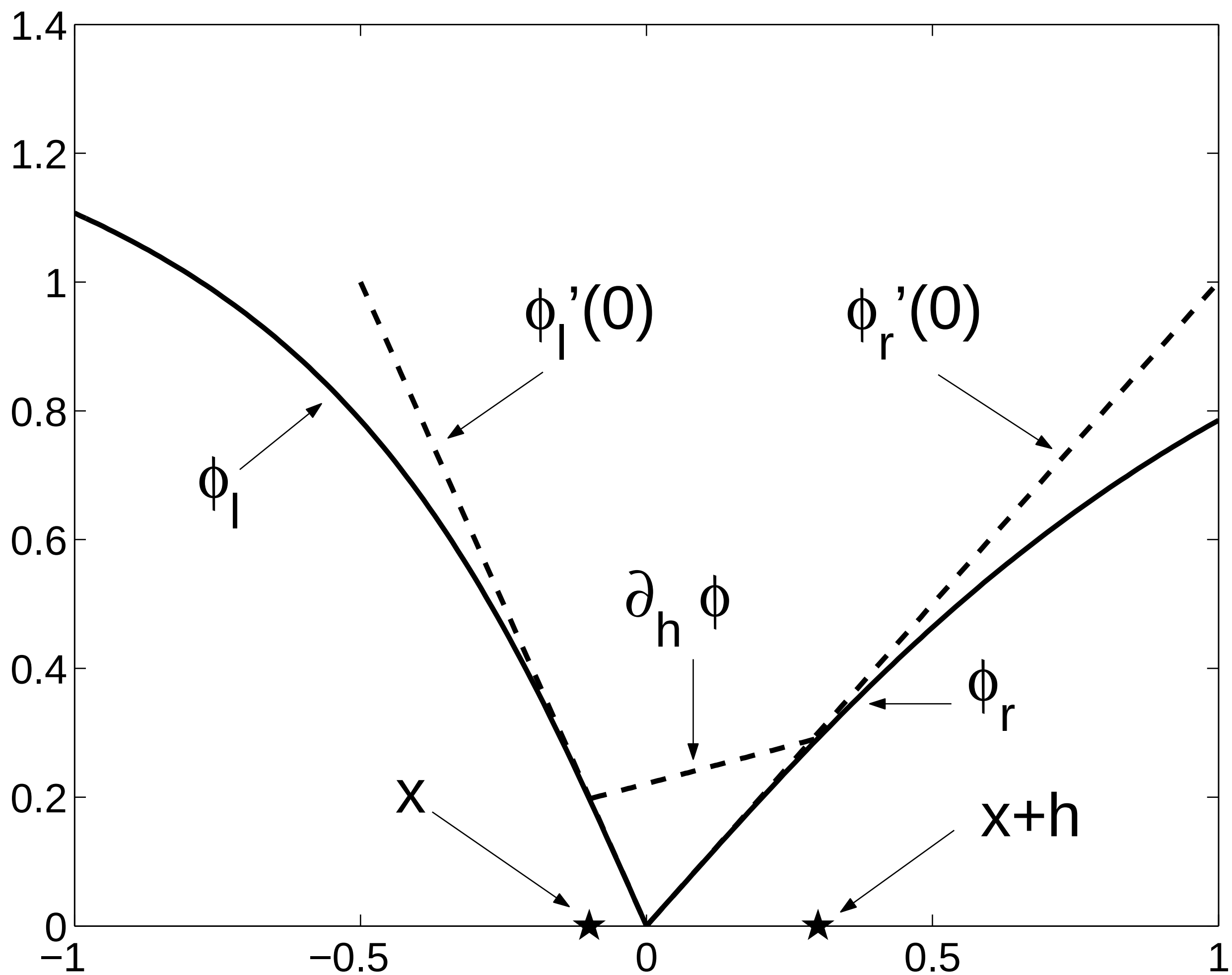
For Lipschitz functions:

$$\partial_h \phi(x) \in \partial \phi(\bar{x}) + O(h)$$

where $|x - \bar{x}| \leq h$.
Same story for scalar constitutive laws in PDEs.
If you differentiate in coordinate directions!

Difference approximation accuracy

$\phi_l'(0) + O(h) \leq \partial_h \phi(x) \leq \phi_r'(0) + O(h)$, so $\partial_h \phi(x) \in \partial \phi(0) + O(h)$



Semismoothness

A Lipschitz function F is semismooth (Mifflin, Pang, Qi) if

$$\lim_{w \to 0, V \in \partial F(x+w)} \frac{\|F(x+w) - F(x) - Vw\|}{\|w\|} = 0.$$

and semismooth of order p at z if

$$F(z+w) - F(z) - Vw = O(\|w\|^{1+p})$$

for all $w \in R^N$ and $V \in \partial F(x+w)$ as $w \to 0$.
What you need for local convergence of Newton's method.
Piecewise smooth functions are semismooth of order 1.

Why semismoothness?

If

- F semismooth of order p,
- $F(x^*) = 0$, and
- everything in $\partial F(x^*)$ uniformly nonsingular,
- x_c near x^*,

then if

$$x_+ = x_c - V^{-1}F(x_c), \text{ where } V \in \partial F(x_c),$$

you get fast local convergence

$$\|x_+ - x^*\| = O(\|x_c - x^*\|^{1+p}).$$

Convergence Proof, $e = x - x^*$

Semismoothness ($z = x^*, w = e_c, z + w = x_c$) implies

$$F(x_c) - Ve_c = O(\|e_c\|^{1+p})$$

Subtract x^* from both sides of

$$x_+ = x_c - V^{-1}F(x_c),$$

to get

$$e_+ = e_c - V^{-1}F(x_c) = e_c - e_c + O(\|e_c\|^{1+p}) = O(\|e_c\|^{1+p}).$$

Things get more complicated if x_c is far from x^*.
Armijo may fail.

Formulation of Ψtc

$$x_{n+1} = x_n + s_n$$

where

$$\|(\delta_n^{-1} D + V(x_n)) s_n + F(x_n)\| \le \eta_n \|F(x_n)\|$$

and

$$V(x) \in \partial F(\overline{x}) + O(h), \|x - \overline{x}\| \le h.$$

Local Convergence: $e_n = x_n - x^* \to 0$

Once close, grow the time step and get fast convergence.
If $\delta_{max} = \infty$

- F semismooth of order 1.
- $F(x^*) = 0$. Everything in $\partial F(x^*)$ nonsingular.
- $\|(D + \delta V(x))^{-1} D\| \leq 1/(1 + \beta\delta)$, for all $\delta > 0$.
- x_0 sufficiently near x^*.
- h sufficiently small.

then $\delta_n \to \infty$ and

$$\|e_{n+1}\| = O(\|e_n\|^2 + (\eta_n + \delta_n^{-1})\|e_n\| + h).$$

Early stagnation comes from the difference.

Stable steady state

$$Dx' = F(x), x(0) = x_0$$

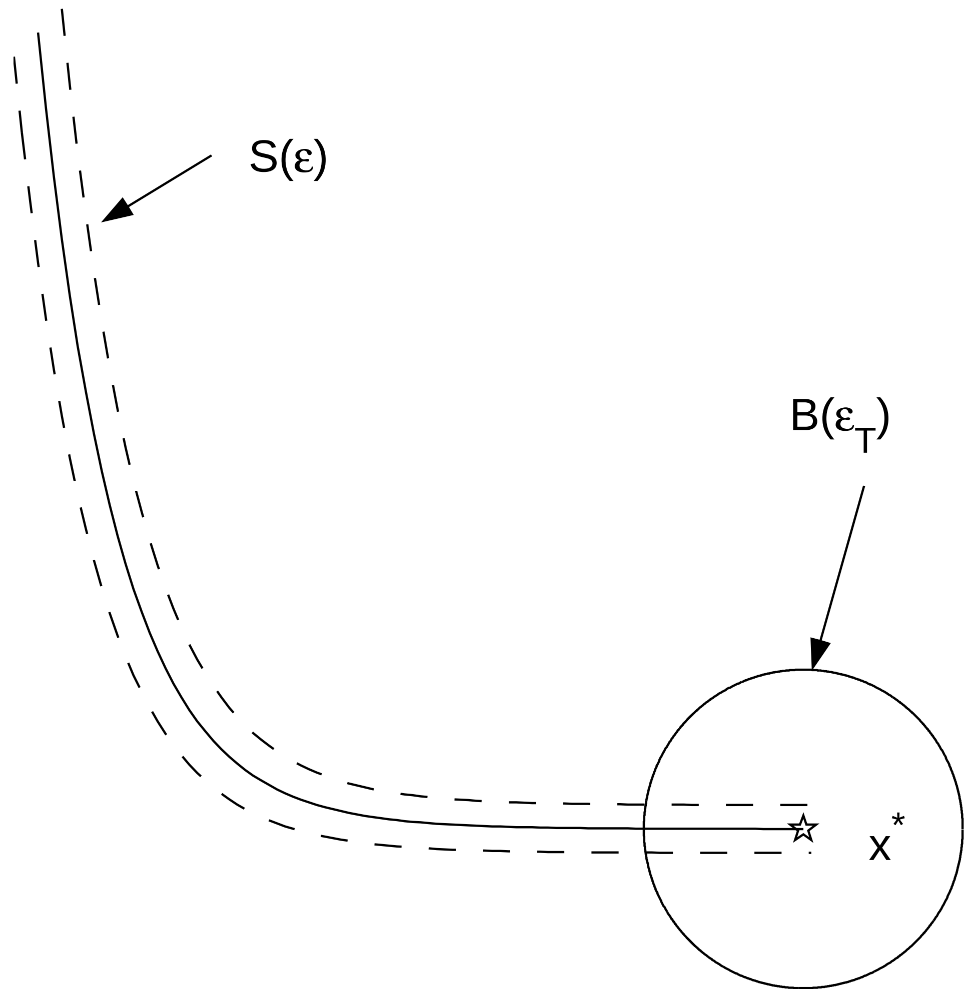
has consistent initial data and

$$x(t) \rightarrow x^* \text{ as } t \rightarrow \infty$$

Iteration confined to a neighborhood of the trajectory $x(t) : t > 0$.

$$S(\varepsilon) = \{z \mid \inf_{t \geq 0} \|z - x(t)\| \leq \varepsilon\}.$$

Iterations hug trajectory



Assumptions in $S(\varepsilon)$

- $(\delta^{-1}D + V(x))$ is uniformly bounded and well-conditioned.
- $V_{vv}(x)$ is uniformly bounded and well conditioned.

We partition V consistently with F.

$$F(x) = \begin{pmatrix} f(u,v) \\ g(u,v) \end{pmatrix} \text{ and } V(x) = \begin{pmatrix} V_{uu} & V_{uv} \\ V_{vu} & V_{vv} \end{pmatrix}.$$

Bottom line: $x_n \to x^*$, $\delta_n \to \infty$, everything works.

Example

$$-u_{zz} + \lambda \max(0,u)^p = 0$$

$$z \in (0,1), u(0) = u(1) = 0,$$

where $p \in (0,1)$.
Reformulate as a DAE to make the nonlinearity Lipschitz.
Let

$$v = \begin{cases} u^p & \text{if } u \geq 0 \\ u & \text{if } u < 0 \end{cases}$$

Reformulation

Set $x = (u,v)^T$ and solve

$$F(x) = \left(\begin{array}{c} f(u,v) \\ g(u,v) \end{array} \right) = \left(\begin{array}{c} -u_{zz} + \lambda \max(0,v) \\ u - \omega(v) \end{array} \right) = 0,$$

The nonlinearity is

$$\omega(v) = \begin{cases} v^{1/p} & \text{if } v \geq 0 \\ v & \text{if } v < 0 \end{cases}$$

DAE Dynamics

$$D\begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} u' \\ 0 \end{pmatrix}$$

$$= -\begin{pmatrix} f(u,v) \\ g(u,v) \end{pmatrix} = -F(x), \quad x(0) = x_0,$$

Why not ODE dynamics?

Original time-dependent problem is

$$u_t = u_{zz} - \lambda \max(0, u)^p.$$

Applying Ψtc to

$$v_t = u - \omega(v)$$

rather than using $u - \omega(v) = 0$ as an algebraic constraint

- adds non-physical time dependence,
- changes the problem, and
- doesn't work.

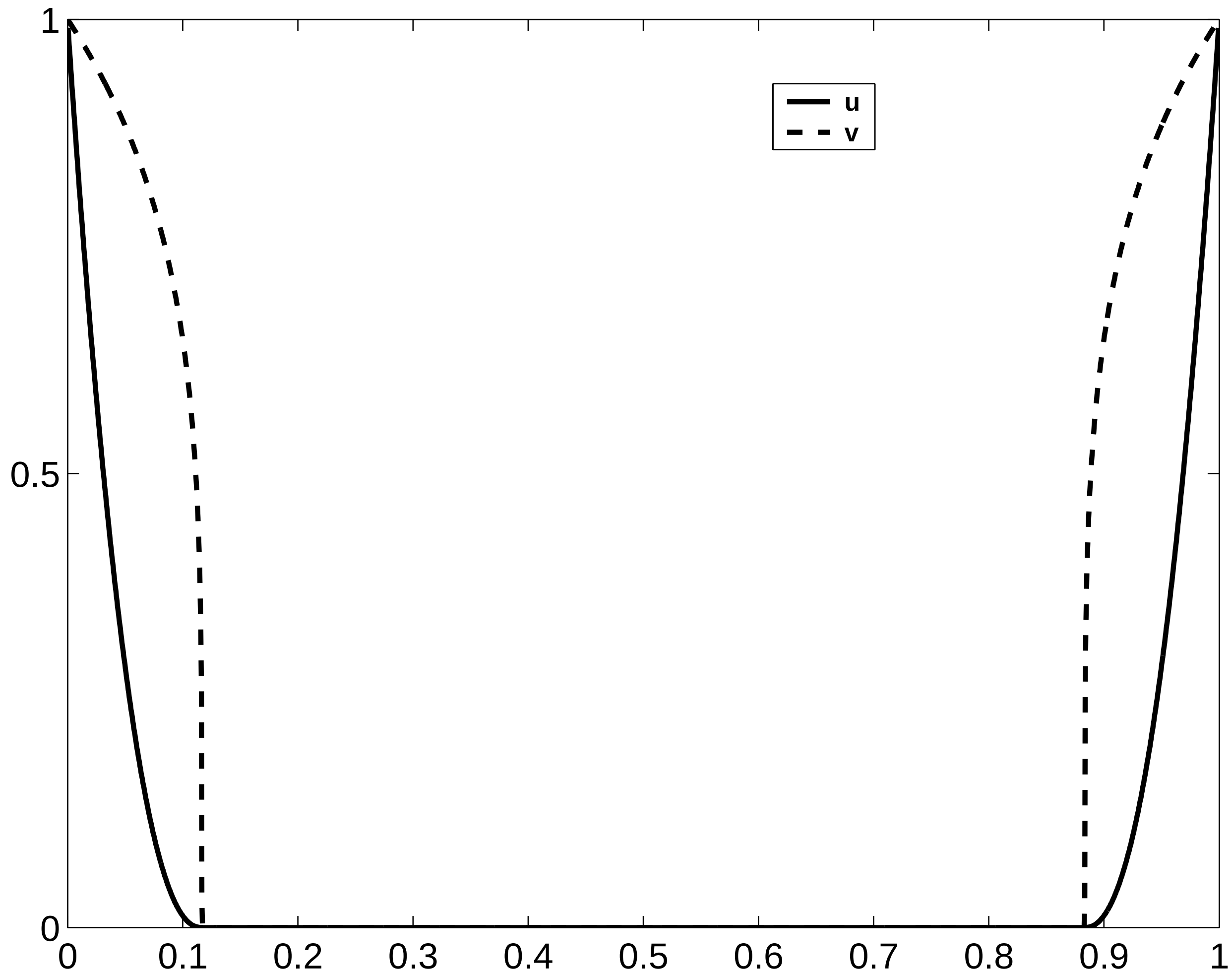
Parameters

- $p = .1$ and $\lambda = 200$. Leads to "dead core".
- $\delta_0 = 1.0$, $\delta_{max} = 10^6$.
- Spatial mesh size $\delta_z = 1/2048$; discrete Laplacian L_{δ_z}
- Terminate nonlinear iteration when either

$$\|F(x_n)\|/\|F(x_0)\| < 10^{-13} \text{ or } \|s_n\| < 10^{-10}.$$

Step is an accurate estimate of error (semismoothness).

Solution



Analytic ∂F

$$
\begin{aligned}
F(x) &= \begin{pmatrix} f(u,v) \\ g(u,v) \end{pmatrix} \\
&= \begin{pmatrix} -L_{\delta_z} u \\ u - v - max(0, v^{1/p}) \end{pmatrix} + \begin{pmatrix} \lambda \\ 1 \end{pmatrix} \max(0,v).
\end{aligned}
$$

Since

$$
\partial \max(0,v) = \begin{cases} 0, & \text{if } v < 0 \\ [0,1], & \text{if } v = 0 \\ 1, & \text{if } v > 0, \end{cases}
$$

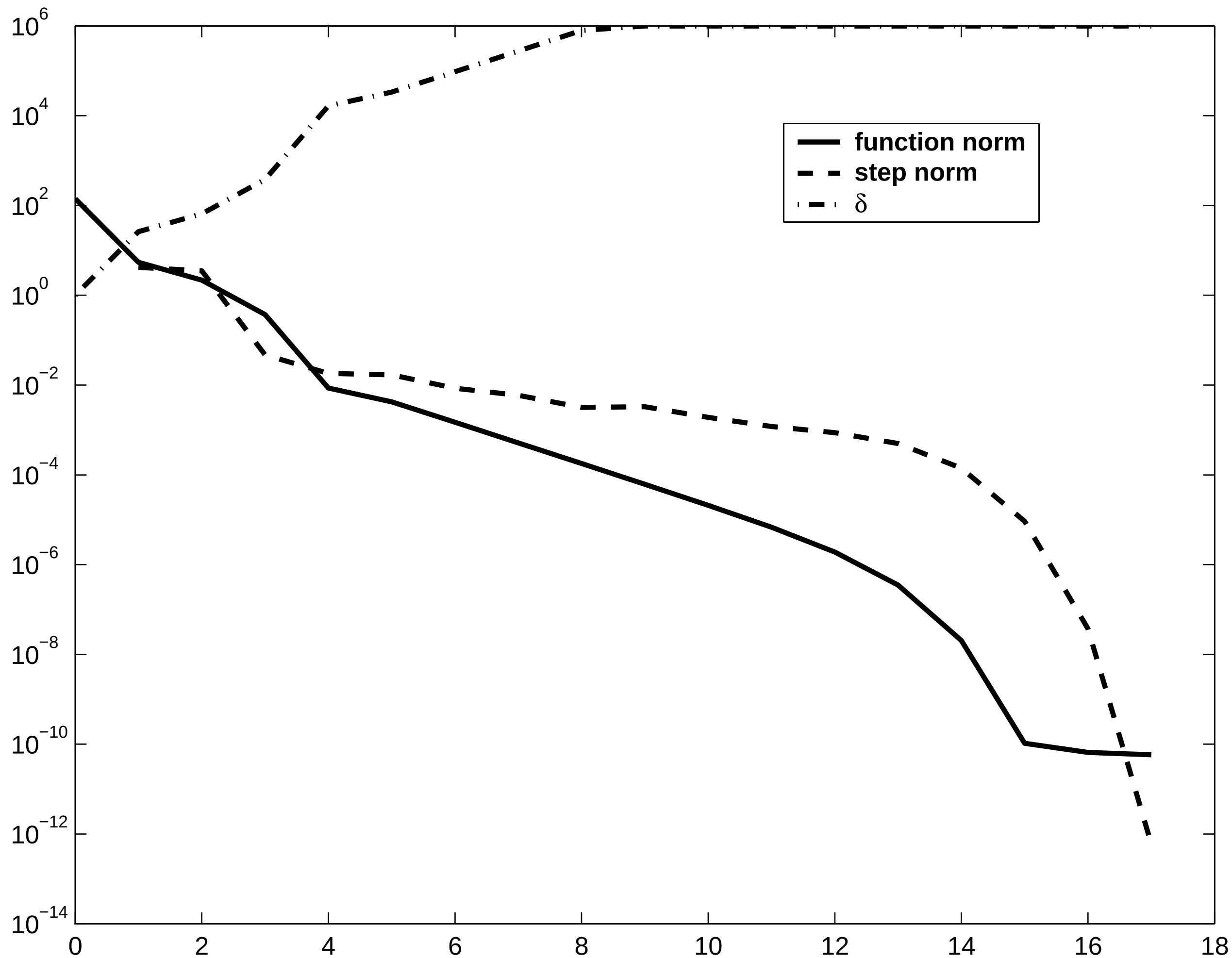
we get ...

∂F

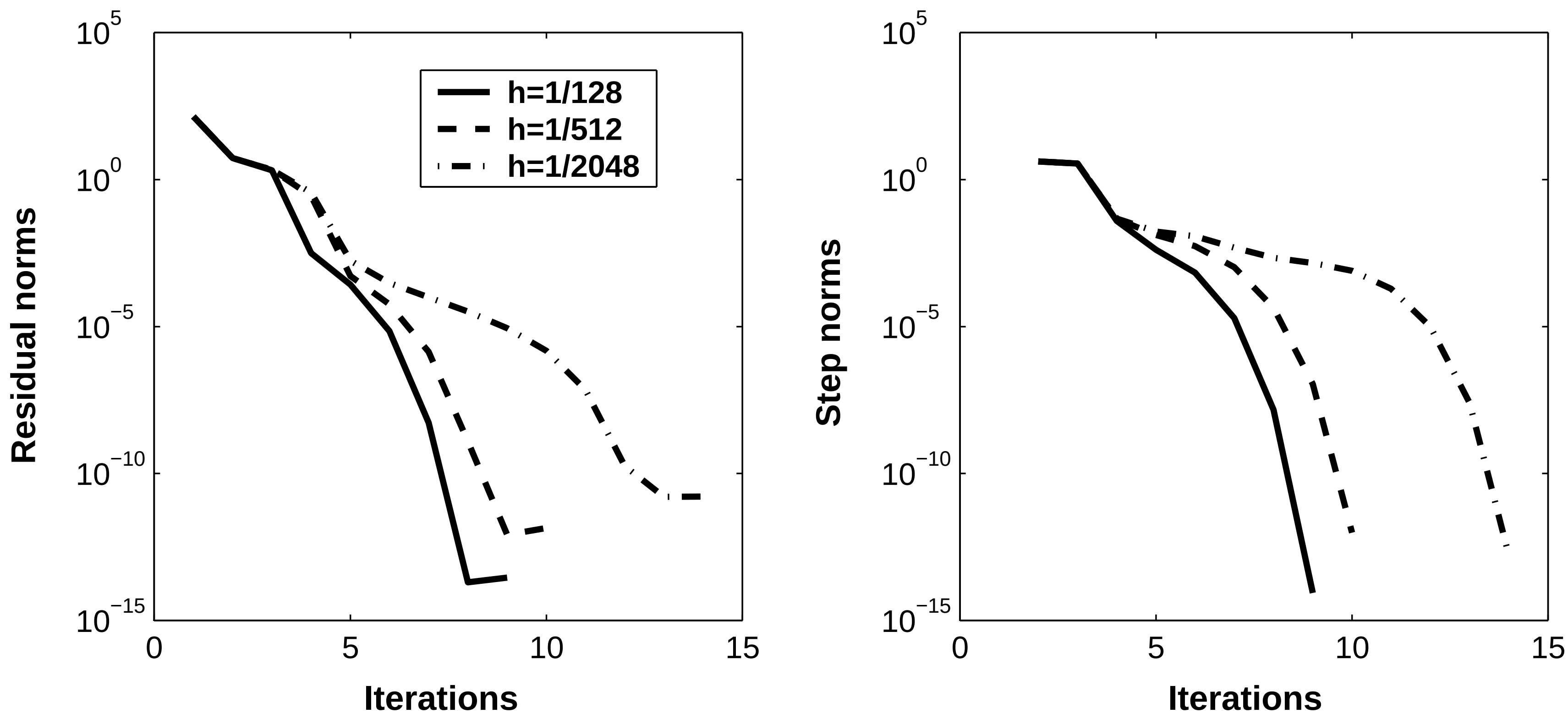
$$\partial F = \begin{pmatrix} -L_{\delta_z} & 0 \\ 1 & -1-(1/p)\max(0, v^{(1-p)/p}) \end{pmatrix}$$

$$+\begin{pmatrix} 0 & \lambda \\ 0 & 1 \end{pmatrix} \partial \max(0, v).$$

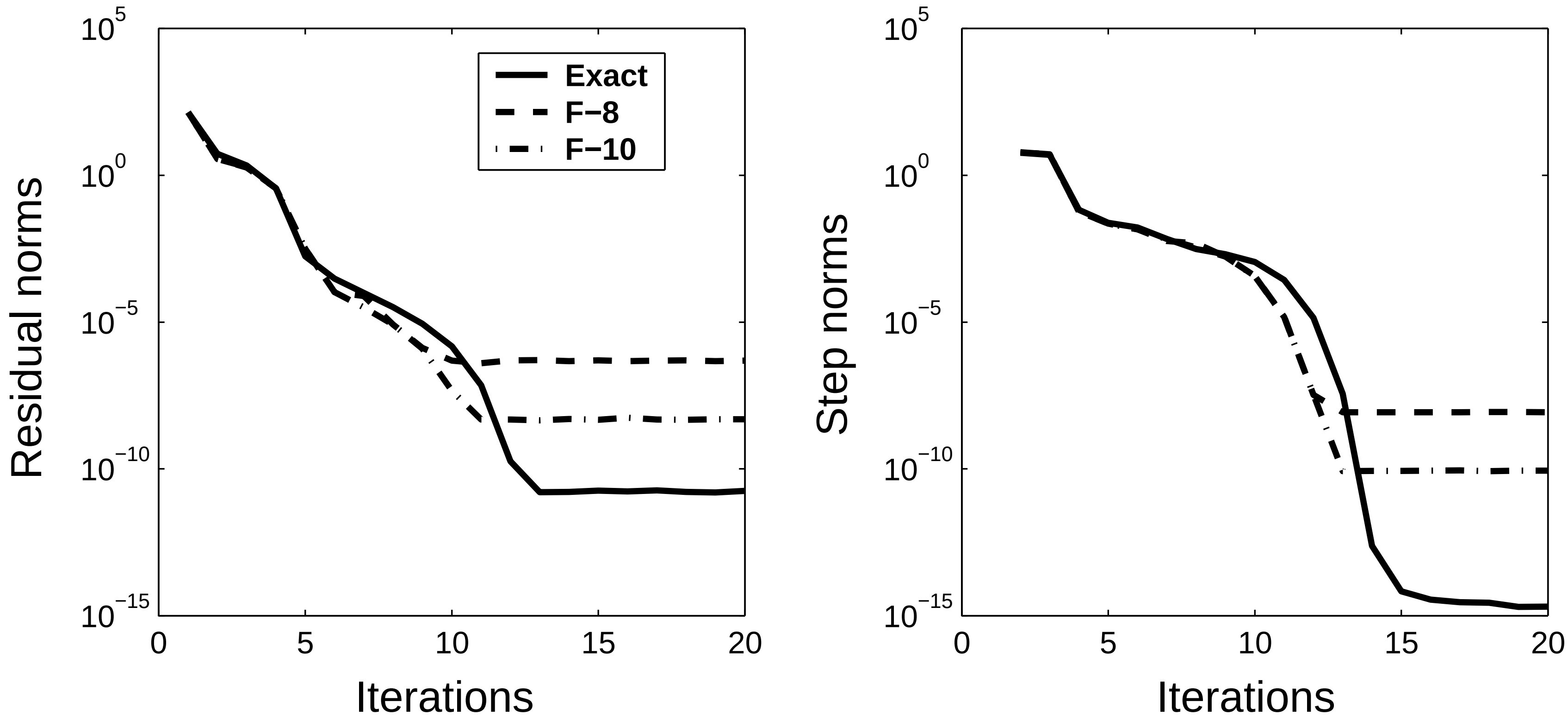
Convergence



Mesh Dependence



Forward Difference ∂F



Optimal difference increment

Let ε_F be floating point roundoff. Include this and

$$V(x) \in \partial F(\overline{x}) + O(h + \varepsilon_F / h)$$

So, if $\|e_n\| = \sqrt{h}$, then

$$\begin{aligned} e_{n+1} &= O((h + \varepsilon_F / h)\|e_n\| + \|e_n\|^2 + h) \\ &= O\left(\frac{\varepsilon_F}{h^{1/2}} + h\right) \end{aligned}$$

which is minimized if $h = O(\varepsilon_F^{2/3}) \approx 10^{-10}$ in IEEE.

Conclusions

- Ψtc can help if Newton-Armijo fails
- Generalized derivatives can be used in Ψtc
- Difference approximations work well with care
  Scalar functions and substitution operators
  Differentiate in coordinate directions
- Finite-difference Newton-Krylov needs more structure (in the works)
- Stagnation tied to difference increment
- Many applications