Composing Nonlinear Solvers

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Numerical Methods for
Large-Scale Nonlinear Problems and Their Applications
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Programming with Options

ex55: Allen-Cahn problem in 2D

- constant mobility
- triangular elements

Geometric multigrid method for saddle point variational inequalities:

```
./ex55 -ksp_type fgmres -pc_type mg -mg_levels_ksp_type fgmres
-mg_levels_pc_type fieldsplit -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_pc_fieldsplit_type schur -da_grid_x 65 -da_grid_y 65
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition user
-mg_levels_fieldsplit_1_ksp_type gmres -mg_coarse_ksp_type preonly
-mg_levels_fieldsplit_1_pc_type none   -mg_coarse_pc_type svd
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor    -pc_mg_levels 5
-mg_levels_fieldsplit_0_pc_sor_forward -pc_mg_galerkin
-snes_vi_monitor -ksp_monitor_true_residual -snes_atol 1.e-11
-mg_levels_ksp_monitor -mg_levels_fieldsplit_ksp_monitor
-mg_levels_ksp_max_it 2 -mg_levels_fieldsplit_ksp_max_it 5
```

Programming with Options

ex55: Allen-Cahn problem in 2D

Run flexible GMRES with 5 levels of multigrid as the preconditioner

```
./ex55 -ksp_type fgmres -pc_type mg -pc_mg_levels 5
  -da_grid_x 65 -da_grid_y 65
```

Use the Galerkin process to compute the coarse grid operators

```
-pc_mg_galerkin
```

Use SVD as the coarse grid saddle point solver

```
-mg_coarse_ksp_type preonly -mg_coarse_pc_type svd
```

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Programming with Options

ex55: Allen-Cahn problem in 2D

Smoother: Flexible GMRES (2 iterates) with a Schur complement PC

```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```

Schur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

Programming with Options

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```

Magma FAS Options

Top level

```
-snes_monitor -snes_converged_reason
-snes_type fas -snes_fas_type full -snes_fas_levels 4
 -fas_levels_3_snes_monitor -fas_levels_3_snes_converged_reason
  -fas_levels_3_snes_atol 1.0e-9 -fas_levels_3_snes_max_it 2
  -fas_levels_3_snes_type newtonls -fas_levels_3_snes_linesearch_type bt
  -fas_levels_3_snes_fd_color -fas_levels_3_snes_fd_color_use_mat
  -fas_levels_3_ksp_rtol 1.0e-10 -mat_coloring_type greedy
  -fas_levels_3_ksp_gmres_restart 50 -fas_levels_3_ksp_max_it 200
   -fas_levels_3_pc_type fieldsplit
    -fas_levels_3_pc_fieldsplit_0_fields 0,2
    -fas_levels_3_pc_fieldsplit_1_fields 1
    -fas_levels_3_pc_fieldsplit_type schur
     -fas_levels_3_pc_fieldsplit_schur_precondition selfp
     -fas_levels_3_pc_fieldsplit_schur_factorization_type full
      -fas_levels_3_fieldsplit_0_pc_type lu
      -fas_levels_3_fieldsplit_pressure_ksp_rtol 1.0e-9
       -fas_levels_3_fieldsplit_pressure_pc_type gamg
       -fas_levels_3_fieldsplit_pressure_ksp_gmres_restart 100
       -fas_levels_3_fieldsplit_pressure_ksp_max_it 200
```

Magma FAS Options

2nd level

```
-fas_levels_2_snes_monitor -fas_levels_2_snes_converged_reason
 -fas_levels_2_snes_atol 1.0e-9 -fas_levels_2_snes_max_it 2
 -fas_levels_2_snes_type newtonls -fas_levels_2_snes_linesearch_type bt
 -fas_levels_2_snes_fd_color -fas_levels_2_snes_fd_color_use_mat
 -fas_levels_2_ksp_rtol 1.0e-10 -fas_levels_2_ksp_gmres_restart 50
 -fas_levels_2_pc_type fieldsplit
  -fas_levels_2_pc_fieldsplit_0_fields 0,2
  -fas_levels_2_pc_fieldsplit_1_fields 1
  -fas_levels_2_pc_fieldsplit_type schur
   -fas_levels_2_pc_fieldsplit_schur_precondition selfp
   -fas_levels_2_pc_fieldsplit_schur_factorization_type full
    -fas_levels_2_fieldsplit_0_pc_type lu
    -fas_levels_2_fieldsplit_pressure_ksp_rtol 1.0e-9
     -fas_levels_2_fieldsplit_pressure_pc_type gamg
     -fas_levels_2_fieldsplit_pressure_ksp_gmres_restart 100
     -fas_levels_2_fieldsplit_pressure_ksp_max_it 200
```

Magma FAS Options

1st level

```
-fas_levels_1_snes_monitor -fas_levels_1_snes_converged_reason
 -fas_levels_1_snes_atol 1.0e-9
 -fas_levels_1_snes_type newtonls -fas_levels_1_snes_linesearch_type bt
 -fas_levels_1_snes_fd_color -fas_levels_1_snes_fd_color_use_mat
 -fas_levels_1_ksp_rtol 1.0e-10 -fas_levels_1_ksp_gmres_restart 50
 -fas_levels_1_pc_type fieldsplit
  -fas_levels_1_pc_fieldsplit_0_fields 0,2
  -fas_levels_1_pc_fieldsplit_1_fields 1
  -fas_levels_1_pc_fieldsplit_type schur
   -fas_levels_1_pc_fieldsplit_schur_precondition selfp
   -fas_levels_1_pc_fieldsplit_schur_factorization_type full
    -fas_levels_1_fieldsplit_0_pc_type lu
    -fas_levels_1_fieldsplit_pressure_ksp_rtol 1.0e-9
    -fas_levels_1_fieldsplit_pressure_pc_type gamg
```

Magma FAS Options

Coarse level

```
-fas_coarse_snes_monitor -fas_coarse_snes_converged_reason
 -fas_coarse_snes_atol 1.0e-9
 -fas_coarse_snes_type newtonls -fas_coarse_snes_linesearch_type bt
 -fas_coarse_snes_fd_color -fas_coarse_snes_fd_color_use_mat
 -fas_coarse_ksp_rtol 1.0e-10 -fas_coarse_ksp_gmres_restart 50
 -fas_coarse_pc_type fieldsplit
  -fas_coarse_pc_fieldsplit_0_fields 0,2
  -fas_coarse_pc_fieldsplit_1_fields 1
  -fas_coarse_pc_fieldsplit_type schur
   -fas_coarse_pc_fieldsplit_schur_precondition selfp
   -fas_coarse_pc_fieldsplit_schur_factorization_type full
    -fas_coarse_fieldsplit_0_pc_type lu
    -fas_coarse_fieldsplit_pressure_ksp_rtol 1.0e-9
    -fas_coarse_fieldsplit_pressure_pc_type gamg
```

Outline

Abstract System

Out prototypical nonlinear equation is:

$$\mathbf{F}(\mathbf{x}) = \mathbf{b}$$

and we define the residual as

$$\mathbf{r}(\mathbf{x}) = \mathbf{F}(\mathbf{x}) - \mathbf{b}$$

Abstract System

Out prototypical nonlinear equation is:

$$\mathbf{F}(\mathbf{x}) = \mathbf{b}$$

and we define the (linear) residual as

$$\mathbf{r}(\mathbf{x}) = A\mathbf{x} - \mathbf{b}$$

Linear Left Preconditioning

The modified equation becomes

$$P^{-1}(A\mathbf{x} - \mathbf{b}) = 0 \tag{1}$$

Linear Left Preconditioning

The modified defect correction equation becomes

$$P^{-1}\left(A\mathbf{x}_i - \mathbf{b}\right) = \mathbf{x}_{i+1} - \mathbf{x}_i \tag{2}$$

Additive Combination

The linear iteration

$$\mathbf{x}_{i+1} = \mathbf{x}_i - (\alpha P^{-1} + \beta Q^{-1})(A\mathbf{x}_i - \mathbf{b}) \tag{3}$$

becomes the nonlinear iteration

Additive Combination

The linear iteration

$$\mathbf{x}_{i+1} = \mathbf{x}_i - (\alpha P^{-1} + \beta Q^{-1})\mathbf{r}_i \tag{4}$$

becomes the nonlinear iteration

Additive Combination

The linear iteration

$$\mathbf{x}_{i+1} = \mathbf{x}_i - (\alpha P^{-1} + \beta Q^{-1})\mathbf{r}_i \tag{4}$$

becomes the nonlinear iteration

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha(\mathcal{N}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}) - \mathbf{x}_i) + \beta(\mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}) - \mathbf{x}_i) \tag{5}$$

Nonlinear Left Preconditioning

From the additive combination, we have

$$P^{-1}\mathbf{r} \Longrightarrow \mathbf{x}_i - \mathcal{N}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}) \tag{6}$$

so we define the preconditioning operation as

$$\mathbf{r}_L \equiv \mathbf{x} - \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}) \tag{7}$$

Multiplicative Combination

The linear iteration

$$\mathbf{x}_{i+1} = \mathbf{x}_i - (P^{-1} + Q^{-1} - Q^{-1}AP^{-1})\mathbf{r}_i \qquad (8)$$

becomes the nonlinear iteration

Multiplicative Combination

The linear iteration

$$\mathbf{x}_{i+1/2} = \mathbf{x}_i - P^{-1}\mathbf{r}_i \tag{9}$$

$$\mathbf{x}_i = \mathbf{x}_{i+1/2} - Q^{-1}\mathbf{r}_{i+1/2} \tag{10}$$

becomes the nonlinear iteration

Multiplicative Combination

The linear iteration

$$\mathbf{x}_{i+1/2} = \mathbf{x}_i - P^{-1}\mathbf{r}_i \tag{9}$$

$$\mathbf{x}_i = \mathbf{x}_{i+1/2} - Q^{-1}\mathbf{r}_{i+1/2} \tag{10}$$

becomes the nonlinear iteration

$$\mathbf{x}_{i+1} = \mathcal{M}(\mathbf{F}, \mathcal{N}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}), \mathbf{b}) \tag{11}$$

Nonlinear Right Preconditioning

For the linear case, we have

$$AP^{-1}\mathbf{y} = \mathbf{b} \tag{12}$$

$$\mathbf{x} = P^{-1}\mathbf{y} \tag{13}$$

so we define the preconditioning operation as

$$\mathbf{y} = \mathcal{M}(\mathbf{F}(\mathcal{N}(\mathcal{F}, \cdot, \mathbf{b})), \mathbf{x}_i, \mathbf{b}) \tag{14}$$

$$\mathbf{x} = \mathcal{N}(\mathbf{F}, \mathbf{y}, \mathbf{b}) \tag{15}$$

Nonlinear Preconditioning

Type	Sym	Statement	Abbreviation
Additive	$+$	$\mathbf{x} + \alpha(\mathcal{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}) - \mathbf{x})$ $+ \beta(\mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}) - \mathbf{x})$	$\mathcal{M} + \mathcal{N}$
Multiplicative	$*$	$\mathcal{M}(\mathbf{F}, \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{b})$	$\mathcal{M} * \mathcal{N}$
Left Prec.	$-_L$	$\mathcal{M}(\mathbf{x} - \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}, \mathbf{b})$	$\mathcal{M} -_L \mathcal{N}$
Right Prec.	$-_R$	$\mathcal{M}(\mathbf{F}(\mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b})), \mathbf{x}, \mathbf{b})$	$\mathcal{M} -_R \mathcal{N}$
Inner Lin. Inv.	$\backslash$	$\mathbf{y} = J(\mathbf{x})^{-1}\mathbf{r}(\mathbf{x}) = \mathrm{K}(J(\mathbf{x}), \mathbf{y}_0, \mathbf{b})$	$\mathcal{N} \backslash \mathrm{K}$

Composing Scalable Nonlinear Algebraic Solvers (Brune et al. 2015)

Outline

Additive Composition

We can represent the additive update rule

$$\vec{x}_{i+1} = \vec{x}_i + \alpha(\mathcal{M}(\mathcal{F}, \vec{x}_i,) - \vec{x}_i) + \beta(\mathcal{N}(\mathcal{F}, \vec{x}_i,) - \vec{x}_i)$$

as

$$\vec{x}_{i+1} = (\mathcal{M} + \mathcal{N})(\mathcal{F}, \vec{x}_i,)$$

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as

$$\vec{x}_{i+1} = (\mathcal{M} + \mathcal{N})(\mathcal{F}, \vec{x}_i,)$$

Additive Composition

If $\alpha = \beta = 1$, this has an identity operation 0 (the identity map),

$$\begin{aligned}\vec{x}_{i+1} &= \vec{x}_i + \alpha(\mathcal{M}(\mathcal{F}, \vec{x}_i,) - \vec{x}_i) + \beta(0(\mathcal{F}, \vec{x}_i,) - \vec{x}_i) \\ &= \vec{x}_i + (\mathcal{M}(\mathcal{F}, \vec{x}_i,) - \vec{x}_i) + \left(\vec{x}_i - \vec{x}_i\right) \\ &= \mathcal{M}(\mathcal{F}, \vec{x}_i,)\end{aligned}$$

so that $(\mathcal{M}, +)$ is an abelian group.

Multiplicative Composition

We can represent the multiplicative update rule

$$\vec{x}_{i+1} = \mathcal{M}(\mathcal{F}, \mathcal{N}(\mathcal{F}, \vec{x}_i,),)$$

as

$$\vec{x}_{i+1} = (\mathcal{M} * \mathcal{N})(\mathcal{F}, \vec{x}_i,)$$

which is clearly associative.

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Algebraic Structure

If we look at the distributive case,

$$\vec{x}_{i+1} = ((\mathcal{M} + \mathcal{N}) * \mathcal{Q})(\mathcal{F}, \vec{x}_i,)$$

we get the update rule

$$\begin{aligned}\vec{x}_{i+1} = \vec{x}_i &+ \alpha(\mathcal{M}(\mathcal{F}, \mathcal{Q}(\mathcal{F}, \vec{x}_i,),) - \vec{x}_i) \\ &+ \beta(\mathcal{N}(\mathcal{F}, \mathcal{Q}(\mathcal{F}, \vec{x}_i,),) - \vec{x}_i)\end{aligned}$$

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$$\vec{x}_{i+1} = ((\mathcal{M} + \mathcal{N}) * \mathcal{Q})(\mathcal{F}, \vec{x}_i,)$$

which we can write as

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Note however that

$$\mathcal{Q} * (\mathcal{M} + \mathcal{N}) \neq \mathcal{Q} * \mathcal{M} + \mathcal{Q} * \mathcal{N}$$

which means $(\mathcal{M}, +, *)$ is a near ring.

Algebraic Structure

If we combine it using our left NPC operation

$$\vec{x}_{i+1} = ((\mathcal{M} + \mathcal{N}) -_L \mathcal{Q})(\mathcal{F}, \vec{x}_i,)$$

we get the update rule

$$\begin{aligned}\vec{x}_{i+1} = \vec{x}_i &+ \alpha(\mathcal{M}(\vec{x} - \mathcal{Q}(\mathcal{F}, \vec{x}_i,), \vec{x}_i,) - \vec{x}_i) \\ &+ \beta(\mathcal{N}(\vec{x} - \mathcal{Q}(\mathcal{F}, \vec{x}_i,), \vec{x}_i,) - \vec{x}_i)\end{aligned}$$

Algebraic Structure

If we combine it using our left NPC operation

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which we can write as

$$\vec{x}_{i+1} = (\mathcal{M} -_L \mathcal{Q} + \mathcal{N} -_L \mathcal{Q})(\mathcal{F}, \vec{x}_i,)$$

we we again have a near ring.

Algebraic Structure

In the same way, we can combine it with our right NPC operation

$$\vec{x}_{i+1} = ((\mathcal{M} + \mathcal{N}) -_R \mathcal{Q})(\mathcal{F}, \vec{x}_i,)$$

and get the update rule

$$\begin{aligned}\vec{x}_{i+1} = \vec{x}_i &+ \alpha(\mathcal{M}(\mathcal{F}(\mathcal{Q}(\mathcal{F}, \vec{x}_i,)), \vec{x}_i,) - \vec{x}_i) \\ &+ \beta(\mathcal{N}(\mathcal{F}(\mathcal{Q}(\mathcal{F}, \vec{x}_i,)), \vec{x}_i,) - \vec{x}_i)\end{aligned}$$

Algebraic Structure

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$$\vec{x}_{i+1} = (\mathcal{M} -_R \mathcal{Q} + \mathcal{N} -_R \mathcal{Q})(\mathcal{F}, \vec{x}_i,)$$

we we again have a near ring.

Polynomial solution through decomposition

Let us solve

$$x^8 - 4x^6 - 11x^4 + 30x^2 + 56 = 0$$

which can be decomposed

$$\left(x^4 - 4x^3 - 11x^2 + 30x + 56\right) \circ x^2 = 0$$
$$\left(x^2 - 15x + 56\right) \circ \left(x^2 - 2x\right) \circ x^2 = 0.$$

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$$\left(x^2 - 15x + 56\right) \circ \left(x^2 - 2x\right) \circ x^2 = 0.$$

We solve the first equation, to get

$$x_{00} = 7 \qquad x_{01} = 8,$$

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and then solve

$$x^2 - 2x = 7 \text{ or } 8,$$

to get

$$x_{10} = 1 + 2\sqrt{2} \qquad x_{11} = 1 - 2\sqrt{2} \qquad x_{12} = 4 \qquad x_{13} = -2.$$

Polynomial solution through decomposition

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which can be decomposed

$$\left(x^4 - 4x^3 - 11x^2 + 30x + 56\right) \circ x^2 = 0$$
$$\left(x^2 - 15x + 56\right) \circ \left(x^2 - 2x\right) \circ x^2 = 0.$$

At the end, we have $x^2 = x_{1j}$, so that

$$x_{0,1,2,3} = \pm\sqrt{1 \pm 2\sqrt{2}}$$
$$x_{5,6} = \pm 2$$
$$x_{7,8} = \pm i\sqrt{2}.$$

There is an $\mathcal{O}(d \ln d)$ algorithm for finding the unique decomposition.

Outline

Outline

Nonlinear Richardson

procedure NRICH($\mathbf{F}, \mathbf{x}_i, \mathbf{b}$)
$\mathbf{d} := -\mathbf{r}(\mathbf{x}_i)$
$\quad \mathbf{x}_{i+1} = \mathbf{x}_i + \lambda \mathbf{d}$ ▷ λ determined by line search
end procedure
return $\mathbf{x}_{i+1}$

L Adds line search to $\mathcal{N}$

R Uses $\mathcal{N}$ to improve search direction

Nonlinear Richardson

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R Uses $\mathcal{N}$ to improve search direction

Line Search

Equivalent to NRICH $-_L \mathcal{N}$:

$$\text{NRICH} -_L \mathcal{N}$$

Line Search

Equivalent to NRICH $-_L \mathcal{N}$:

$$\text{NRICH} -_L \mathcal{N}$$
$$\text{NRICH}(\mathbf{x} - \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}, \mathbf{b})$$

Line Search

Equivalent to NRICH $-_L \mathcal{N}$:

$$
\begin{aligned}
\text{NRICH} &-_L \mathcal{N} \\
\text{NRICH}(\mathbf{x} &- \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}, \mathbf{b}) \\
\mathbf{x}_{i+1} &= \mathbf{x}_i - \lambda \mathbf{r}_L
\end{aligned}
$$

Line Search

Equivalent to NRICH $-_L \mathcal{N}$:

$$\begin{aligned} &\text{NRICH} -_L \mathcal{N} \\ &\text{NRICH}(\mathbf{x} - \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}, \mathbf{b}) \\ \mathbf{x}_{i+1} &= \mathbf{x}_i - \lambda \mathbf{r}_L \\ \mathbf{x}_{i+1} &= \mathbf{x}_i + \lambda(\mathcal{N}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}) - \mathbf{x}_i) \end{aligned}$$

Line Search

Equivalent to NRICH $-_L \mathcal{N}$:

$$\begin{aligned}
\text{NRICH} -_L \mathcal{N} \\
\text{NRICH}(\mathbf{x} - \mathcal{N}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}, \mathbf{b}) \\
\mathbf{x}_{i+1} = \mathbf{x}_i - \lambda \mathbf{r}_L \\
\mathbf{x}_{i+1} = \mathbf{x}_i + \lambda(\mathcal{N}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}) - \mathbf{x}_i)
\end{aligned}$$

Let R_1 be Richardson iteration with a unit step scaling (no damping). Then we have

$$\mathcal{M} -_L \mathbb{R}_1 = \mathcal{M} \qquad \mathbb{R}_1 -_L \mathcal{M} = \mathcal{M} \tag{16}$$

so that $\mathbb{R}_1$ is the identity operation for left preconditioning, whereas for right preconditioning this is just the identity map.

Outline

3 Solvers
- Richardson
- Newton
- Generalized Broyden

Newton-Krylov

1: **procedure** $\mathcal{N}\backslash\mathrm{K}(\mathbf{F}, \mathbf{x}_i, \mathbf{b})$
2: $\mathbf{d} = J(\mathbf{x}_i)^{-1}\mathbf{r}(\mathbf{x}_i, \mathbf{b})$ ▷ solve by Krylov method
3: $\mathbf{x}_{i+1} = \mathbf{x}_i + \lambda\mathbf{d}$ ▷ λ determined by line search
4: **end procedure**
5: **return** $\mathbf{x}_{i+1}$

Left Preconditioned Newton-Krylov

procedure $\mathcal{N}\backslash\mathrm{K}(\mathbf{x} - \mathcal{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}_i, 0)$

  $\mathbf{d} = \frac{\partial(\mathbf{x}_i - \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}))}{\partial \mathbf{x}_i}^{-1} (\mathbf{x}_i - \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}))$

  $\mathbf{x}_{i+1} = \mathbf{x}_i + \lambda \mathbf{d}$

end procedure

return $\mathbf{x}_{i+1}$

Jacobian Computation

$$\frac{\partial(\mathbf{x} - \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}))}{\mathbf{x}_i} = I - \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b})}{\partial \mathbf{x}_i},$$

Direct differencing would require

- one inner nonlinear iteration

per **Krylov** iteration.

Jacobian Computation

$$\frac{\partial(\mathbf{x} - \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}))}{\mathbf{x}_i} = I - \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b})}{\partial \mathbf{x}_i},$$

Direct differencing would require

- one inner nonlinear iteration

per **Krylov** iteration.

Jacobian Computation

Impractical!

$$\frac{\partial(\mathbf{x} - \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b}))}{\mathbf{x}_i} = I - \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{x}_i, \mathbf{b})}{\partial \mathbf{x}_i},$$

Direct differencing would require

- one inner nonlinear iteration

per **Krylov** iteration.

Jacobian Computation

Approximation for NASM

$$\frac{\partial(\mathbf{x} - \mathcal{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}))}{\partial \mathbf{x}} = \frac{\partial(\mathbf{x} - (\mathbf{x} - \sum_b J_b(\mathbf{x}_b)^{-1}\mathbf{F}_b(\mathbf{x}_b)))}{\partial \mathbf{x}}$$

$$\approx \sum_b J_b(\mathbf{x}_{b*})^{-1} J(\mathbf{x})$$

This would require

- one inner nonlinear iteration
- small number of block solves

per **outer nonlinear** iteration.

Nonlinearly preconditioned inexact Newton algorithms (X.-C. Cai and Keyes 2002)

Right Preconditioned Newton-Krylov

procedure $\mathrm{NK}(\mathbf{F}(\mathcal{M}(\mathbf{F}, \cdot, \mathbf{b})), \mathbf{y}_i, \mathbf{b})$

$\qquad \mathbf{x}_i = \mathcal{M}(\mathbf{F}, \mathbf{y}_i, \mathbf{b})$

$\qquad \mathbf{d} = J(\mathbf{x})^{-1}\mathbf{r}(\mathbf{x}_i)$

$\qquad \mathbf{x}_{i+1} = \mathbf{x}_i + \lambda\mathbf{d}$ $\quad \triangleright$ λ determined by line search

end procedure

return $\mathbf{x}_{i+1}$

Jacobian Computation

First-Order Approximation

Only the action of the original Jacobian is needed at first order:

$$\mathbf{y}_{i+1} = \mathbf{y}_i - \lambda \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i}^{-1} J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))$$

$$\begin{aligned}
\mathcal{M}(\mathbf{F}, \mathbf{y}_{i+1}) &= \mathcal{M}(\mathbf{F}, \mathbf{y}_i - \lambda \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i}^{-1} J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))) \\
&\approx \mathcal{M}(\mathbf{F}, \mathbf{y}_i) \\
&\quad - \lambda \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i} \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i}^{-1} J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))) \\
&= \mathcal{M}(\mathbf{F}, \mathbf{y}_i) - \lambda J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i)) \\
\mathbf{x}_{i+1} &= \mathbf{x}_i - \lambda J(\mathbf{x}_i)^{-1} \mathbf{F}(\mathbf{x}_i)
\end{aligned}$$

$\mathcal{N}\backslash\mathrm{K} -_R \vec{M}$ is equivalent to $\mathcal{N}\backslash\mathrm{K} * \vec{M}$ at first order

A parallel adaptive nonlinear elimination preconditioned inexact Newton method for transonic full

Jacobian Computation

First-Order Approximation

Only the action of the original Jacobian is needed at first order:

$$\mathbf{y}_{i+1} = \mathbf{y}_i - \lambda \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i}^{-1} J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))$$

$$\begin{aligned}
\mathcal{M}(\mathbf{F}, \mathbf{y}_{i+1}) &= \mathcal{M}(\mathbf{F}, \mathbf{y}_i - \lambda \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i}^{-1} J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))) \\
&\approx \mathcal{M}(\mathbf{F}, \mathbf{y}_i) \\
&\quad - \lambda \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i} \frac{\partial \mathcal{M}(\mathbf{F}, \mathbf{y}_i)}{\partial \mathbf{y}_i}^{-1} J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))) \\
&= \mathcal{M}(\mathbf{F}, \mathbf{y}_i) - \lambda J(\mathcal{M}(\mathbf{F}, \mathbf{y}_i))^{-1} \mathbf{F}(\mathcal{M}(\mathbf{F}, \mathbf{y}_i)) \\
\mathbf{x}_{i+1} &= \mathbf{x}_i - \lambda J(\mathbf{x}_i)^{-1} \mathbf{F}(\mathbf{x}_i)
\end{aligned}$$

$\mathcal{N}\backslash\mathrm{K} -_R \vec{M}$ is equivalent to $\mathcal{N}\backslash\mathrm{K} * \vec{M}$ at first order

A parallel adaptive nonlinear elimination preconditioned inexact Newton method for transonic full

Jacobian Computation

Direct Approximation

$$
\begin{aligned}
\mathbf{F}(\mathcal{M}(\mathbf{F},\mathbf{y}_i,\mathbf{b})) &= J(\mathcal{M}(\mathbf{F},\mathbf{y}_i,\mathbf{b}))\frac{\partial\mathcal{M}(\mathbf{F},\mathbf{y}_i,\mathbf{b})}{\partial\mathbf{y}_i}(\mathbf{y}_{i+1}-\mathbf{y}_i) \\
&\approx J(\mathcal{M}(\mathbf{F},\mathbf{y}_i,\mathbf{b}))(\mathcal{M}(\mathbf{F},\mathbf{y}_i+\mathbf{d},\mathbf{b})-\mathbf{x}_i)
\end{aligned}
$$

- Solve for **d**
- Requires inner nonlinear solve for each Krylov iterate
- Needs FGMRES

On nonlinear preconditioners in Newton-Krylov methods for unsteady flows (Birken and Jameson 2010)

Outline

Anderson

1: **procedure** ANDERSON($\mathbf{F}, \mathbf{x}_i, \mathbf{b}$)
2: $\gamma_i = (\mathbf{F}_i^T \mathbf{F}_i)^{-1} \mathbf{F}_i^T \mathbf{r}(\mathbf{x}_i, \mathbf{b})$ ▷ solve LS by SVD
3: $\mathbf{x}_{i+1} = \mathbf{x}_i + \beta \mathbf{r}(\mathbf{x}_i, \mathbf{b}) - (\mathbf{x}_k + \beta \mathbf{F}_k)\gamma_k$
4: **end procedure**
5: **return** $\mathbf{x}_{i+1}$

Iterative procedures for nonlinear integral equations (Anderson 1965)

Generalized Broyden

procedure GB($\mathbf{F}, \mathbf{x}_i, \mathbf{b}$)

  $\gamma_i = (\mathbf{F}_i^T \mathbf{F}_i)^{-1} \mathbf{F}_i^T \mathbf{r}(\mathbf{x}_i, \mathbf{b})$ ▷ solve LS by SVD

  $\mathbf{x}_{i+1} = \mathbf{x}_i - G_0 \mathbf{r}(\mathbf{x}_i, \mathbf{b}) - (\mathbb{X}_k - G_0 \mathbf{F}_k)\gamma_k$

end procedure

return $\mathbf{x}_{i+1}$

Two classes of multisecant methods for nonlinear acceleration (Fang and Saad 2009)

Left Preconditioned Generalized Broyden

1: **procedure** GB($\mathbf{x} - \vec{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}_i, \mathbf{b}$)
2: $\gamma_i = (\mathbf{F}_i^T \mathbf{F}_i)^{-1} \mathbf{F}_i^T (\mathbf{x} - \vec{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}))$ ▷ solve LS by SVD
3: $\mathbf{x}_{i+1} = \mathbf{x}_i - G_0(\mathbf{x} - \vec{M}(\mathbf{F}, \mathbf{x}, \mathbf{b})) - (\mathbb{X}_k - G_0 \mathbf{F}_k)\gamma_k$
4: **end procedure**
5: **return** $\mathbf{x}_{i+1}$

We change the minimization problem,
since we minimize over different residuals.

Anderson acceleration for fixed-point iterations (Walker and Ni 2011)

Left Preconditioned Generalized Broyden

procedure $\mathrm{GB}(\mathbf{x} - \vec{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}), \mathbf{x}_i, \mathbf{b})$

  $\gamma_i = (\mathbf{F}_i^T \mathbf{F}_i)^{-1} \mathbf{F}_i^T (\mathbf{x} - \vec{M}(\mathbf{F}, \mathbf{x}, \mathbf{b}))$ ▷ solve LS by SVD

  $\mathbf{x}_{i+1} = \mathbf{x}_i - G_0(\mathbf{x} - \vec{M}(\mathbf{F}, \mathbf{x}, \mathbf{b})) - (\mathbb{X}_k - G_0 \mathbf{F}_k)\gamma_k$

end procedure

return $\mathbf{x}_{i+1}$

We change the minimization problem,
since we minimize over different residuals.

Anderson acceleration for fixed-point iterations (Walker and Ni 2011)

Right Preconditioned Generalized Broyden

1: **procedure** GB($\mathbf{F}(\mathcal{M}(\mathbf{F}, \cdot, \mathbf{b})), \mathbf{x}_i, \mathbf{b}$)
2: $\gamma_i = (\mathbf{F}_i^T \mathbf{F}_i)^{-1} \mathbf{F}_i^T \mathbf{r}(\mathcal{M}(\mathbf{x}_i), \mathbf{b})$ ▷ solve LS by SVD
3: $\mathbf{x}_{i+1} = \mathbf{x}_i - G_0 \mathbf{r}(\mathcal{M}(\mathbf{x}_i), \mathbf{b}) - (\mathbb{X}_k - G_0 \mathbf{F}_k)\gamma_k$
4: **end procedure**
5: **return** $\mathbf{x}_{i+1}$

We change the minimization problem,
since we use candidate solutions from the inner solver.

Krylov Subspace Acceleration for Nonlinear Multigrid Schemes with Application to Recirculating Flow (Washio and Oosterlee 2000)

Right Preconditioned Generalized Broyden

1: **procedure** GB($\mathbf{F}(\mathcal{M}(\mathbf{F}, \cdot, \mathbf{b})), \mathbf{x}_i, \mathbf{b}$)
2: $\gamma_i = (\mathbf{F}_i^T \mathbf{F}_i)^{-1} \mathbf{F}_i^T \mathbf{r}(\mathcal{M}(\mathbf{x}_i), \mathbf{b})$ ▷ solve LS by SVD
3: $\mathbf{x}_{i+1} = \mathbf{x}_i - G_0 \mathbf{r}(\mathcal{M}(\mathbf{x}_i), \mathbf{b}) - (\mathbb{X}_k - G_0 \mathbf{F}_k)\gamma_k$
4: **end procedure**
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We change the minimization problem,
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Krylov Subspace Acceleration for Nonlinear Multigrid Schemes with Application to Recirculating Flow (Washio and Oosterlee 2000)

Outline

I ran NPC on some problem and it worked.

Outline

Rate of Convergence

What should be a Rate of Convergence? [Ptak, 1977]:

1. It should relate quantities which may be measured or estimated during the actual process
2. It should describe accurately in particular the initial stage of the process, not only its asymptotic behavior . . .

$$\|x_{n+1} - x^*\| \leq c\|x_n - x^*\|^q$$

Rate of Convergence

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$$\|x_{n+1} - x_n\| \leq c\|x_n - x_{n-1}\|^q$$

Rate of Convergence

What should be a Rate of Convergence? [Ptak, 1977]:

1. It should relate quantities which may be measured or estimated during the actual process
2. It should describe accurately in particular the initial stage of the process, not only its asymptotic behavior ...

$$\|x_{n+1} - x_n\| \leq \omega(\|x_n - x_{n-1}\|)$$

where we have for all $r \in (0, R]$

$$\sigma(r) = \sum_{n=0}^{\infty} \omega^{(n)}(r) < \infty$$

Nondiscrete Induction

Define an approximate set $Z(r)$, where $x^* \in Z(0)$ implies $f(x^*) = 0$.

Nondiscrete Induction

Define an approximate set $Z(r)$, where $x^* \in Z(0)$ implies $f(x^*) = 0$.

For Newton's method, we use

$$Z(r) = \left\{ x \middle| \|f'(x)^{-1} f(x)\| \leq r, d(f'(x)) \geq h(r), \|x - x_0\| \leq g(r) \right\},$$

where

$$d(A) = \inf_{\|x\| \geq 1} \|Ax\|,$$

and $h(r)$ and $g(r)$ are positive functions.

Nondiscrete Induction

Define an approximate set $Z(r)$, where $x^* \in Z(0)$ implies $f(x^*) = 0$.

For $r \in (0, R]$,

$$Z(r) \subset U(Z(\omega(r)), r)$$

implies

$$Z(r) \subset U(Z(0), \sigma(r)).$$

Nondiscrete Induction

For the fixed point iteration

$$x_{n+1} = Gx_n,$$

if I have

$$x_0 \in Z(r_0)$$

and for $x \in Z(r)$,

$$\begin{aligned} \|Gx - x\| &\leq r \\ Gx &\in Z(\omega(r)) \end{aligned}$$

then

Nondiscrete Induction

For the fixed point iteration

$$x_{n+1} = Gx_n,$$

if I have

$$x_0 \in Z(r_0)$$

and for $x \in Z(r)$,

$$\begin{aligned} \|Gx - x\| &\leq r \\ Gx &\in Z(\omega(r)) \end{aligned}$$

then

$$\begin{aligned} x^* &\in Z(0) \\ x_n &\in Z(\omega^{(n)}(r_0)) \end{aligned}$$

Nondiscrete Induction

For the fixed point iteration

$$x_{n+1} = G x_n,$$

if I have

$$x_0 \in Z(r_0)$$

and for $x \in Z(r)$,

$$\begin{aligned} \|Gx - x\| &\leq r \\ Gx &\in Z(\omega(r)) \end{aligned}$$

then

$$\begin{aligned} \|x_{n+1} - x_n\| &\leq \omega^{(n)}(r_0) \\ \|x_n - x^*\| &\leq \sigma(\omega^{(n)}(r_0)) \end{aligned}$$

Nondiscrete Induction

For the fixed point iteration

$$x_{n+1} = G x_n,$$

if I have

$$x_0 \in Z(r_0)$$

and for $x \in Z(r)$,

$$\begin{aligned} \|Gx - x\| &\leq r \\ Gx &\in Z(\omega(r)) \end{aligned}$$

then

$$\begin{aligned} \|x_n - x^*\| &\leq \sigma(\omega(\|x_n - x_{n-1}\|)) \\ &= \sigma(\|x_n - x_{n-1}\|) - \|x_n - x_{n-1}\| \end{aligned}$$

Newton's Method

$$\omega_{\mathcal{N}}(r) = cr^2$$

Newton's Method

$$\omega_{\mathcal{N}}(r) = \frac{r^2}{2\sqrt{r^2 + a^2}}$$
$$\sigma_{\mathcal{N}}(r) = r + \sqrt{r^2 + a^2} - a$$

where

$$a = \frac{1}{k_0}\sqrt{1 - 2k_0 r_0},$$

k_0 is the (scaled) Lipschitz constant for f', and
r_0 is the (scaled) initial residual.

Newton's Method

$$\omega_{\mathcal{N}}(r) = \frac{r^2}{2\sqrt{r^2 + a^2}}$$
$$\sigma_{\mathcal{N}}(r) = r + \sqrt{r^2 + a^2} - a$$

This estimate is *tight* in that the bounds hold with equality for some function f,

$$f(x) = x^2 - a^2$$

using initial guess

$$x_0 = \frac{1}{k_0}.$$

Also, if equality is attained for some n_0, this holds for all $n \geq n_0$.

Newton's Method

$$\omega_{\mathcal{N}}(r) = \frac{r^2}{2\sqrt{r^2 + a^2}}$$
$$\sigma_{\mathcal{N}}(r) = r + \sqrt{r^2 + a^2} - a$$

If $r \gg a$, meaning we have an inaccurate guess,

$$\omega_{\mathcal{N}}(r) \approx \frac{1}{2} r,$$

whereas if $r \ll a$, meaning we are close to the solution,

$$\omega_{\mathcal{N}}(r) \approx \frac{1}{2a} r^2.$$

Left vs. Right

Left:

$$\mathcal{F}(x) \Longrightarrow x - \mathcal{N}(\mathcal{F}, x, b)$$

Right:

$$x \Longrightarrow y = \mathcal{N}(\mathcal{F}, x, b)$$

Heisenberg vs. Schrödinger Picture

Left vs. Right

Left:

$$\mathcal{F}(x) \Longrightarrow x - \mathcal{N}(\mathcal{F}, x, b)$$

Right:

$$x \Longrightarrow y = \mathcal{N}(\mathcal{F}, x, b)$$

Heisenberg vs. Schrödinger Picture

$\mathcal{M} -_R \mathcal{N}$

We start with $x \in Z(r)$, apply $\mathcal{N}$ so that

$$y \in Z(\omega_{\mathcal{N}}(r)),$$

and then apply $\mathcal{M}$ so that

$$x' \in Z(\omega_{\mathcal{M}}(\omega_{\mathcal{N}}(r))).$$

Thus we have

$$\omega_{\mathcal{M} -_R \mathcal{N}} = \omega_{\mathcal{M}} \circ \omega_{\mathcal{N}}$$

Non-Abelian

$\mathcal{N} -_R$ NRICH

$$\begin{aligned}
\omega_{\mathcal{N}} \circ \omega_{\text{NRICH}} &= \frac{1}{2} \frac{r^2}{\sqrt{r^2 + a^2}} \circ cr, \\
&= \frac{1}{2} \frac{c^2 r^2}{\sqrt{c^2 r^2 + a^2}}, \\
&= \frac{1}{2} \frac{cr^2}{\sqrt{r^2 + (a/c)^2}}, \\
&= \frac{1}{2} c \frac{r^2}{\sqrt{r^2 + \tilde{a}^2}},
\end{aligned}$$

Non-Abelian

$$\mathcal{N} -_R \text{NRICH: } \frac{1}{2}c\frac{r^2}{\sqrt{r^2+\tilde{a}^2}}$$

NRICH $-_R \mathcal{N}$

$$\begin{aligned}
\omega_{\text{NRICH}} \circ \omega_{\mathcal{N}} &= cr \circ \frac{1}{2}\frac{r^2}{\sqrt{r^2+a^2}}, \\
&= \frac{1}{2}c\frac{r^2}{\sqrt{r^2+a^2}}, \\
&= \frac{1}{2}c\frac{r^2}{\sqrt{r^2+a^2}}.
\end{aligned}$$

Non-Abelian

$$\mathcal{N} -_R \text{NRICH}: \frac{1}{2} c \frac{r^2}{\sqrt{r^2 + \tilde{a}^2}}$$

$$\text{NRICH} -_R \mathcal{N}: \frac{1}{2} c \frac{r^2}{\sqrt{r^2 + a^2}}$$

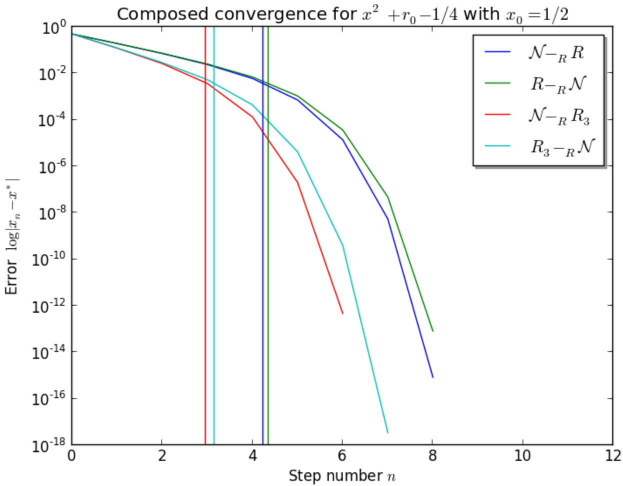
The first method also changes the onset of second order convergence.

Example

$$f(x) = x^2 + (0.0894427)^2$$

n	$\|x_{n+1} - x_n\|$	$\|x_{n+1} - x_n\| - w^{(n)}(r_0)$	$\|x_n - x^*\| - s(w^{(n)}(r_0))$
0	1.9990e+00	$< 10^{-16}$	$< 10^{-16}$
1	9.9850e-01	$< 10^{-16}$	$< 10^{-16}$
2	4.9726e-01	$< 10^{-16}$	$< 10^{-16}$
3	2.4470e-01	$< 10^{-16}$	$< 10^{-16}$
4	1.1492e-01	$< 10^{-16}$	$< 10^{-16}$
5	4.5342e-02	$< 10^{-16}$	$< 10^{-16}$
6	1.0251e-02	$< 10^{-16}$	$< 10^{-16}$
7	5.8360e-04	$< 10^{-16}$	$< 10^{-16}$
8	1.9039e-06	$< 10^{-16}$	$< 10^{-16}$
9	2.0264e-11	$< 10^{-16}$	$< 10^{-16}$
10	0.0000e+00	$< 10^{-16}$	$< 10^{-16}$

Example



Matrix iterations also 1D scalar once you diagonalize

Pták's nondiscrete induction and its application to matrix iterations, Liesen, IMA J. Num. Anal., 2014.

Outline

Further Questions

- Can we say something general about left preconditioning?
- Can the composed iteration have a larger region of convergence?
- What should be a nonlinear smoother?
- Can we usefully predict the convergence of NPC solvers?