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Adaptive Nonlinear Preconditioning for PDEs with Error Bounds on Output Functionals

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From a nonlinear guy to a linear guy at his 71^{st}, with deep gratitude

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Outline

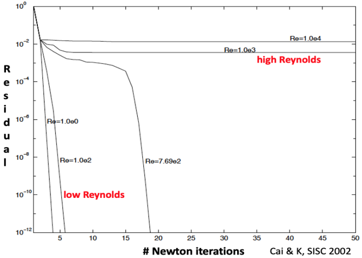
Introduction

Consider a nonlinear problem $F(x) = 0, \; F : \hat{D} \subset R^n \to R^n$.

Taking the Taylor expansion,

$$\boxed{F(x) = F(x_k) + F'(x_k)(x - x_k)} + O(\|x - x_k\|^2).$$

- When high-order terms dominate, the linear model is not a suitable approximation to $F(x)$.
- Strong nonlinearities result in a long plateau period of the residual $\|F(x_k)\|$.
- Only a small number of components of the solution may undergo significant updates in Newton corrections that are highly damped by linesearch backtracking or trust region globalization.



Newton methods may thus waste considerable computational resources solving global linear systems in problems that are "nonlinearly stiff" until they find the convergence domain. Examples include shocks, combustion fronts, recirculation bubbles, etc.

Enter nonlinear preconditioning

- A nonlinear "preconditioner" performs nonlinear relaxation within one or more subspaces, inside the context of an outer Newton method "accelerator."
  - Analogous to linear preconditioners, such as domain decomposition or multigrid, inside a Krylov accelerator.
  - Preconditioned Krylov methods are often used inside *both* the nonlinear subproblems and the global problem.
- A prime consideration in selecting a nonlinear preconditioner is whether the resulting outer problem is amenable to linear preconditioning.
- Left nonlinear preconditioners ASPIN and MSPIN complicate linear preconditioning by replacing a sparse Jacobian with a dense one.
- Right preconditioners like INB-NE retain the original Jacobian.
- Left preconditioner NEPIN (introduced here) can also employ the original Jacobian.

Nonlinear preconditioning

- **Left preconditioning:** solve equivalent system with better balanced nonlinearities

$$\mathcal{F}(x) = G(F(x)) = 0,$$

  - e.g., Additive Schwarz Preconditioned Inexact Newton (ASPIN), Cai & K (SISC, 2002), Multiplicative Schwarz Preconditioned Inexact Newton (MSPIN), Liu & K (SISC, 2015), Restricted Additive Schwarz Preconditioned Exact Newton (RASPEN), Dolean *et al.* (SISC, 2016), Nonlinear Elimination Preconditioning Inexact Newton (NEPIN), Liu *et al.* (2021, submitted)

- **Right preconditioning:** start from a better initial guess by correction within a subspace:

$$F(G(\tilde{x})) = 0, x = G(\tilde{x}),$$

  - e.g., Nonlinear FETI-DP and BDDC, Klawonn *et al.* (SISC, 2014), Nonlinear Elimination (NE), Hwang *et al.* (Comp & Fl, 2015), Luo *et al.* (SISC, 2020)

Co-authors and references for this talk

2015	Liu & K	Field-split preconditioned inexact Newton algorithms	SISC
2016	Liu & K	Convergence analysis for the multiplicative Schwarz preconditioned inexact Newton algorithm	SINUM
2018	Liu, K & Krause	A note on adaptive nonlinear preconditioning techniques	SISC
2021	Liu & K	Approximate error bounds on solutions of nonlinearly preconditioned PDEs	SISC (to appear)
2021	Liu, Hwang, Luo, Cai & K	A nonlinear elimination preconditioned inexact Newton algorithm	(submitted)

Short-cuts for a 10-minute peek

- We illustrate on standard 2D PDE models
  - transonic potential flow over an airfoil
  - velocity-vorticity incompressible Navier-Stokes in a cavity
  - velocity-vorticity-energy incompressible Boussinesq in a cavity
- Some other applications, not discussed here:
  - porous media flows, arterial flows, two-phase flows, combustion
- Discretizations are suppressed, being primitive
  - second-order finite differences
  - 2-point upwinding from Boeing in transonic potential example
- Derivations are suppressed
  - please see references
- Parallel scaling and parameter tuning are suppressed
  - PETSc, on KAUST's Shaheen Cray SC-40
  - nonlinear preconditioning has imbalance issues not yet addressed in our software, but Newton-Krylov scaling is decent within a subproblem or outer Newton iteration
  - inexact Newton uses loose linear convergence tolerances
  - nonlinear convergence tolerances and thresholds for "bad" / "good" component selection can be nontrivial

A simple algebraic example in R^2

$$F(x_1, x_2) = \begin{bmatrix} F_1(x_1, x_2) \\ F_2(x_1, x_2) \end{bmatrix} = \begin{bmatrix} (x_1 - x_2^3 + 1)^5 - x_2^5 \\ x_1 + 2x_2 - 3 \end{bmatrix} = 0 \quad (1)$$

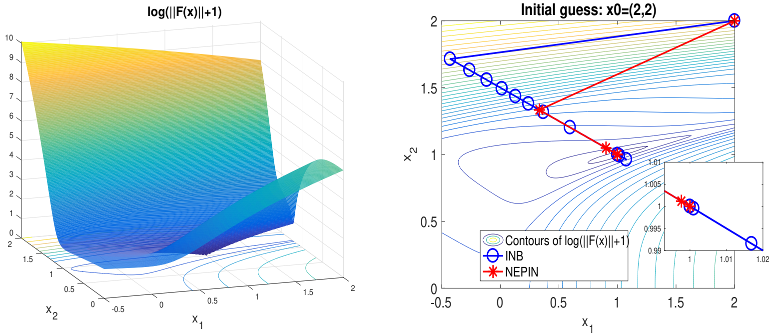


Figure: Contours of $\log(\|F(x)\| + 1)$ for and the path using Inexact Newton with Backtracking (INB) (blue circles) and Nonlinear Elimination Preconditioning Inexact Newton (NEPIN) (red stars) from the same starting point $x^0 = [2, 2]^T$.

Outline

Nonlinear Elimination PIN for unbalanced nonlinearities

The components of the nonlinear system $F(x) = 0$ are partitioned heuristically into two groups, “bad” and “good,” labeled as F_b and F_g, respectively, according to the degree of nonlinear “stiffness.” This is often successfully associated with the components whose absolute residual exceeds some threshold, or for which some physical feature exceeds some threshold. The unknowns principally associated with each equation are split conformally into $x = [x_b, x_g]^T$:

$$F(x) = F(x_b, x_g) = \begin{bmatrix} F_b(x_b, x_g) \\ F_g(x_b, x_g) \end{bmatrix}, \qquad (2)$$

where x_b and x_g are “bad” and “good” components, respectively.

Nonlinear preconditioned function

For a given partitioning, the nonlinear elimination preconditioned function

$$\mathcal{F}(x) = \mathcal{F}(x_b, x_g) = \begin{bmatrix} T_b(x_b, x_g) \\ F_g(x_b, x_g) \end{bmatrix} = \begin{bmatrix} T_b(x) \\ F_g(x) \end{bmatrix}, \tag{3}$$

is obtained by solving the subsystem

$$F_b(x_b - T_b(x), x_g) = 0. \tag{4}$$

for $T_b(x)$. The Jacobian of $\mathcal{F}(x)$ can be written in the form of

$$\mathcal{J}(x) = \begin{bmatrix} \left(\frac{\partial F_b}{\partial u_b}\right)^{-1} & \\ & I_g \end{bmatrix} \begin{bmatrix} \frac{\partial F_b}{\partial u_b} & \frac{\partial F_b}{\partial x_g} \\ \frac{\partial F_g}{\partial x_b} & \frac{\partial F_g}{\partial x_g} \end{bmatrix}, \quad \text{where} \quad u_b = x_b - T_b(x). \tag{5}$$

Then the Newton correction step

$$\mathcal{J}(x)\hat{d} = \mathcal{F}(x) = \begin{bmatrix} T_b(x) \\ F_g(x) \end{bmatrix} \tag{6}$$

is equivalent, upon multiplying the upper block row through by $J_b = R_b J(u_b, x_g) R_b^T$, to

$$J(u_b, x_g)\hat{d} = \begin{bmatrix} J_b T_b(x) \\ F_g(x) \end{bmatrix}. \tag{7}$$

NEPIN algorithm basic step

1. Solve the subspace problem:

$$F_b(z^{(k)}) = F_b(x_b^{(k)} - T_b^{(k)}, x_g^{(k)}) = 0, \tag{8}$$

2. Form the global residual

$$g^{(k)} = \begin{bmatrix} J_b(z^{(k)})T_b^{(k)} \\ F_g(x^{(k)}) \end{bmatrix}, \quad J_b(z^{(k)}) = R_b J(z^{(k)}) R_b^T. \tag{9}$$

3. Solve inexactly for the Newton direction $d^{(k)}$ in

$$J(z^{(k)})d^{(k)} = g^{(k)}, \quad \text{where} \quad J(x) = F'(x) \tag{10}$$

4. Compute the new approximate solution

$$x^{(k+1)} = x^{(k)} - \lambda^{(k)} d^{(k)}. \tag{11}$$

Example: Transonic full potential flow

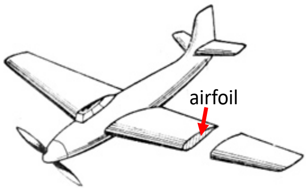
Consider transonic flow around an airfoil, which is described by the scalar full potential equation, derived for inviscid, irrotational, isentropic compressible flow as:

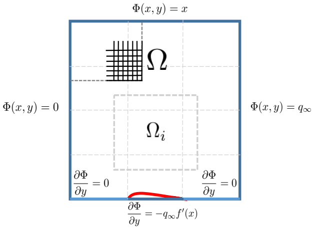
$$\nabla \cdot (\rho(\Phi)\nabla\Phi) = 0, \tag{12}$$

where Φ is the velocity potential, and $\nabla\Phi = [u, v]^T$ is the velocity field. The density function ρ is computed by

$$\rho(\Phi) = \rho_\infty \left(1 + \frac{\gamma - 1}{2} M_\infty^2 \left(1 - \frac{\|\nabla\Phi\|_2^2}{q_\infty^2}\right)\right)^{\frac{1}{\gamma-1}} \tag{13}$$

with suitable upwinding, as in the Boeing TRANAIR code [Young *et al.*, JCP 1991].





Example: Transonic full potential flow

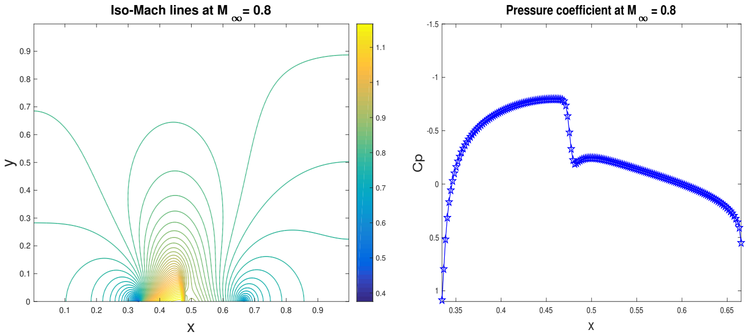


Figure: Mach number countours (left) and the pressure coefficient C_p curve (right) obtained by the final solution at $M_\infty = 0.8$ on a uniform 512×512 mesh.

The distribution of the "bad" components

Define "bad" components as those where the local velocity exceeds a certain cut-off Mach number, $M(x, y) > M_c$.

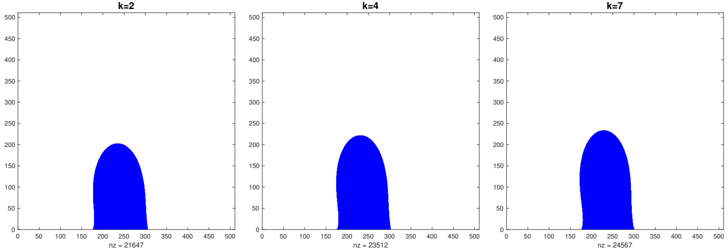
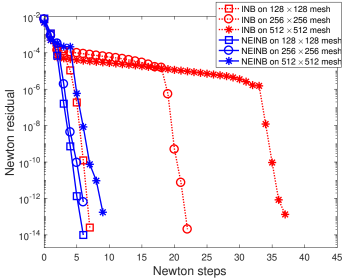
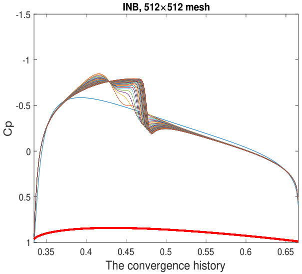
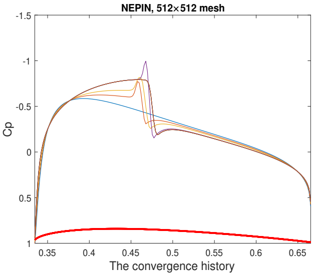


Figure: The evolution of the "bad" component region using NEPIN for $M_\infty = 0.8$ and $M_c = 0.82$, on a uniform 512×512 mesh, on the second, the fourth and the seventh global Newton iterations. Number of bad components: 21,647 at iteration 2; then 23,512 at iteration 4; then 24,567 at iteration 7.

Convergence history for varying mesh size ($M_c = 0.82$)







Outline

Multiplicative Schwarz Preconditioned Inexact Newton algorithm (MSPIN)

A form of nonlinear Gauss-Seidel:

The nonlinear function $F(x)$ is split conformally into 2 nonoverlapping components, representing distinct fields or physical features, as

$$F(x) = F(u, v) = \begin{bmatrix} G(u, v) \\ H(u, v) \end{bmatrix} = 0. \tag{14}$$

The preconditioned system comes from solving subspace nonlinear problems:

$$\mathcal{F}(u, v) = \begin{bmatrix} g(u, v) \\ h(u, v) \end{bmatrix} \tag{15}$$

1. Solve for g in

$$G(u - g, v) = 0$$

2. Solve for h with the new g in

$$H(u - g, v - h) = 0$$

MSPIN, 2-component, non-overlapping

The Jacobian matrix of the preconditioned system is

$$\mathcal{J}(u,v) = \begin{bmatrix} g_u & g_v \\ h_u & h_v \end{bmatrix} = \begin{bmatrix} \frac{\partial G}{\partial p} & \\ \frac{\partial H}{\partial p} & \frac{\partial H}{\partial q} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial G}{\partial p} & \frac{\partial G}{\partial v} \\ \frac{\partial H}{\partial p} & \frac{\partial H}{\partial q} \end{bmatrix}, \qquad (16)$$

where $p = u - g(u,v)$ and $q = v - h(u,v)$.
In practice, since (p,q) approaches (u,v) as the solution converges locally, the preconditioned Jacobian is locally well approximated by the readily computable

$$\hat{\mathcal{J}}_{MSPIN}(u,v) = \begin{bmatrix} G_p & \\ H_p & H_v \end{bmatrix}^{-1} \begin{bmatrix} G_p & G_v \\ H_p & H_v \end{bmatrix} = \begin{bmatrix} G_p & \\ H_p & H_v \end{bmatrix}^{-1} J(p,v). \qquad (17)$$

Generalization to 3 or more components is straightforward.

Example: lid-driven cavity

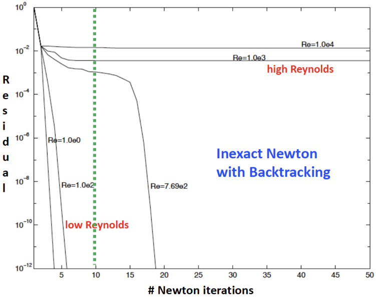
The governing system consists of the nondimensional steady-state incompressible Navier-Stokes equations in vorticity-velocity form:

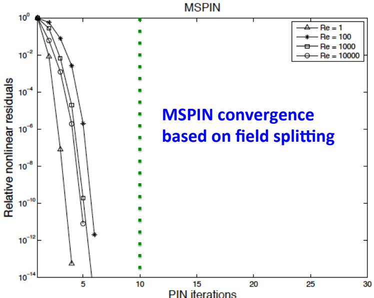
$$\begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0, \\ -\Delta \omega + Re(u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y}) = 0, \end{cases} \tag{18}$$

There are three unknowns: the velocity fields (u, v) in the (x, y) directions, and the vorticity ω. The parameter Re controls the system's only nonlinearity.

We employ MSPIN as the nonlinear preconditioner with two subsystems: the two velocity equations as one subsystem and the vorticity equation as the other.

Example: lid-driven cavity





Some analysis

[Liu & K, SISC, 2015] $F(x)$ and $\mathcal{F}(x)$ are equivalent in the sense that they have the same solution in a neighborhood of x^* in D.

[Liu & K, SINUM, 2016] MSPIN's local convergence is guaranteed

- superlinear if the forcing tolerance approaches 0
- quadratically if the forcing tolerance approaches 0 like $\mathcal{O}(\|\mathcal{F}(\cdot)\|)$

Outline

Adaptive preconditioning motivation

- Asymptotically, nonlinear preconditioned Newton approaches Newton.
- A preconditioned Newton step is more expensive because of the nonlinear subiterations.
- Nonlinear preconditioning should be “on” only when needed and “off” when not.
- A scalar manipulation of norms available as by-products of the global iterations can be the switch.
- η_k below reflects the agreement between $F(x)$ and its local linear model at the previous step:

$$\eta_k = \frac{\Big| \|F(x_k)\| - \|F(x_{k-1}) + F'(x_{k-1})s_{k-1}\| \Big|}{\|F(x_{k-1})\|}, \quad k = 1, 2, \ldots, \tag{19}$$

Adaptive preconditioning algorithm

Set initial iterate $x^{(0)}$
Set $\eta_0 = 1$ and switch tolerance ϵ
While $k = 0, 1, 2, \ldots$ until convergence
    Update $x^{(k+1)}$ starting from $x^{(k)}$ based on η_k:
    If $\eta_k < \epsilon$
        Implement one step of plain INB
    Else
        Implement one step of nonlinearly preconditioned INB
    EndIf
    Step 2. Compute η_{k+1}
    Step 3. $k \leftarrow k + 1$
EndWhile

Example: lid-driven cavity

We compare the number of nonlinear iterations using MSPIN and MSPIN-adapt at different Reynolds numbers. MSPIN-adapt suspends preconditioning for the terminal step(s), but converges in the same number of Newton iterations as MSPIN.

INB fails to converge from the same "cold" start for large Reynolds numbers.

Number of global Newton iterations				
Algorithm	$Re = 100$	$Re = 1000$	$Re = 5000$	$Re = 10000$
INB	5	-	-	-
MSPIN	4	3	3	3
MSPIN-adapt	4	3	3	3

Example: lid-driven cavity

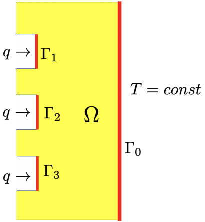
History of η_k for the lid-driven cavity with $\epsilon = 0.2$.

$Re = 100$		
Iter	η_k	step
0	1.0	MSPIN
1	0.580156	MSPIN
2	0.132696	INB
3	0.028887	INB
$Re = 1000$		
Iter	η_k	step
0	1.0	MSPIN
1	0.272078	MSPIN
2	0.025135	INB
$Re = 10000$		
Iter	η_k	step
0	1.0	MSPIN
1	0.061412	INB
2	0.034303	INB

Outline

Motivation

- In applications, we are are often happy with selected functionals of the overall field solution.
- Some of these, particularly integral functionals, may converge faster than the primitive variables.
- Can we directly bound the functionals with by-products of the iteration and stop early?



- The field solution $[\boldsymbol{u}, p, T]^T$
- Given an input heat flux q, we wish to determine whether

$$T_{mean} = \int_{\Gamma_1} T ds.$$

is within an acceptable design interval.

The problem of cooling electronic components in a computer by natural convection of air in the enclosure. $\partial\Omega / \bigcup_{i=0}^{3} \Gamma_i$ is isolated.

Output linear functional of the coupled solution

As in MSPIN, the nonlinear system $F(x)$ is split as

$$F(x) = F(u,v) = \begin{bmatrix} G(u,v) \\ H(u,v) \end{bmatrix} = 0, \quad x = [u,v]^T, \qquad (20)$$

We are interested in a linear functional of the coupled solution:

$$J(u,v) = \langle \psi_1, u \rangle + \langle \psi_2, v \rangle, \qquad (21)$$

for prescribed $\psi_1 \in R^{n_1}$ and $\psi_2 \in R^{n_2}$.

Approximate error bounds for MSPIN

We can bound the error in the linear functional in terms of the component residuals and some Jacobian blocks

$$
\begin{aligned}
& J(u,v) - J(\hat{u}^{(k)}, \hat{v}^{(k)}) \\
= \;& \langle \psi_1, u - \hat{u}^{(k)} \rangle + \langle \psi_2, v - \hat{v}^{(k)} \rangle \\
\approx \;& -\langle \psi_1, R_1^{(k)} \rangle + \langle \psi_1, {\mathcal{B}_{11}^{(k)}}^{-1} \mathcal{B}_{12}^{(k)} (I - \mathcal{C}_2^{(k)})^{-1} R_2^{(k)} \rangle \\
& -\langle \psi_2, (I - \mathcal{C}_2^{(k)})^{-1} R_2^{(k)} \rangle,
\end{aligned}
$$

where $\mathcal{C}_2^{(k)} = {\mathcal{B}_{22}^{(k)}}^{-1} \mathcal{B}_{21}^{(k)} {\mathcal{B}_{11}^{(k)}}^{-1} \mathcal{B}_{12}^{(k)}$.

Approximate error bounds for MSPIN

In the MSPIN algorithm, the submodels are solved sequentially for the physical variable corrections, which implicitly forms the preconditioned system. For any given $x = [u, v]^T \in R^n$, the preconditioned nonlinear system

$$\mathcal{F}(x) = \begin{bmatrix} g(u, v) \\ h(u, v) \end{bmatrix} = 0 \tag{22}$$

is obtained by solving

$$G(u - g, v) = 0, \tag{23}$$

for g. With values of u, v, g, the system

$$H(u - g, v - h) = 0, \tag{24}$$

is solved for h.

Approximate error bounds for MSPIN

Let $p = u - g(u,v)$ and $q = v - h(u,v)$. We define

$$\mathcal{B} = \begin{bmatrix} \frac{\partial G}{\partial p} & \frac{\partial G}{\partial v} \\ \frac{\partial H}{\partial p} & \frac{\partial H}{\partial q} \end{bmatrix} = \begin{bmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} \\ \mathcal{B}_{21} & \mathcal{B}_{22} \end{bmatrix}. \quad (25)$$

The derivatives of g and h with respect to u and v are written as

$$\frac{\partial g}{\partial u} = I_u, \quad \frac{\partial g}{\partial v} = \mathcal{B}_{11}^{-1}\mathcal{B}_{12}, \quad (26)$$

$$\frac{\partial h}{\partial u} = 0, \quad \frac{\partial h}{\partial v} = I_v - \mathcal{B}_{22}^{-1}\mathcal{B}_{21}\mathcal{B}_{11}^{-1}\mathcal{B}_{12}, \quad (27)$$

where I_u and I_v are the identity matrices that have the same dimension as the u and v blocks, respectively.

Approximate error bounds for MSPIN

Theorem

At the k-th iteration in the MSPIN algorithm, the approximate solution is denoted by $\hat{x}^{(k)} = [\hat{u}^{(k)}, \hat{v}^{(k)}]^T$ and let $\mathcal{C}_2^{(k)} = \mathcal{B}_{22}^{(k)\,-1}\mathcal{B}_{21}^{(k)}\mathcal{B}_{11}^{(k)\,-1}\mathcal{B}_{12}^{(k)}$. We define the error induced in the linear functional (21) as

$$\Delta J_k = |J(u,v) - J(\hat{u}^{(k)}, \hat{v}^{(k)})|. \tag{28}$$

Then the approximate error bound is given by

$$\begin{aligned} \Delta J_k \quad &\lesssim \quad |\langle \psi_1, R_1^{(k)} \rangle| + \|(I - \mathcal{C}_2^{(k)})^{-1} R_2^{(k)}\| \|\mathcal{B}_{12}^{(k)\,T} \mathcal{B}_{11}^{(k)\,-T} \psi_1\| \\ &+ \quad \|R_2\| \|(I - \mathcal{C}_2^{(k)})^{-T} \psi_2\|. \end{aligned} \tag{29}$$

If $\|\mathcal{C}_2^{(k)}\| < 1$, we further derive

$$\Delta J_k \lesssim |\langle \psi_1, R_1^{(k)} \rangle| + \|R_2^{(k)}\| (\|\mathcal{B}_{12}^{(k)\,T} \mathcal{B}_{11}^{(k)\,-T} \psi_1\| + \|\psi_2\|) \frac{1}{1 - \|\mathcal{C}_2^{(k)}\|}. \tag{30}$$

Example: buoyancy-driven cavity

The governing system consists of the nondimensional steady-state incompressible Navier-Stokes equations in vorticity-velocity form with Boussinesq bouyancy and the energy equation:

$$\begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0, \\ -\Delta \omega + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} - Gr\frac{\partial T}{\partial x} = 0, \\ -\Delta T + Pr(u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}) = 0, \end{cases} \tag{31}$$

There are four unknowns: the velocity fields (u, v) in the (x, y) directions, the vorticity ω and the temperature T.

Example: buoyancy-driven cavity

For this example, we are interested in the following four linear functionals of u, v, ω and T:

$$J_1 = \int_0^1 u(0.5, y)dy, \tag{32}$$

$$J_2 = v_x(0.5, 0.5), \tag{33}$$

$$J_3 = \omega(0.5, 0.5), \tag{34}$$

$$J_4 = \int_0^1 \int_0^1 T dx dy. \tag{35}$$

- J_1 is the mass flux across the vertical line through geometric center of the cavity;
- J_2 is the partial derivative of v along the horizontal line through the center point;
- J_3 is the vorticity at the center point;
- J_4 is the average temperature in the cavity.

Error bounds using MSPIN with different Gr

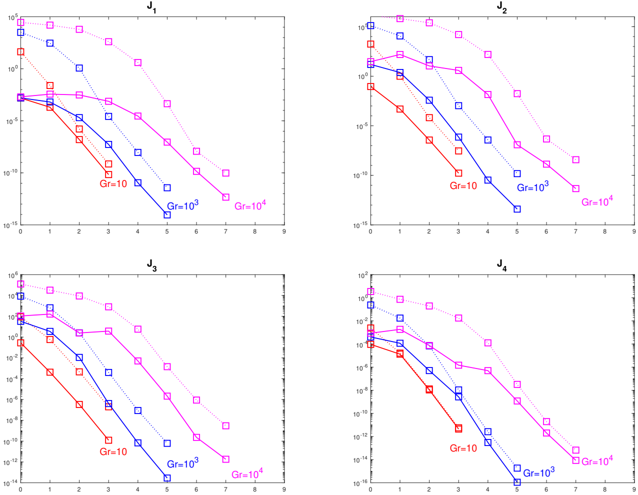


Figure: The absolute errors (solid) in J_1, J_2, J_3 and J_4 with $Gr = 10, 10^3, 10^4$, $Pr = 1$ and the lid velocity $V_{lid} = 0.1$ on uniform 256×256 mesh, with the corresponding error bounds (dotted).

Outline

Conclusions

- Experiments demonstrate that left-preconditioned methods NEPIN (threshold-split) and MSPIN (field-split) can each be effective in improving on the convergence of global Inexact Newton with Backtracking (INB) iterations.
- Nonlinear preconditioning expends extra local computational cost for the solution of nonlinear subproblems to reduce the computation, communication, and synchronization costs of the global outer iterations, by reducing their number.
- A simple adaptive framework is useful to switch nonlinear preconditioning on and off during the outer Newton iterations.
- *A posteriori* approximate error bounds on the linear functionals of interest are available using by-products of the nonlinear preconditioning split systems.

Future Work

- Use of dynamic runtime systems to better sequence the irregularity of the nonlinear subiterations
- More automated identification of “bad” components systems, perhaps using machine learning


Thank you!

Questions