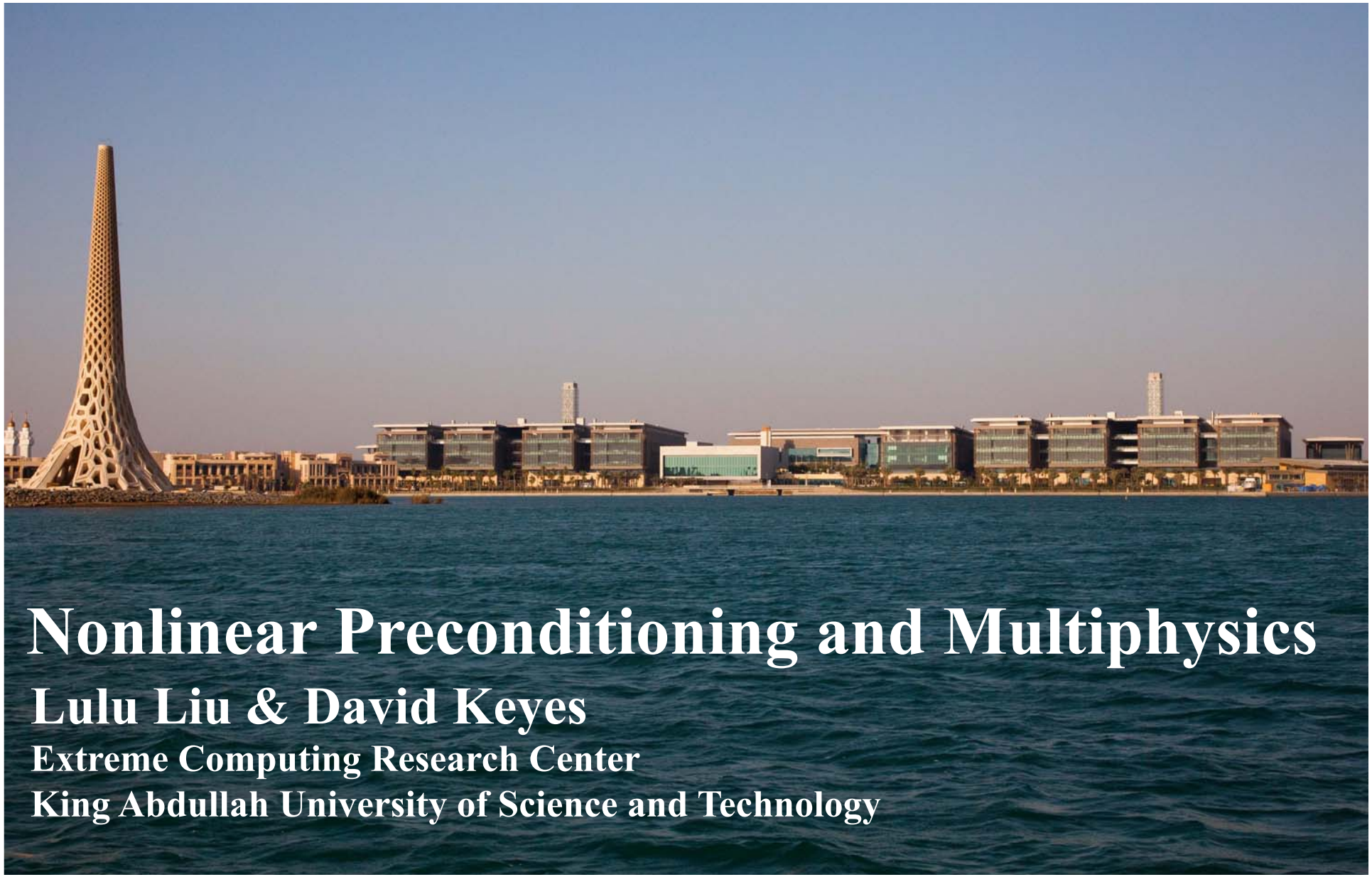
SPPEXA

German Priority Programme 1648
Software for Exascale Computing



Nonlinear Preconditioning and Multiphysics

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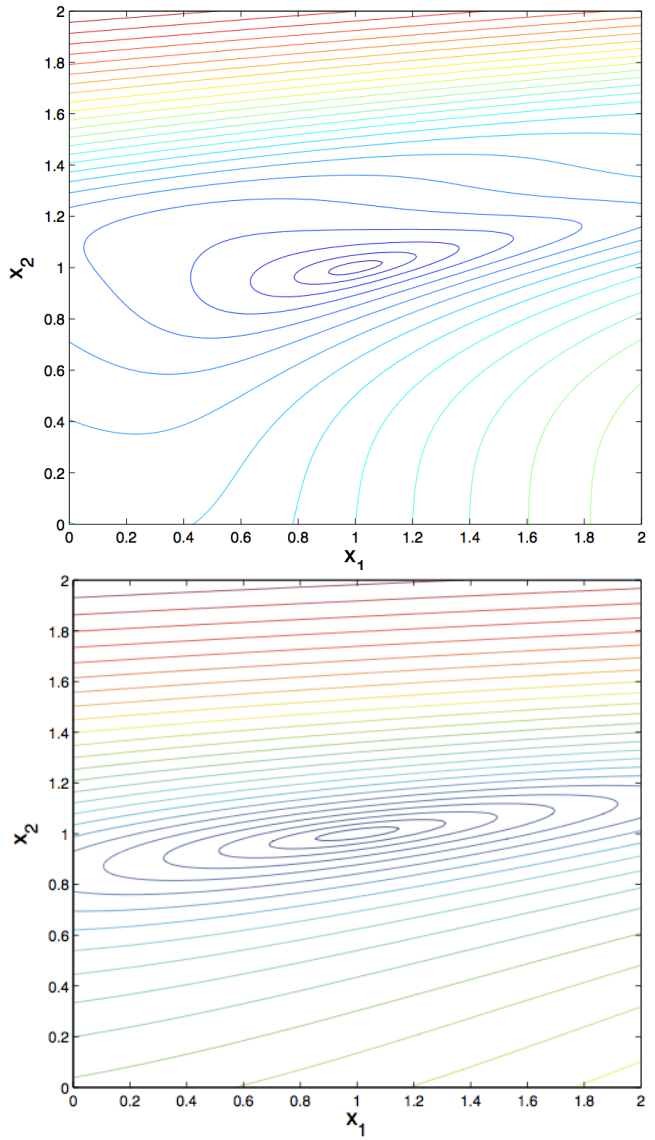
Original motivation for nonlinear preconditioning

- **A nonlinear system $F(u) = 0$ may be "stiff," in the sense that the iso-contours of the merit function, e.g., $f(u) = ||F(u)||^2$, are far from hyperellipsoidal, giving a small domain of guaranteed local convergence for Newton**

- **This may be combined with linear ill-conditioning, in the sense that the hyperellipsoids are locally badly stretched**



Typical causes of nonlinear stiffness

[Cai, K, Young, 2000] **: shocks, reaction zones, boundary layers, interior layers**

$$(A\rho u_x)_x = 0, \;\; 0 < x < 2$$

$$A = A(x) = 0.4 + 0.6(x-1)^2,$$

$$\rho = \rho(v) = (c^2)^{1/(\gamma-1)} = \left(1 + \frac{\gamma-1}{2}(1-v^2)\right)^{1/(\gamma-1)}$$

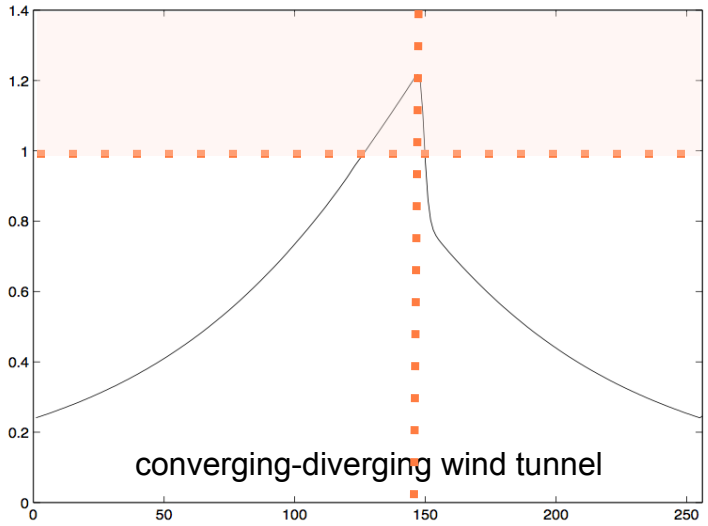


Figure 1: Mach distribution and the shock location.

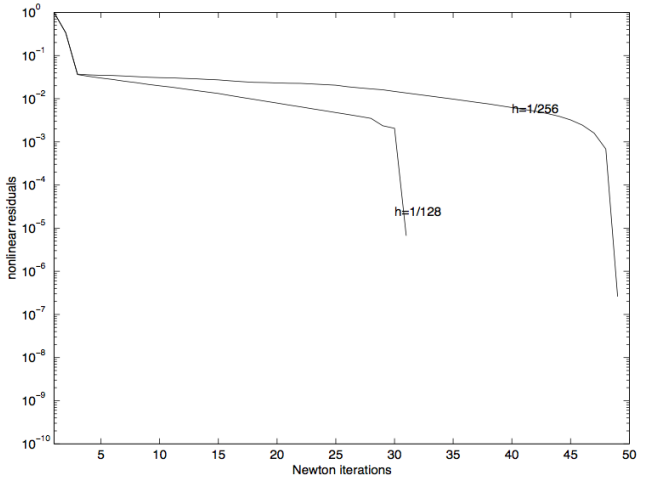


Figure 2: Nonlinear residual history of the inexact Newton's algorithm for the flow problem with mesh sizes $h = 1/128$ and $h = 1/256$.

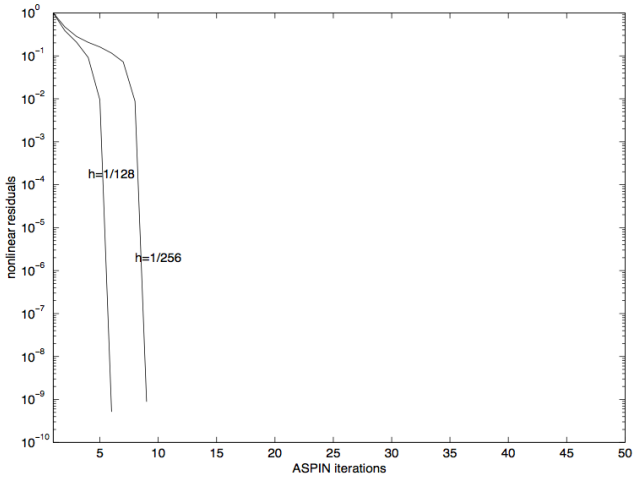


Figure 3: Nonlinear residual history of the additive Schwarz preconditioned inexact Newton's algorithm for the flow problem with mesh sizes $h = 1/128$ and $h = 1/256$.

Key idea

- **Newton's method for a nonlinear system solves** $F(u) = 0$
  - **computes a *global* Jacobian matrix, and a *global* Newton step by solving the *global* linear system**
  - **Krylov iteration on global linear systems is expensive**
  - **wasteful when the resulting correction is significant only on a small set**
  - **also, "global" is a bad word with a billion cores**
- **Nonlinearly preconditioned Newton solves** $\mathcal{F}(u) = 0$
  - **implemented Jacobian-free through set of *local* problems on subsets of the original global nonlinear system**
  - **each of the linear systems for *local* Newton updates has only *local* scope and coordination**
  - **still global coordination in outer steps, hopefully *many fewer* than required in the original Newton method**

Selective background context

[Lions, 1988] **:** ***On the Schwarz Alternating Method. I*****, 2-subdomain procedure for monotone nonlinear problems by alternating variational minimization in each subdomain**

[Cai, Gropp, K & Tidriri, 1994] **:** ***Newton-Krylov-Schwarz Methods in CFD*****, a matrix-free method based on global linearization and local preconditioning**

[Cai & Dryja, 1994] **:** ***Domain decomposition methods for monotone nonlinear elliptic problems*****, quadratic convergence proof for Newton, based on global linearization and local preconditioning**

[Dryja & Hackbusch, 1997] **:** ***On the nonlinear domain decomposition method*****, an additive nonlinear Richardson iteration based on the solution of local nonlinear problems**

[Cai & K, 2002] **:** ***Nonlinearly preconditioned inexact Newton algorithms,*** **matrix-free Newton acceleration of** [Dryja & Hackbusch, 1997]

Requirements for an equivalent system

- **Find solution u^* of $F(u^*) = 0$ from $\mathcal{F}(u^*) = 0$**
  - **using inexact Newton**
  - **linear systems solved with matrix-free Krylov**
  - **globalized with backtracking line search or trust region, etc.**

- **$F(u) = 0$ and $\mathcal{F}(u^*) = 0$ have the same solution**
- **$\mathcal{F}(w)$ is easily computable for w in R^n**
- **$\mathcal{F}'(w)v$ is also easily computable for w, v in R^n**

Why nonlinear Schwarz preconditioning?

2000: Robustify Newton and improve its efficiency

- Additive Schwarz Preconditioned Inexact Newton (ASPIN)
- interchange order of linearization and decomposition
- spend majority of effort on local problems
- local problems are smaller and better nonlinearly conditioned
- create better nonlinearly conditioned global problem, Jacobian-free
- high concurrency through domain decomposition

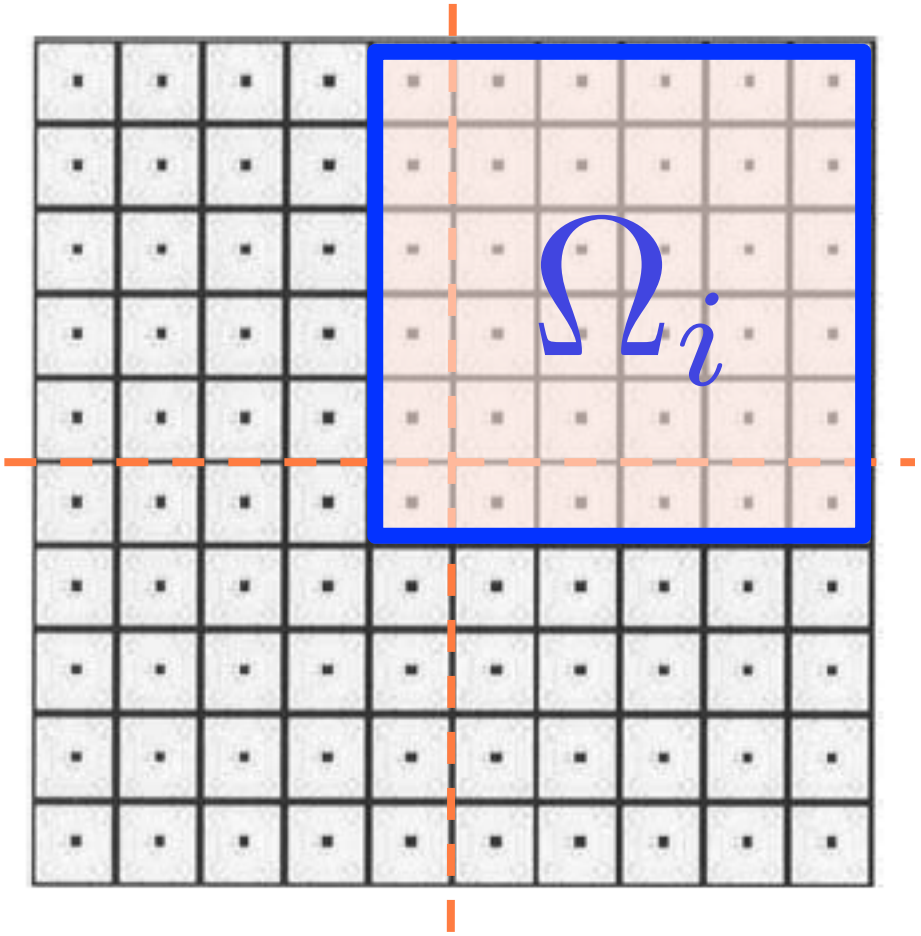
2010: Relax global synchronization requirements of Newton

- fewer global synchronizations
- local synchronizations, asynchronous to each other

2015: Further robustify Newton for multiphysics systems

- Multiplicative Schwarz Preconditioned Inexact Newton (MSPIN)
- precondition multiphysics through (sequential) uniphysics solves
- nest ASPIN (on subdomains) inside MSPIN, for reasons above

ASPIN: nonlinear domain decomposition



$$\Omega = \bigcup_{i=1}^{N} \Omega_i, \quad i = 1, \ldots, N$$

ASPIN: construction through local solves

- **Concurrent (possibly overlapping) local solves for local corrections, using existing code**

$$F_{\Omega_i}(u - T_{\Omega_i}(u)) = 0, \qquad i = 1, \ldots, N$$

- **Sum for global residual**

$$\mathcal{F}(u) = \sum_{i=1}^{N} T_{\Omega_i}(u), \qquad \bigcup_{i=1}^{N} \Omega_i = \Omega$$

- **Finite difference for global Jacobian-vector product**
- **No new code required for $\mathcal{F}$ or its Jacobian $\mathcal{J}$**

Inexact Newton w/Backtracking

ALGORITHM 1 (INB).
An initial iterate $x^{(0)}$ is given. For $k = 0, 1, 2, \ldots$ until convergence:

1. Find an inexact Newton direction $d^{(k)}$ such that

$$\|F(x^{(k)}) - F'(x^{(k)})d^{(k)}\| \leq \eta_k \|F(x^{(k)})\|. \tag{1.2}$$

2. Determine a step size $\lambda^{(k)}$ using a backtracking linesearch technique based on the function $f(x) = \frac{1}{2}\|F(x)\|^2$.
3. Compute a new approximate solution

$$x^{(k+1)} = x^{(k)} - \lambda^{(k)} d^{(k)}. \tag{1.3}$$

- **For strict Newton, $\eta_k = 0$ *and* $\lambda^{(k)} = 1$**
- **loose tolerance on forcing term η_k when INB used as an outer method**
- **tight tolerance when used as an inner method**
- **dependence on η_k characterized later**

ASPIN: 2-component example
(nonoverlapping)

Original system

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

Transformed system

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

where (u,v) are obtained implicitly by solving independently

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

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

ASPIN: 2-component example (cont.)

Jacobian of preconditioned system

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

where $p = u - g(u,v)$ **and** $q = v - h(u,v)$

Since (p,q) **approach** (u,v) **as the solution converges locally, the preconditioned Jacobian is locally well approximated by the readily computable**

$$\hat{\mathcal{J}}(u,v) = \begin{bmatrix} G_u^{-1} & \\ & H_v^{-1} \end{bmatrix} \begin{bmatrix} G_u & G_v \\ H_u & H_v \end{bmatrix} = \begin{bmatrix} G_u & \\ & H_v \end{bmatrix}^{-1} J(u,v)$$

Diagonal blocks of this product are identities, so linear conditioning depends on coupling strength in the off-diagonals

ASPIN: 2-component example (cont.)

Operationally, the approximate preconditioned matvec

$$\hat{\mathcal{J}}x = y$$

is straightforward, in terms of code for the original problem:

1. Perform the multiplication $w = Jx$, $w = [w_1, w_2]^T$.
2. Solve $G_u y_1 = w_1$ and $H_v y_2 = w_2$.
3. Form the result $y = [y_1, y_2]^T$.

Generalization to 3 or more components is natural

Multiplicative generalizations

- [Kahou et al., 2007, 2008] **: multiplicative generalization of linear additive Schwarz (Richardson and Krylov-accelerated)**
  - **applied to standard sparse test matrices**
  - **of limited interest due to lack of exploitation of concurrency**
- [Ernst et al., 2007] **: multiplicative generalization of nonlinear additive Schwarz (Richardson)**
  - **applied to acoustic-structure interaction (the structure being nonlinear)**
  - **remarked: "inexact Newton generalization is future work"**
- [Liu & Keyes, 2015] **: multiplicative Schwarz preconditioned inexact Newton (MSPIN)**
  - **interesting for multicomponent problems, where the number of multiplicative stages is small**
  - **each stage represents a different component of the physics, for which an individual solver is presumed available**

Source of today's talk

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FIELD-SPLIT PRECONDITIONED INEXACT NEWTON ALGORITHMS*

LULU LIU† AND DAVID E. KEYES†

Abstract. The multiplicative Schwarz preconditioned inexact Newton (MSPIN) algorithm is presented as a complement to additive Schwarz preconditioned inexact Newton (ASPIN). At an algebraic level, ASPIN and MSPIN are variants of the same strategy to improve the convergence of systems with unbalanced nonlinearities; however, they have natural complementarity in practice. MSPIN is naturally based on partitioning of degrees of freedom in a nonlinear PDE system by field type rather than by subdomain, where a modest factor of concurrency can be sacrificed for physically motivated convergence robustness. ASPIN, originally introduced for decompositions into subdomains, is natural for high concurrency and reduction of global synchronization. We consider both types of inexact Newton algorithms in the field-split context, and we augment the classical convergence theory of ASPIN for the multiplicative case. Numerical experiments show that MSPIN can be significantly more robust than Newton methods based on global linearizations, and that MSPIN can be more robust than ASPIN and maintain fast convergence even for challenging problems, such as high Reynolds number Navier–Stokes equations.

Key words. nonlinear equations, nonlinear preconditioning, field splitting, Newton method, Navier–Stokes equations

AMS subject classifications. 65H10, 65H20, 65N22, 65N55

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MSPIN: 2-component example
(nonoverlapping)

Original system

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

Transformed system

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

where (u,v) are obtained implicitly by solving *sequentially*

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

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

MSPIN: 2-component example (cont.)

Jacobian of preconditioned system

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

where $p = u - g(u,v)$ **and** $q = v - h(u,v)$

As before, since (p,q) **approaches** (u,v) **as the solution converges locally, the preconditioned Jacobian is locally well approximated by the readily computable**

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

MSPIN: 2-component example (cont.)

Operationally, the approximate preconditioned matvec

$$\hat{\mathcal{J}} x = y$$

is again natural, in terms of code for the original problem:

1. Perform the multiplication $w = Jx$, $w = [w_1, w_2]^T$.
2. Let $z_2 = w_2$ and solve $G_p z_1 = w_1$.
3. Perform $z_2 = z_2 - H_p z_1$ and set $y_1 = z_1$.
4. Solve $H_v y_2 = z_2$.
5. Form the result $y = [y_1, y_2]^T$.

Generalization to 3 or more components is block triangular, as expected

Nonlinear preconditioning: theory

- **Assume original Jacobian $J = F'(u)$ is continuous in a neighborhood D of the exact solution u^* and nonsingular at u^***
- [Dryja & Hackbusch, 1997] **: the original subproblems for $T_{\Omega i}$ are all uniquely solvable in a neighborhood of u^* in D**
- [Dryja & Hackbusch, 1997] **: the matrix $\Sigma_i (J_i^+) J$, where J_i represents the Jacobian of the i^{th} subdomain extended to the full space, and J_i^+ denotes its generalized inverse, is nonsingular in a neighborhood of u^* in D**
- Remark **: if $F(u) = b - Au$, this is the usual additive Schwarz preconditioned operator, $\Sigma_i (A_i^+) A$**
- **The Jacobian of the ASPIN modified system $\mathcal{J} = \mathcal{F}'(u)$ approaches $\Sigma_i (J_i^+) J$ as u approaches u^***

Nonlinear preconditioning: theory

- [Cai & K, 2002] : $F(u)$ **and ASPIN's** $\mathcal{F}(u)$ **are equivalent in that they possess the same solution in a neighborhood of** D
- [An, 2005] **: ASPIN local convergence guaranteed**
  - **superlinear if forcing term in inexact Newton approaches** 0
  - **quadratic if forcing term approaches** 0 **like** $O(\|\mathcal{F}(\bullet)\|)$

- [Liu & K, 2014] : $F(u)$ **and MSPIN's** $\mathcal{F}(u)$ **are equivalent in that they possess the same solution in a neighborhood of** D
- [Liu & K, 2015] **: MSPIN local convergence guaranteed**
  - **superlinear if forcing term in inexact Newton approaches** 0
  - **quadratic if forcing term approaches** 0 **like** $O(\|\mathcal{F}(\bullet)\|)$

2-unknown algebraic example [Hwang, 2004]

For ease of manipulation and visualization, consider

$$F_1(x_1, x_2) = (x_1 - x_2^3 + 1)^3 - x_2^3,$$
$$F_2(x_1, x_2) = 2x_1 + 3x_2 - 5.$$

For ASPIN (Jacobi-like)

$$F_1(x_1 - \delta_1^J, x_2) = 0$$
$$F_2(x_1, x_2 - \delta_2^J) = 0$$

$$\Longrightarrow$$

$$\delta_1^J(x_1, x_2) = x_1 - x_2^3 + 1 - x_2,$$
$$\delta_2^J(x_1, x_2) = \frac{2}{3}x_1 + x_2 - \frac{5}{3}.$$

For MSPIN (Gauss-Seidel-like)

$$F_1(x_1 - \delta_1^{GS}, x_2) = 0$$
$$F_2(x_1 - \delta_1^*, x_2 - \delta_2^{GS}) = 0$$

$$\Longrightarrow$$

$$\delta_1^{GS}(x_1, x_2) = x_1 - x_2^3 + 1 - x_2,$$
$$\delta_2^{GS}(x_1, x_2) = \frac{2}{3}x_2^3 + \frac{5}{3}x_2 - \frac{7}{3}.$$

Original vs. ASPIN vs. MSPIN

$$F_1(x_1, x_2) = (x_1 - x_2^3 + 1)^3 - x_2^3,$$
$$F_2(x_1, x_2) = 2x_1 + 3x_2 - 5.$$

One ninth-order, one linear, both equations couple unknowns

$$\delta_1^J(x_1, x_2) = x_1 - x_2^3 + 1 - x_2,$$
$$\delta_2^J(x_1, x_2) = \frac{2}{3}x_1 + x_2 - \frac{5}{3}.$$

All have same root, namely (1,1)

One third-order, one linear, both equations couple unknowns

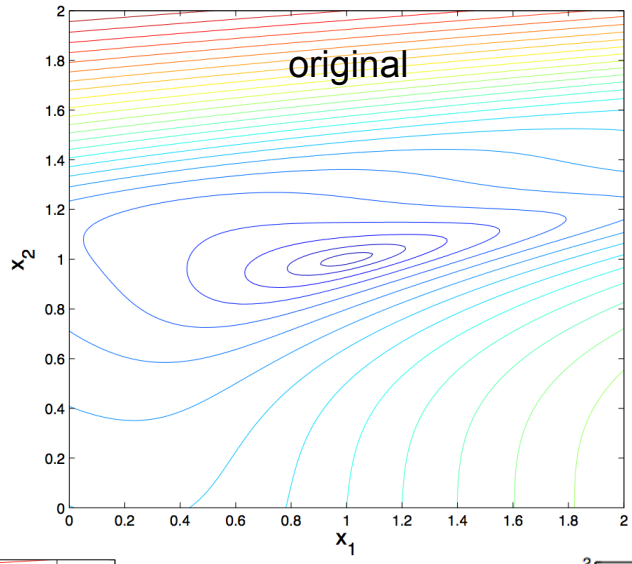
$$\delta_1^{GS}(x_1, x_2) = x_1 - x_2^3 + 1 - x_2,$$
$$\delta_2^{GS}(x_1, x_2) = \frac{2}{3}x_2^3 + \frac{5}{3}x_2 - \frac{7}{3}.$$

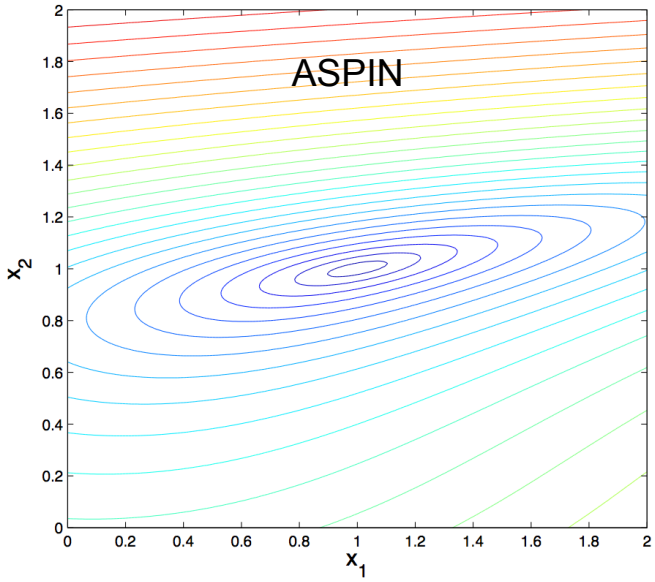
Both third-order, one equation decouples

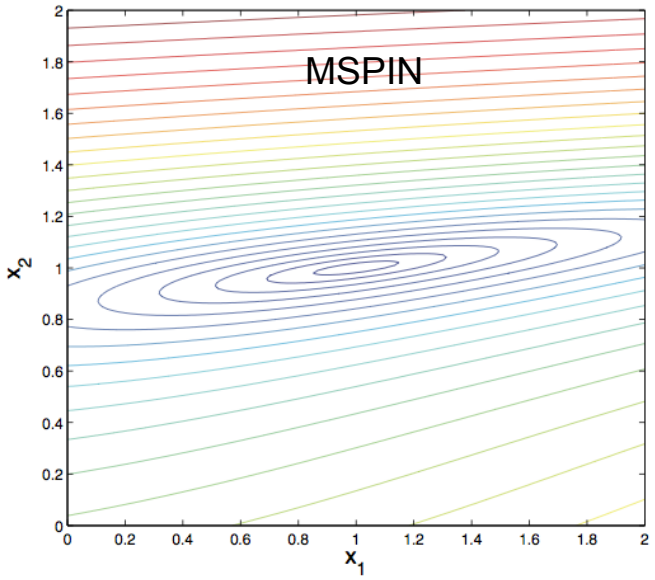
Original vs. ASPIN vs. MSPIN

Contours of

$\log(\|F(x_1,x_2)\| + 1)$







Original vs. ASPIN vs. MSPIN

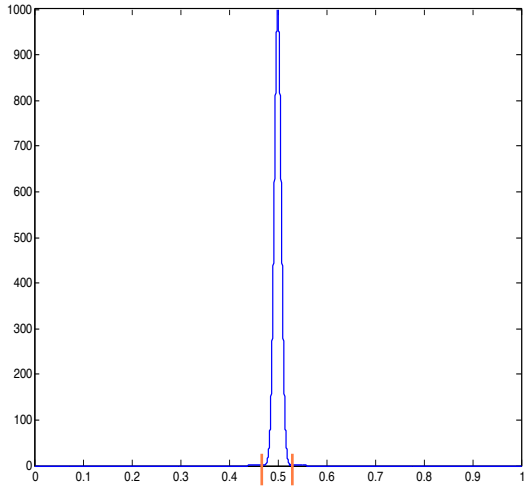
TABLE 1

The number of nonlinear iterations. The outer global tolerance is 10^{-8}*, and the inner component tolerances are both* 10^{-3}.

Initial guess x_0	INB	ASPIN	MSPIN
$x_0 = (0,0)^T$	11	7	6
$x_0 = (0,2)^T$	10	7	5
$x_0 = (2,0)^T$	1	8	6
$x_0 = (2,2)^T$	11	7	5

1D BVP example

[Lanzkron, Rose & Wilkes, 1997]



$$-u'' + u^3 + (4 \times 10^8 (x - 0.5)^2 - 2 \times 10^4) u - 10^9 e^{-3(\frac{x-0.5}{0.01})^2} = 0$$

$$x \in (0, 1), \qquad u(0) = 0, \qquad u(1) = 0$$

$$u(x) = 10^3 e^{-(\frac{x-0.5}{0.01})^2}$$

Comparison of the number of nonlinear iterations for different methods in the rightmost three columns. "No. points" indicates the number of grid points used to discretize the ODE. The points between G_{left} and G_{right} are unknowns in G.

No. points	G_{left}	G_{right}	Its. INB	Its. ASPIN	Its. MSPIN
100	48	53	5	2	1
500	236	265	5	2	2
1000	471	530	6	2	1
5000	2351	2650	5	2	2

DAE example (decoupled by component)

[PETSc, ex28]

$$-(vu_x)_x + \lambda u^2 = 1 \text{ on } (0,1), \quad \text{subject to } u(0) = 0,\ u(1) = 1, \tag{5.4}$$

$$\exp(v-1) + v = \frac{1}{\frac{1}{1+u} + \frac{1}{1+u_x^2}}, \tag{5.5}$$

Global nonlinear and linear iterations using globalized INB, ASPIN and MSPIN. $\epsilon_{global-nonlinear-rtol} = 10^{-10}$, $\epsilon_{global-linear-rtol} = 10^{-8}$, $\epsilon_{sub-nonlinear-rtol} = 10^{-3}$. *"$*$" indicates that linear iterations are not available, since the nonlinear methods stagnate at the line search.*

	Number of PIN iterations				
Methods	$\lambda = 0$	$\lambda = 100$	$\lambda = 1000$	$\lambda = 3000$	$\lambda = 5000$
INB	6	6	15	-	9
ASPIN	6	-	-	-	-
MSPIN	5	5	5	5	5
	Average number of GMRES iterations per PIN				
INB	12	18	14	*	7
ASPIN	21	*	*	*	*
MSPIN	10	9	8	8	7

3-field PDE example

[PETSc, ex19]

$$(5.6)\qquad \begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0, \\ -\frac{1}{Re}\Delta \omega + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} = 0. \end{cases}$$

Here $u = 1, v = 0$ on the top boundary and $u = 0, v = 0$ on the other boundaries. The boundary condition on ω is given by its definition:

$$(5.7)\qquad \omega(x,y) = -\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}.$$

MSPIN splitting

$$G: \quad \begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0, \end{cases}$$

$$H: \quad -\frac{1}{Re}\Delta \omega + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} = 0.$$

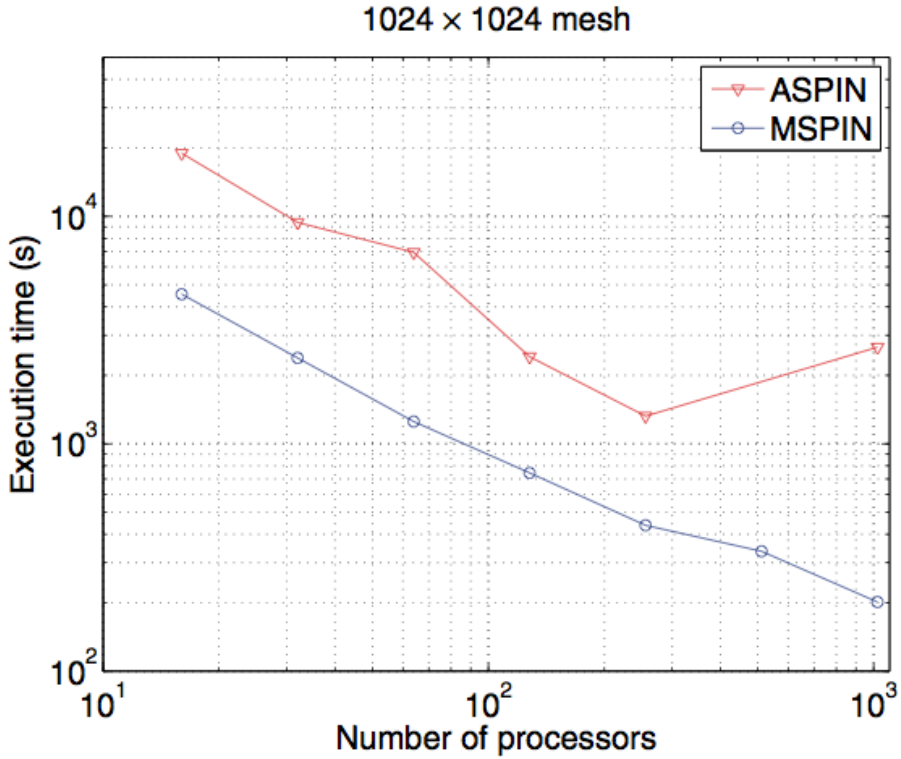
***G, H* systems are now linear among their "own" unknowns**

MSPIN: 3-field PDE example

Global nonlinear and linear iterations using globalized INB, ASPIN, and MSPIN on different mesh sizes. The initial guess is zero for u, v, and ω. $\epsilon_{global-linear-rtol} = 10^{-6}$, $\epsilon_{global-nonlinear-rtol} = 10^{-10}$. The finite difference step size for the matrix-free Jacobian applications is 10^{-8}. "$**$" indicates that nonlinear iterations are not available, because linear iterations fail to converge after $10,000$ steps.

64×64 mesh			
Number of PIN iterations			
Methods	$Re = 10$	$Re = 100$	$Re = 1000$
INB	3	5	17
ASPIN	4	9	10
MSPIN	4	5	4
Average number of GMRES iterations per PIN			
INB	19	24	26
ASPIN	23	37	39
MSPIN	13	18	15
128×128 mesh			
Number of PIN iterations			
Methods	$Re = 10$	$Re = 100$	$Re = 1000$
INB	3	5	$**$
ASPIN	4	9	13
MSPIN	4	5	5
Average number of GMRES iterations per PIN			
INB	37	62	-
ASPIN	41	42	64
MSPIN	14	21	20
256×256 mesh			
Number of PIN iterations			
Methods	$Re = 10$	$Re = 100$	$Re = 1000$
INB	3	5	$**$
ASPIN	4	10	18
MSPIN	4	6	6
Average number of GMRES iterations per PIN			
INB	93	200	-
ASPIN	75	47	129
MSPIN	15	24	28

MSPIN: 3-field PDE example



Linear subsystems solved with hypre's BoomerAMG

FIG. 5. *Strong scaling for the driven cavity flow problem on a* 1024×1024 *mesh at Reynolds number* 1000. *The initial guess is still zero for* u, v, ω. $\epsilon_{global-linear-rtol} = 10^{-3}$, $\epsilon_{global-nonlinear-rtol} = 10^{-8}$, $\epsilon_{sub-rtol} = 10^{-3}$, *and* $\epsilon_{Jac-rtol} = 10^{-3}$. $\epsilon_{sub-rtol}$ *denotes the relative tolerance for the subproblems (which are linear in this example), and we specify* $\epsilon_{Jac-rtol}$ *as the relative tolerance for the linear problems in* (2.13) *and* (2.29). *The finite difference step size for the matrix-free Jacobian applications is* 10^{-8}. *Execution time for ASPIN using* 512 *processors is not shown since it fails to converge on this mesh and this Reynolds number from a zero initial guess.*

MSPIN: 3-field PDE example

Execution times for strong scaling of the lid-driven cavity for ASPIN and MSPIN on a 256×256 *mesh at Reynolds number 1000, for tight and loose relative convergence tolerances on the subproblems and global preconditioner linear systems solutions. The initial guess is zero for* u, v, *and* ω. $\epsilon_{global-linear-rtol} = 10^{-6}$, $\epsilon_{global-nonlinear-rtol} = 10^{-8}$. $\epsilon_{sub-rtol}$ *denotes the relative tolerance for the subproblems (which are linear in this example), and we specify* $\epsilon_{Jac-rtol}$ *as the relative tolerance for the linear problems in* (2.13) *and* (2.29). *The finite difference step size for the matrix-free Jacobian applications is* 10^{-8}. *"* N_p*" indicates the number of processors, which does not have to be square. Performance for INB is not shown since it fails to converge on this mesh and this Reynolds number from a zero initial guess.*

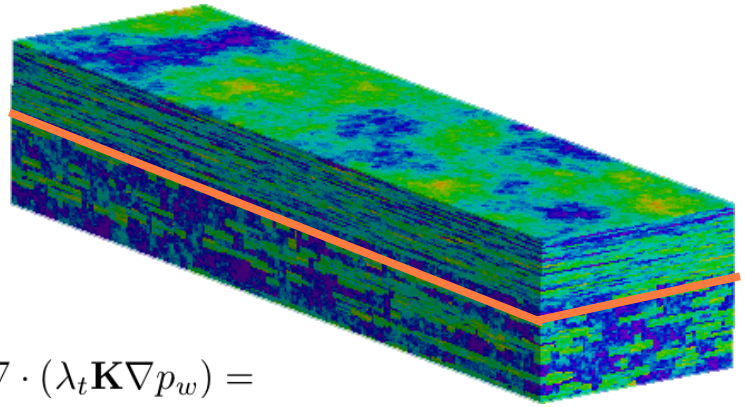
Execution time (s)					
	256 × 256 mesh				
Methods	N_p	$\epsilon_{sub-rtol} = 10^{-3}$ $\epsilon_{Jac-rtol} = 10^{-3}$	$\epsilon_{sub-rtol} = 10^{-3}$ $\epsilon_{Jac-rtol} = 10^{-6}$	$\epsilon_{sub-rtol} = 10^{-6}$ $\epsilon_{Jac-rtol} = 10^{-3}$	$\epsilon_{sub-rtol} = 10^{-6}$ $\epsilon_{Jac-rtol} = 10^{-6}$
ASPIN	4	2363.98	3273.88	2194.43	3219.34
	16	687.68	943.91	654.32	976.95
	32	397.12	589.86	395.26	588.95
	64	272.4	412.27	276.03	405.92
MSPIN	4	175.31	245.59	199.64	248.18
	16	57.04	74.06	56.74	74.48
	32	32.17	45.86	34.55	46.33
	64	22.31	31.64	23.90	31.79

Examples

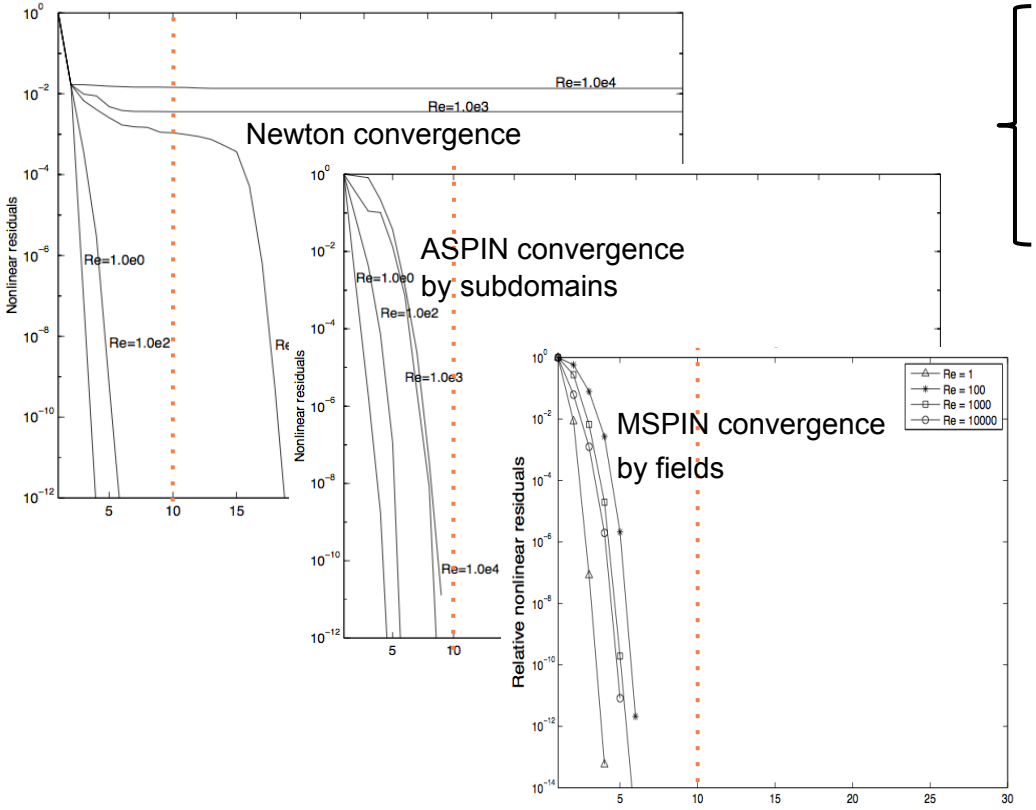
Driven cavity model (ex19 in PETSc)

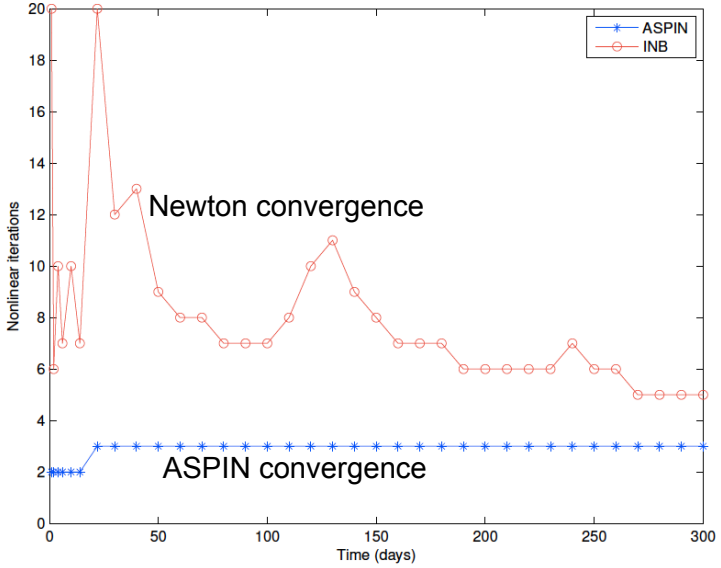
$$\begin{cases} -\Delta u - \dfrac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \dfrac{\partial \omega}{\partial x} = 0, \\ -\frac{1}{Re}\Delta \omega + u\dfrac{\partial \omega}{\partial x} + v\dfrac{\partial \omega}{\partial y} = 0. \end{cases}$$

reservoir model (SPE10)



$$\begin{cases} -\nabla \cdot (\lambda_t \mathbf{K} \nabla p_w) = \\ q_t + \nabla \cdot (\lambda_n \mathbf{K} \nabla p_c) - \nabla \cdot ((\lambda_n \rho_n + \lambda_w \rho_w)\mathbf{K}\mathbf{g}), \\ \phi \dfrac{\partial S_w}{\partial t} - \nabla \cdot (\lambda_w \mathbf{K}(\nabla p_w - \rho_w \mathbf{g})) = q_w. \end{cases}$$





MSPIN: an alternative multiphysics solver

- Given a two-component multiphysics system

$$G(u, v) = 0$$
$$H(u, v) = 0$$

- Each physics component typically has its own implicit solver, e.g.,

$$u = \mathcal{G}(v)$$

- One can do nonlinear elimination by nesting solvers, e.g.,

$$H(\mathcal{G}(v), v) = 0$$

- Or one can do Newton on the full system

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

- The first is likely inefficient; the second likely non-robust

Comment

- **Newton was not doomed before nonlinear preconditioning**
- **Other relevant globalization methods**
  - **mesh continuation: approach the problem on the mesh of desired resolution by initial guesses recursively built up from easier Newton problems on coarser meshes**
  - **pseudo-transient continuation: approach the steady state by a transient approach in the vorticity equation, with implicit time step eventually approaching infinity**
  - **Parameter homotopy: approach the problem at the desired parameter value by initial guesses projected by Davidenko's method from an easier value**
- **These may also be *combined* with nonlinear preconditioning**

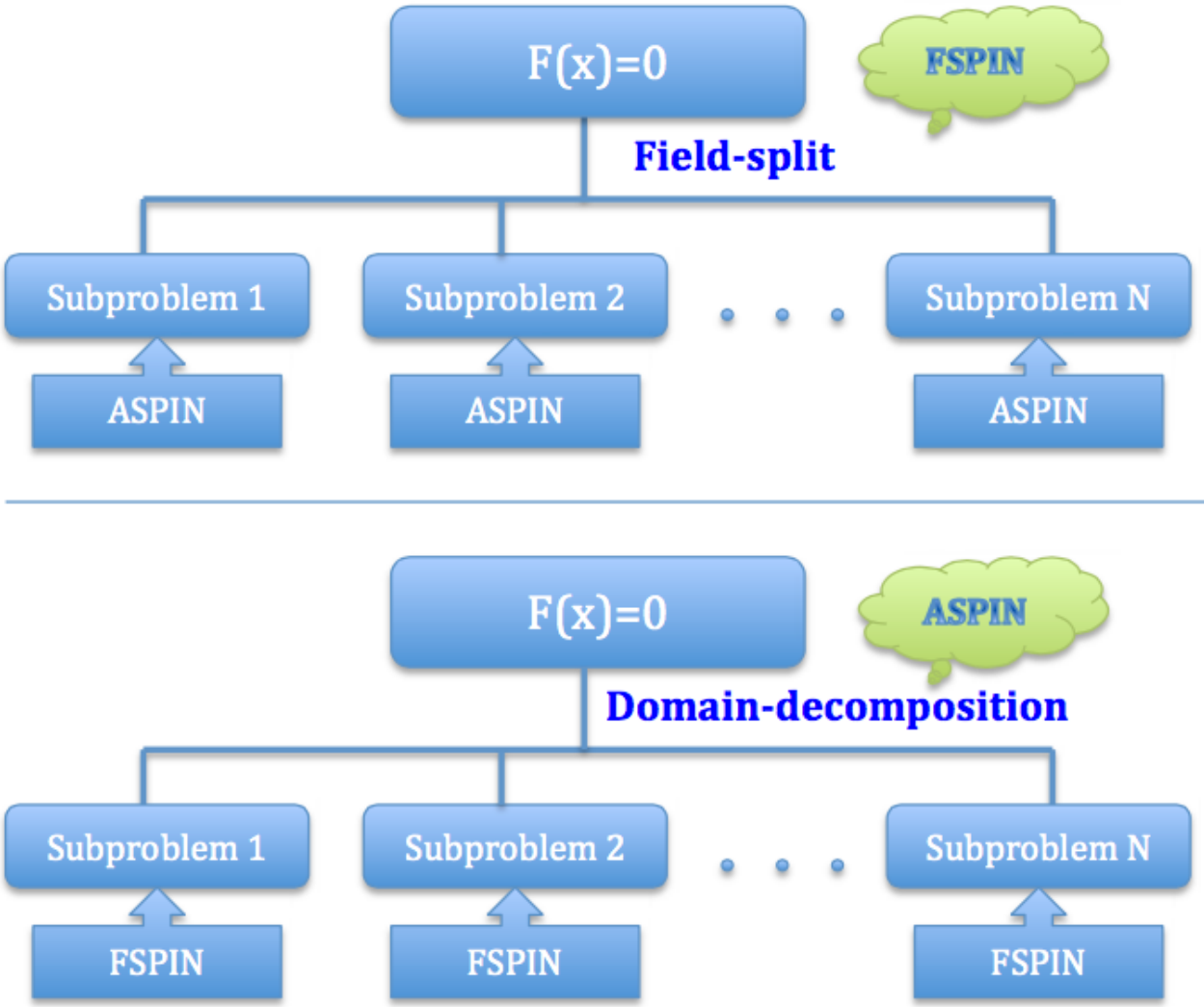
Caveat

- **Newton is ever more art than science…**
- **Picking** $u, v, \ldots$ **and corresponding** $G, H, \ldots$ **is not trivial**
- **Different groupings and different orderings can change the quality of the preconditioning – even dramatically**
  - **generally good to order the linear subsystem (or the "least" nonlinear subsystems) first**
  - **generally good to try to keep the "most" nonlinear subsystems as small as possible and order last**
  - **sometimes splitting the systems by component yields equations that are linear among their own local unknowns**

Future work

- **Applications: gain more experience on problems difficult to converge globally any other way**
- **Improvements: the modified Jacobian is known only in the form of matvecs and is therefore a challenge to precondition further**
  - **should inner preconditioning therefore include a spatially hierarchical component?**
- **Theory: try to come up with measures of nonlinearity for different subsystems**
  - **will vary with input arguments**
  - **cannot deduce from form of equations alone**
- **Software: create high performance implementations**
  - **exploit the permitted asynchrony of inner Newton subproblems, with work-stealing**
  - **nest domain-split ASPIN inside of field-split MSPIN**

Field splitting and domain decomposition




Thank you
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Extra Slides

Algorithms motivated by exascale roadmap

www.exascale.org/iesp

INTERNATIONAL EXASCALE SOFTWARE PROJECT ROADMAP 1.0

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The International Exascale Software Roadmap, J. Dongarra, P. Beckman, et al., *International Journal of High Performance Computer Applications* **25**(1), 2011, ISSN 1094-3420.

ECRC's algorithmic agenda

- **Reformulate bulk-synchronous homogeneous algs for**
  - **reduced synchronization and communication**
    - **less frequent *and/or* less global** ← Nonlinear Schwarz Preconditioning
  - **greater arithmetic intensity (flops per byte moved into and out of registers and upper cache)**
    - **including assured accuracy with (adaptively) less floating-point precision**
  - **greater SIMD-style thread concurrency for accelerators**
  - **algorithmic resilience to various types of faults**
- **To undertake the exciting applications that exascale is meant to exploit**
  - **"post-forward" problems: optimization, data assimilation, parameter inversion, uncertainty quantification, etc.**

ASPIN: PETSc implementation

petsc-3.6.0 2015-06-09
Report Typos and Errors

SNESASPIN

Helper SNES type for Additive-Schwarz Preconditioned Inexact Newton

Options Database

-npc_snes_ - options prefix of the nonlinear subdomain solver (must be of type NASM)
-npc_sub_snes_ - options prefix of the subdomain nonlinear solves
-npc_sub_ksp_ - options prefix of the subdomain Krylov solver
-npc_sub_pc_ - options prefix of the subdomain preconditioner

Notes: This routine sets up an instance of NETWONLS with nonlinear left preconditioning. It differs from other

similar functionality in SNES as it creates a linear shell matrix that corresponds to the product

\sum_{i=0}^{N_b}J_b({X^b_{converged}})^{-1}J(X + \sum_{i=0}^{N_b}(X^b_{converged} - X^b))

which is the ASPIN preconditioned matrix. Similar solvers may be constructed by having matrix-free differencing of nonlinear solves per linear iteration, but this is far more efficient when subdomain sparse-direct preconditioner factorizations are reused on each application of J_b^{-1}.

See Also

SNESCreate(), SNES, SNESSetType(), SNESNEWTONLS, SNESNASM, SNESGetNPC(), SNESGetNPCSide()

Level:intermediate
Location:src/snes/impls/nasm/aspin.c

Parting quotations

"All linear problems are alike; each nonlinear problem is nonlinear in its own way."

– *K, with apologies to Tolstoy (1878)*

"Every numerical analyst has a favorite preconditioner and you have a perfect chance to find a better one."

– *Gil Strang (1986)*