Nonlinear Multiplicative Schwarz Preconditioning in Natural Convection Cavity Flow

Lulu Liu[1], Wei Zhang[2], and David Keyes[3]

1 Introduction

The multiplicative Schwarz preconditioned inexact Newton (MSPIN) algorithm, as a complement to additive Schwarz preconditioned inexact Newton (ASPIN), provides a Gauss-Seidel-like way to improve the global convergence of systems with unbalanced nonlinearities. To demonstrate, a natural convection cavity flow PDE system is solved using nonlinear multiplicative Schwarz preconditioners resulting from different groupings and orderings of the PDEs and their associated fields, and convergence results are reported over a range of Rayleigh number, a dimensionless parameter representing the ratio of convection to diffusion, and in this case, of the magnitude of nonlinear to the linear terms in the transport PDEs. The robustness of nonlinear convergence with respect to Rayleigh number is sensitive to the grouping strategy.

Globally nonlinearly implicit methods, such as Newton-Krylov-Schwarz, work well for many problems, but they may be frustrated by "nonlinear stiffness," which results in stagnation of residual norms or even failure of global Newton iterations. Nonlinear preconditioning may improve global convergence of nonlinearly stiff problems by changing coordinates and solving a different system possessing the same root by an outer Jacobian-free [8] Newton method.

Though algebraically related, ASPIN and MSPIN arise from different motivations. Additive Schwarz preconditioned inexact Newton [1], was based on domain decomposition when proposed in 2002. It is shown in, e.g., [1, 2, 3, 7, 11] that ASPIN is effective in reducing the number of globally synchronizing outer Newton iterations, at the price of solving in parallel

[1] Program in Applied Mathematics and Computational Science and Extreme Computing Research Center, lulu.liu@kaust.edu.sa · [2] Program in Mechanical Engineering, wei.zhang@kaust.edu.sa · [3] Program in Applied Mathematics and Computational Science and Extreme Computing Research Center, david.keyes@kaust.edu.sa. King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia.

many smaller subdomain-scale nonlinear systems. Motivated instead by splitting physical fields, multiplicative Schwarz preconditioned inexact Newton algorithm [9] was introduced in 2015. MSPIN solves physical submodels sequentially, and different groupings and different orderings result in different preconditioned functions. These two types of preconditioning can be nested.

2 MSPIN

Given the discrete nonlinear function $F : R^n \to R^n$, we want to find $x^* \in R^n$ such that

$$F(x^*) = 0, \tag{1}$$

where $F(x) = [F_1(x), F_2(x), \ldots, F_n(x)]^T$ and $x = [x_1, x_2, \ldots, x_n]^T$. We assume that $F(x)$ in (1) is continuously differentiable. The function $F(x)$ is split into $2 \leqslant N \leqslant n$ nonoverlapping components representing distinct physical features as

$$F(x) = F(u_1, \ldots, u_N) = \begin{bmatrix} \hat{F}_1(u_1, \ldots, u_N) \\ \vdots \\ \hat{F}_N(u_1, \ldots, u_N) \end{bmatrix} = 0, \tag{2}$$

where $x = [x_1, \ldots, x_n]^T = [u_1, \ldots, u_N]^T \in R^n$. u_i and $\hat{F}_i$ denote conformal subpartitions of x and F, respectively, $i = 1, \ldots, N$.

The inexact Newton method with backtracking (INB) [5, 6, 10] serves as the basic component of MSPIN, so we first review the framework of INB.

Algorithm 1 (INB).

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

1. Choose η_k and find an approximate Newton step $d^{(k)}$ such that

$$\|F(x^{(k)}) - F'(x^{(k)})d^{(k)}\| \leq \eta_k \|F(x^{(k)})\|. \tag{3}$$

2. Determine $\lambda^{(k)}$ using a backtracking linesearch technique [5].

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

$\eta_k \in [0, 1)$ is a "forcing term," and determines how accurately we solve $F'(x^{(k)})d^{(k)} = F(x^{(k)})$. As η_k approaches 0, INB becomes ordinary Newton with backtracking (NB).

In the MSPIN algorithm, the submodels are solved sequentially for the physical variable corrections, and the preconditioned system consists of the sum of these corrections. The multiplicative Schwarz preconditioned function

$$\mathcal{F}(x) = \begin{bmatrix} T_1(u_1, \ldots, u_N) \\ \vdots \\ T_N(u_1, \ldots, u_N) \end{bmatrix} \tag{4}$$

is obtained by solving the following equations:

$$\begin{aligned} &\hat{F}_1(u_1 - T_1(x), u_2, u_3, \ldots, u_N) = 0, \\ &\hat{F}_2(u_1 - T_1(x), u_2 - T_2(x), u_3, \ldots, u_N) = 0, \\ &\qquad \vdots \\ &\hat{F}_N(u_1 - T_1(x), u_2 - T_2(x), u_3 - T_3(x), \ldots, u_N - T_N(x)) = 0. \end{aligned} \tag{5}$$

As with ASPIN, MSPIN solves the global preconditioned problem in (4) using INB in Algorithm 1, which requires only Jacobian-vector multiplication.

In general, the Jacobian $\mathcal{F}'(x) = \mathcal{J}(x)$ is dense. Fortunately, as shown in [9], the Jacobian of preconditioned function $\mathcal{F}(x)$ can be written as follows:

$$\mathcal{J}(x) = \begin{bmatrix} \frac{\partial \hat{F}_1}{\partial \delta_1} & & & \\ \frac{\partial \hat{F}_2}{\partial \delta_1} & \frac{\partial \hat{F}_2}{\partial \delta_2} & & \\ \vdots & \vdots & \ddots & \\ \frac{\partial \hat{F}_N}{\partial \delta_1} & \frac{\partial \hat{F}_N}{\partial \delta_2} & \cdots & \frac{\partial \hat{F}_N}{\partial \delta_N} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial \hat{F}_1}{\partial \delta_1} & \frac{\partial \hat{F}_1}{\partial u_2} & \frac{\partial \hat{F}_1}{\partial u_3} & \cdots & \frac{\partial \hat{F}_1}{\partial u_N} \\ \frac{\partial \hat{F}_2}{\partial \delta_1} & \frac{\partial \hat{F}_2}{\partial \delta_2} & \frac{\partial \hat{F}_2}{\partial u_3} & \cdots & \frac{\partial \hat{F}_2}{\partial u_N} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{\partial \hat{F}_N}{\partial \delta_1} & \frac{\partial \hat{F}_N}{\partial \delta_2} & \frac{\partial \hat{F}_N}{\partial \delta_3} & \cdots & \frac{\partial \hat{F}_N}{\partial \delta_N} \end{bmatrix}, \tag{6}$$

where $\delta_i = u_i - T_i(x)$. Due to the continuity of $F(x)$, we know that $T_i(x) \to 0$ and $\delta_i \to x$ when x approaches the exact solution x^*. In practical implementations, it is more convenient to use the following approximate Jacobian

$$\hat{\mathcal{J}}(x) = L(x)^{-1} J(x)|_{x=[\delta_1,\ldots,\delta_N]^T}, \tag{7}$$

where $J(x) = F'(x) = \left(\frac{\hat{F}_i}{u_j}\right)_{N\times N}$ and $L(x)$ is the lower triangular part of $J(x)$. Functions from the original code may be used to compute $\hat{\mathcal{J}}(y)z$ for any given vectors y, z, matrix-free, rather than forming Jacobian $\mathcal{J}(x)$ explicitly.

3 Natural Convection Cavity Flow Problem

We consider a benchmark problem [4] that describes the two-dimensional natural convection cavity flow of a Boussinesq fluid with Prandtl number 0.71 in an upright square cavity $\Omega = (0,1) \times (0,1)$. Following [12], the nondimensional steady-state Navier-Stokes equations in vorticity-velocity form and energy equation are formulated as:

$$\begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0, \\ -(\frac{Pr}{Ra})^{0.5}\Delta\omega + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} - \frac{\partial T}{\partial x} = 0, \\ -(\frac{1}{PrRa})^{0.5}\Delta T + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = 0, \end{cases} \tag{8}$$

where Pr and Ra denote the Prandtl number and the Rayleigh number, respectively. There are four unknowns: the velocities u, v, the vorticity ω, and the temperature T.

The upright square cavity is filled with air ($Pr = 0.71$). Boundary conditions are described as follows. On the solid walls, both velocity components u, v are zero, and the vorticity is determined from its definition:

$$\omega(x, y) = -\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}. \tag{9}$$

The horizontal (top and bottom) walls are insulated, $\frac{\partial T}{\partial y} = 0$, and the vertical walls are maintained at temperatures $T = 0.5$ (left) and $T = -0.5$ (right). The temperature difference drives circulation in the cavity through the Boussinesq buoyancy term in the vorticity equation. In Figure 1, we compare contours of temperature T at different Rayleigh numbers, where higher Ra boosts the buoyant convection relative to diffusion.

Considering the partition with respect to velocity unknowns, the vorticity unknown, and the temperature unknown, we split the system (8) into three submodels:

$$F_T : \quad -(\frac{1}{PrRa})^{0.5}\Delta T + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = 0, \tag{10}$$

$$F_\omega : \quad -(\frac{Pr}{Ra})^{0.5}\Delta\omega + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} - \frac{\partial T}{\partial x} = 0, \tag{11}$$

$$F_{u,v} : \quad \begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0. \end{cases} \tag{12}$$

A finite difference scheme with the 5-point stencil is used to discretize the PDEs, and the first order upwinding is used in both the vorticity equation and the temperature equation.

3.1 Effect of Ordering

In the framework of MSPIN, even when the partition of unknowns and equations is determined, different orderings for solving subproblems result in different nonlinear preconditioners.

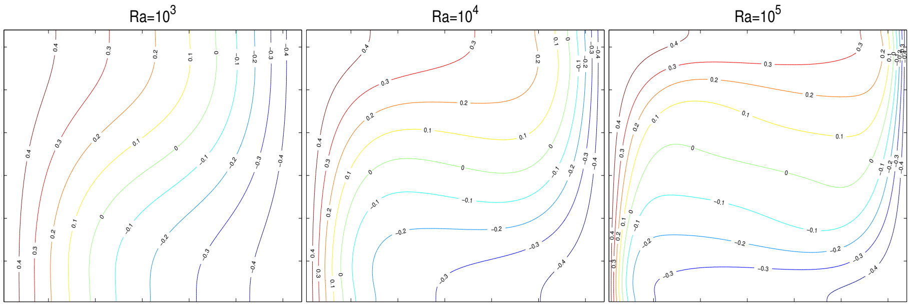

Fig. 1 Contours of temperature T at Rayleigh numbers over 2 orders of magnitude.

We consider two different orderings in the MSPIN algorithm for the natural convection cavity flow problem:

- Ordering A:
$$\hat{F}_1(x) = \begin{bmatrix} F_T \\ F_\omega \end{bmatrix}, \qquad \hat{F}_2(x) = F_{u,v}. \tag{13}$$
- Ordering B:
$$\hat{F}_1(x) = F_{u,v}, \qquad \hat{F}_2(x) = \begin{bmatrix} F_T \\ F_\omega \end{bmatrix}. \tag{14}$$

Independent of ordering, $\hat{F}_1(x)$ and $\hat{F}_2(x)$ are both linear among their own unknowns, and are thus solved by GMRES alone with the tolerance $\epsilon_{sub-lin-rtol}$ ($\equiv \epsilon_{sub-nonlin-rtol}$) $= 10^{-5}$. The nonlinear system (8) is discretized on 100×100 mesh. We set the tolerances for outer Newton iterations as $\epsilon_{global-lin-rtol} = 10^{-6}$ and $\epsilon_{global-nonlin-rtol} = 10^{-10}$. The initial guess is zero for u, v, and ω, and linear interpolation in x for T. Figure 2 compares the convergence history of nonlinear preconditioners corresponding to Ordering A and Ordering B at different Rayleigh numbers. Using Ordering A MSPIN converges for all tests, while using Ordering B it fails at $Ra = 8000$ due to failure of backtracking. However, performance is inconsistent; compared with B, A requires fewer global Newton iterations at $Ra = 30000$, but more iterations at $Ra = 50000$. As shown in Table 1, for this high a Rayleigh number on this fine a grid, with a "cold" initial iterate as above, unpreconditioned globalized Newton stagnates outside of the zone of quadratic convergence.

3.2 Effect of Grouping

For the natural convection cavity flow problem, we can obtain different nonlinear preconditioners by grouping different PDEs and their corresponding unknowns. We consider four grouping-ordering schemes:

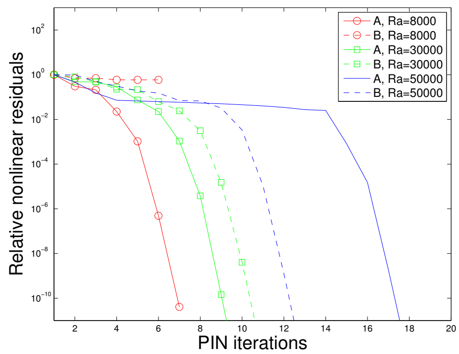

Fig. 2 Convergence history of nonlinear preconditioners using Ordering A (solid lines) and Ordering B (dashed lines).

- Grouping A with two subsystems, $\hat{F}_1 : F_T \;\mid\; \hat{F}_2 : F_\omega,\; F_{u,v}$
- Grouping B with two subsystems, $\hat{F}_1 : F_T,\; F_\omega \;\mid\; \hat{F}_2 : F_{u,v}$
- Grouping C with two subsystems, $\hat{F}_1 : F_T,\; F_{u,v} \;\mid\; \hat{F}_2 : F_\omega$
- Grouping D with three subsystems, $\hat{F}_1 : F_T \;\mid\; \hat{F}_2 : F_\omega \;\mid\; \hat{F}_3 : F_{u,v}$

Table 1 Global nonlinear iterations for NB and MSPIN (plus global linear iterations for MSPIN) at 3 mesh resolutions for each Rayleigh number corresponding to Fig. 1. The initial guess is zero for u, v, and ω, and linear interpolation in x for T. $\epsilon_{global-nonlin-rtol} = 10^{-10}$, $\epsilon_{global-lin-rtol} = 10^{-6}$, $\epsilon_{sub-nonlin-rtol} = 10^{-4}$, and $\epsilon_{sub-lin-rtol} = 10^{-6}$. "*" indicates that one or more subproblems fail to converge or outer backtracking fails. "-" indicates that linear iterations fail to converge within allowed limits.

Ra	No MSPIN NB	Grouping A $F_T \| F_\omega, F_{u,v}$		Grouping B $F_T, F_\omega \| F_{u,v}$		Grouping C $F_T, F_{u,v} \| F_\omega$		Grouping D $F_T \| F_\omega \| F_{u,v}$	
	Newton iter.	Newton	GMRES	Newton	GMRES	Newton	GMRES	Newton	GMRES
64 × 64 mesh, 4 subdomains									
10^3	5	4	5	5	17	4	15	5	17
10^4	*	*		7	27	8	23	6	27
10^5	*	*		18	61		-	17	65
128 × 128 mesh, 16 subdomains									
10^3	5	4	5	5	18	4	16	5	18
10^4	*	*		7	28	10	30	7	28
10^5	*	*		18	110		-	16	83
256 × 256 mesh, 64 subdomains									
10^3	5	4	5	5	18	4	16	4	18
10^4	*	*		7	31	9	32	7	31
10^5	*	*			-		-	19	97

The subproblems corresponding to Groupings B and D are linear, and are solved here by GMRES with BoomerAMG preconditioning. With Groupings A and C, one subproblem is linear and the other one is still nonlinear, which is solved by an internal invocation of INB. The elements of the global MSPIN Jacobians $\hat{\mathcal{J}}$ are not explicitly available, so the global linear problems inherit a conditioning from the subproblem solutions that is hard to improve further; hence, we tabulate the total number of linear iterations required in all of the Newton steps.

Table 1 compares a global Newton method with backtracking (NB), in which the Newton correction is always solved for accurately, with MSPIN algorithms corresponding to different grouping-ordering schemes. When MSPIN algorithms with Groupings B and D converge on a given mesh at a given Rayleigh number, they have similar numbers of Newton iterations and GMRES iterations. In Table 1, MSPIN algorithms with Grouping A, B or C fail to converge in some cases. Sometimes, GMRES on $\hat{\mathcal{J}}$ does not converge within the allowed number of iterations. Sometimes, the outer INB still cannot converge due to failure of the global line search, even though residuals decrease in the early iterations. However, the most decomposed MSPIN algorithm, Grouping D, works in all cases. Experimentally, the groupings play an essential role in determining the quality of nonlinear preconditioning.

Checking corresponding entries for nonlinear iteration count across different mesh densities at the same Rayleigh number in Table 1, we observe that Newton is asymptotically insensitive to the mesh resolution, as expected by theory.

As shown in [9] on a related forced convection problem, additive field-split nonlinear preconditioning can be much less robust than multiplicative. However, classical ASPIN based on domain decomposition can be effective for such problems at high Reynolds or Raleigh numbers, when properly tuned. ASPIN for system (8) with $Ra = 10^5$ on a 128×128 mesh with 16 subdomains and overlap=3, with the same tolerance parameters used in Table 1, converges in 8 Newton iterations. However, this case fails with smaller overlap.

4 Conclusions

MSPIN is used to solve a nonlinear flow problem, with backtracking line-search as the only globalization technique, in the absence of any other physically based globalization strategy normally employed in Newton's method on such problems, such as mesh sequencing or parameter continuation. We experiment with different groups and orderings, since there is not yet a theory for their selection in nonlinear Schwarz preconditioning. Groupings are exhibited that robustify Newton's method even on a fine mesh at high Rayleigh number from a "cold start" initial guess – a regime in which a traditional global Newton method with backtracking alone is completely ineffective.

5 Acknowledgements

The authors acknowledge support from KAUST's Extreme Computing Research Center and the PETSc group of Argonne National Laboratory.

References

[1] X.-C. Cai and D. E. Keyes. Nonlinearly preconditioned inexact Newton algorithms. *SIAM J. Sci. Comput.*, 24(1):183–200, 2002.
[2] X.-C. Cai, D. E. Keyes, and L. Marcinkowski. Nonlinear additive Schwarz preconditioners and application in computational fluid dynamics. *Int. J. Numer. Meth. Fluids*, 40(12):1463–1470, 2002.
[3] X.-C. Cai, D. E. Keyes, and D. P. Young. A nonlinear additive Schwarz preconditioned inexact Newton method for shocked duct flows. In *Domain Decomposition Methods in Science and Engineering (Lyon, 2000)*, pages 345–352. CIMNE, Barcelona, 2002.
[4] G. De Vahl Davis. Natural convection of air in a square cavity: a bench mark numerical solution. *Int. J. Num. Meth. Fluids*, 3(3):249–264, 1983.
[5] J. E. Dennis, Jr. and Robert B. Schnabel. *Numerical methods for unconstrained optimization and nonlinear equations*, volume 16 of *Classics in Applied Mathematics*. SIAM, Philadelphia, 1996.
[6] S. C. Eisenstat and H. F. Walker. Globally convergent inexact Newton methods. *SIAM J. Optim.*, 4(2):393–422, 1994.
[7] F.-N. Hwang and X.-C. Cai. A parallel nonlinear additive Schwarz preconditioned inexact Newton algorithm for incompressible Navier-Stokes equations. *J. Comput. Phys.*, 204(2):666–691, 2005.
[8] D. A. Knoll and D. E. Keyes. Jacobian-free Newton-Krylov methods: a survey of approaches and applications. *J. Comput. Phys.*, 193(2):357–397, 2004.
[9] L. Liu and D. E. Keyes. Field-split preconditioned inexact Newton algorithms. *SIAM J. Sci. Comput.*, 37(3):A1388–A1409, 2015.
[10] M. Pernice and H. F. Walker. NITSOL: a Newton iterative solver for nonlinear systems. *SIAM J. Sci. Comput.*, 19(1):302–318, 1998.
[11] J. O. Skogestad, E. Keilegavlen, and J. M. Nordbotten. Domain decomposition strategies for nonlinear flow problems in porous media. *J. Comput. Phys.*, 234:439–451, 2013.
[12] C.-H. Zhang, W. Zhang, and G. Xi. A pseudospectral multidomain method for conjugate conduction-convection in enclosures. *Numer. Heat. Tr. B-FUND*, 57(4):260–282, 2010.