Block Preconditioners of Trace Gas Sensor Models

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Motivation

- A *trace gas* is a gas which makes up less than **1%** of the Earth's atmosphere.
- A *trace gas sensor* is a very sensitize device for detecting these gases.

- Current Applications:
  1) Monitoring pollutants
  2) Leak detection
  3) Early fire detection
- Future Applications:
  1) Non-invasive disease diagnosis

Mathematical Model

Coupled pressure-temperature equations of gas:

$$\frac{\partial}{\partial t}\left(\mathcal{T} - \frac{\gamma - 1}{\gamma\alpha}\mathcal{P}\right) - \ell_h c\Delta\mathcal{T} = \mathcal{S}, \quad (1a)$$

$$\gamma\left(\frac{\partial^2}{\partial t^2} - \ell_v c\frac{\partial}{\partial t}\Delta\right)(\mathcal{P} - \alpha\mathcal{T}) - c^2\Delta\mathcal{P} = 0. \quad (1b)$$

$\mathbf{T}$: Temperature

$\mathbf{P}$: Pressure

$\mathbf{S}$: Gaussian heat source

ℓ_h: heat conduction parameter

α: $\left(\frac{\partial P}{\partial T}\right)_v$

$\mathbf{c}$: sound speed

ℓ_v: viscosity parameter

γ: $\frac{c_p}{c_v}$

ω: QTF resonance frequency

Helmholtz Equations

With a time harmonic source term, we can simplify (1) to the time-independent Helmholtz equations:

$$-i\beta\omega\left(T - \frac{\gamma - 1}{\gamma\alpha}P\right) - \beta\ell_h c\Delta T = S, \quad (2a)$$

$$-\gamma(\omega^2 - i\ell_v c\omega\Delta)(P - \alpha T) - c^2\Delta P = 0, \quad (2b)$$

where $\beta = \frac{\alpha^2\gamma^2\omega}{\gamma - 1}$, $T = T_1 + iT_2$ and $P = P_1 + iP_2$.

Theory

- **Theorem :** Problem is continuous and coercive.
- **Theorem :** Optimal L^2 and H^1 error estimates.

Automating the Finite Element Method

We employ the Python interface to FEniCS:

- Construct or import a mesh (Dolfin).
- Efficient assembly of global system matrices (FFC).
- Calculate finite element solution (NumPy, SciPy, PyAMG).

Linear System

The system $A_h u = f$ becomes,

$$\begin{pmatrix} a_1K & a_2M & 0 & -a_3M \\ -a_2M & a_1K & a_3M & 0 \\ -a_4K & -a_3M & a_5K & -H \\ a_3M & -a_4K & H & a_5K \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \\ P_1 \\ P_2 \end{pmatrix} = \begin{pmatrix} S \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (3)$$

Where $\mathbf{K}$ and $\mathbf{M}$ are the stiffness and mass matrices, respectively, and $H = K - \kappa^2 M$ is the Helmholtz matrix.

Classical Preconditioning Techniques

N	GMRES	ILU(3)	Block Jacobi	Block Gauss-Seidel
32	1156	12	269	141
64	4320	14	291	154
128	10000+	44	257	143
256		235	245	134
512		429	231	127

Table: Iteration counts for the unpreconditioned GMRES method and GMRES coupled with the block Jacobi, block Gauss Seidel and Incomplete LU factorization preconditioners using realistic physical data.

Custom Block Preconditioner

The effects of fluid viscosity and thermal conduction described by the characteristic lengths ℓ_v and ℓ_h, respectively, are particularly small. Ignoring terms containing these values suggests the following block preconditioner.

$$P = \begin{pmatrix} 0 & a_2M & 0 & -a_3M \\ -a_2M & 0 & a_3M & 0 \\ 0 & -a_3M & 0 & -H \\ a_3M & 0 & H & 0 \end{pmatrix}. \quad (4)$$

- **Eigenvalue Clustering :** $\lambda(P^{-1}A_h) = 1 + Ch^{-2}$, but $C = \mathcal{O}(10^{-10})$.

Complex Shifted Laplacian

Inverting $\mathbf{P}$ can be reduced to solving a block upper triangular system where we must solve the two Helmholtz sub-problems. For this we apply the now common complex shifted Laplacian preconditioner.

$$P_H = K - (\alpha + i\beta)\kappa^2 M \quad (5)$$

where α and β are real numbers chosen such that multigrid methods are known to behave better on P_H than on $\mathbf{H}$ itself.

Numerical Results

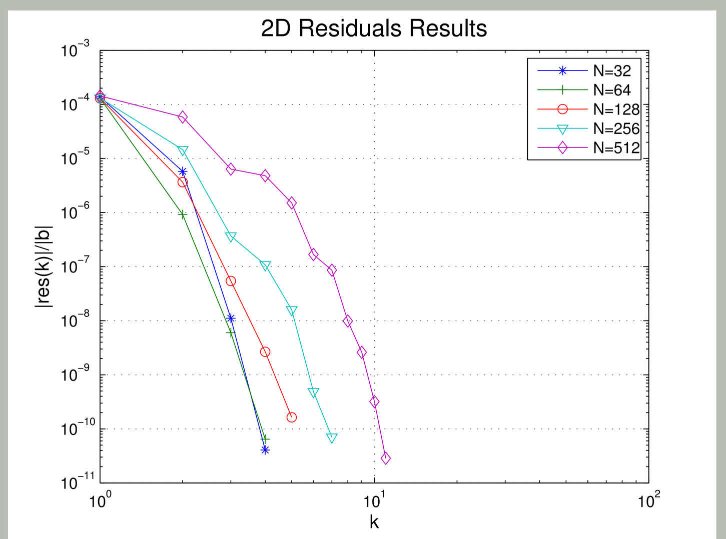

Figure: Preconditioned residual norms at the $\mathbf{k^{th}}$ GMRES iteration for the 2D problem on various $\mathbf{N \times N}$ meshes.

Future Work

- Test with HPC parallel libraries such as Trilinos or PETSc.
- Experiment with alternative methods for Helmholtz problems.
- Couple current problem with an elasticity model for tuning fork boundary.

References

- B. Brennan, R. C. Kirby, J. Zweck, and S. Minkoff, "High Performance Python-based Simulations of Pressure and Temperature Waves in a Trace Gas Sensor," PyHPC 2013.
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