Block Preconditioners for a Coupled Pressure-Temperature Model of Trace Gas Sensors

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Introduction to Trace Gas Sensing

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- **Current Applications**:

  1. Monitoring atmospheric pollutants
  2. Leak detection
  3. Early fire detection on spacecraft

- **Future Applications**:

  1. Non-invasive disease diagnosis

Introduction to Trace Gas Sensing

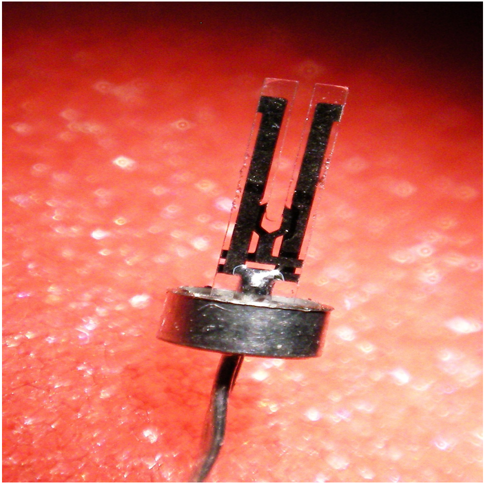
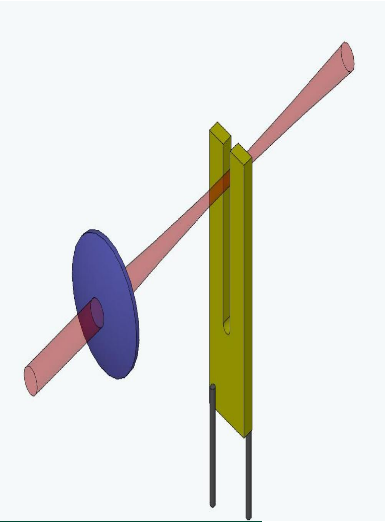


Figure: Trace gas sensor resting on the tip of a finger.

Photo-acoustic Spectroscopy:

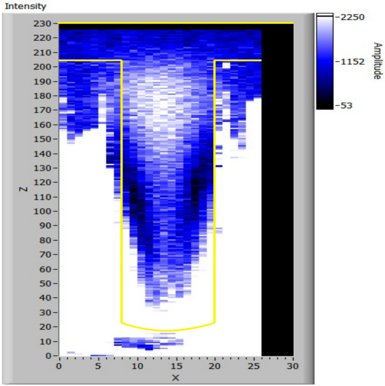


- We fire a modulated laser between the tines of a quartz tuning fork.
- Present gas molecules become excited.
- Thermal and pressure waves are generated.
- Electrodes on the the tuning fork convert waves to electric current.
- The amplitude of the current determines the amount of gas present.

Introduction to Trace Gas Sensing

Current Models:

- Resonant Optothermoacoustic Detection (ROTADE) sensors capture only the thermal wave.
- Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) sensors capture only the pressure wave.



We seek a model which captures both effects simultaneously.

Mathematical Model

Mathematical Model

Coupled pressure-temperature equations of gas:

$$\begin{cases} \dfrac{\partial}{\partial t}\left(T - \dfrac{\gamma - 1}{\gamma\alpha}P\right) - \ell_h c \Delta T = S(x,t) & \text{(1a)} \\ \gamma\left(\dfrac{\partial^2}{\partial t^2} - \ell_v c \dfrac{\partial}{\partial t}\Delta\right)(P - \alpha T) - c^2 \Delta P = 0 \qquad \text{in } \mathbb{R}^2 \backslash \Omega_{TF} & \text{(1b)} \end{cases}$$

- T: temperature
- S: cylindrically sym. Gaussian heat source
- ℓ_h: heat conduction parameter
- α: $\left(\frac{\partial P}{\partial T}\right)_v$
- A: proportional to gas concentration
- P: pressure
- c: sound speed
- ℓ_v: viscosity parameter
- γ: $\frac{c_p}{c_v}$
- ω: QTF resonance frequency

Mathematical Model

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

$$\begin{cases} -i\beta\omega\left(T - \frac{\gamma-1}{\gamma\alpha}P\right) - \beta\ell_h c\Delta T = S & \text{(2a)} \\ -\gamma(\omega^2 - i\ell_v c\omega\Delta)(P - \alpha T) - c^2\Delta P = 0 & \text{(2b)} \end{cases}$$

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

Mathematical Model

It will be convenient to view (2) as a system of four partial differential equations of the form $Au = b$, where

$$A = \begin{pmatrix} -\beta\ell_h c\Delta & \beta\omega & 0 & -\alpha\gamma\omega^2 \\ -\beta\omega & -\beta\ell_h c\Delta & \alpha\gamma\omega^2 & 0 \\ \alpha\gamma\ell_v c\omega\Delta & -\alpha\gamma\omega^2 & -\gamma\ell_v c\omega\Delta & \gamma\omega^2 + c^2\Delta \\ \alpha\gamma\omega^2 & \alpha\gamma\ell_v c\omega\Delta & -(\gamma\omega^2 + c^2\Delta) & -\gamma\ell_v c\omega\Delta \end{pmatrix} \quad (3)$$

where $u = (T_1, T_2, P_1, P_2)^T$ and $b = (S, 0, 0, 0)^T$.

Preliminary Numerical Results

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To mimic a realistic problem, the following set of physical parameters will be used for all tests:

$$\begin{aligned} \ell_h &= \ell_v = 10^{-6} \text{ m} \\ c &= 300 \text{ m/s} \\ \omega &= 3.3e4 \text{ Hz} \\ \gamma &= 1.4 \\ \alpha &= 8.8667 \text{ Pa/K.} \end{aligned}$$

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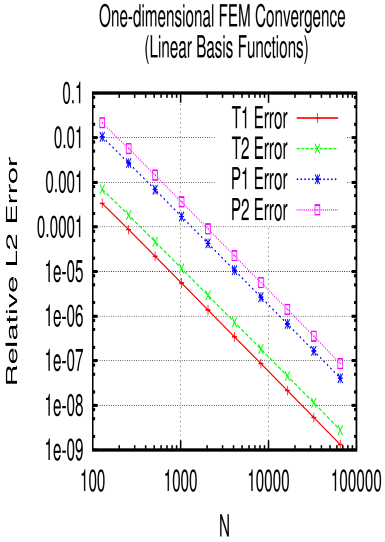
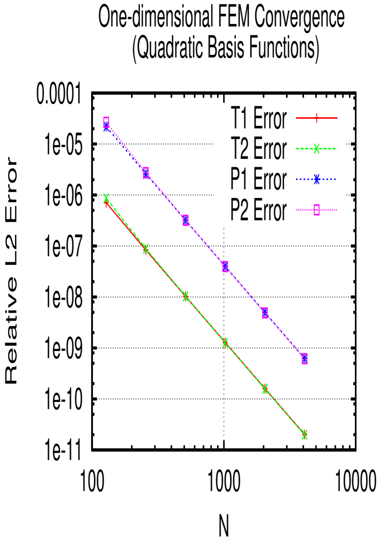
First, we check that our method is converging at the expected rate for order p basis funtions:

$$\|u - u_h\|_{L^2} = Ch^{p+1}.$$

Preliminary Numerical Results





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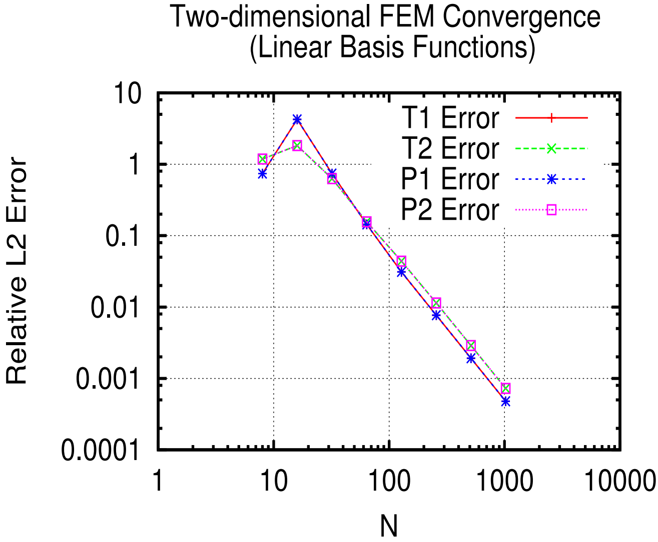

Preconditioning

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For simplicity, we will consolidate the coefficients and define the discrete operator to be

$$A = \left(\begin{array}{cc|cc} a_1 K & a_2 M & 0 & -a_3 M \\ -a_2 M & a_1 K & a_3 M & 0 \\ \hline -a_4 K & -a_3 M & a_5 K & a_6 M - a_7 K \\ a_3 M & -a_4 K & a_7 K - a_6 M & a_5 K \end{array}\right) \tag{4}$$

where K and M are the stiffness and lumped mass matrices, respectively.

Preconditioning

Block Jacobi Preconditioner:

$$P_{Jac} = \left(\begin{array}{cc|cc} a_1 K & a_2 M & 0 & 0 \\ -a_2 M & a_1 K & 0 & 0 \\ \hline 0 & 0 & a_5 K & a_6 M - a_7 K \\ 0 & 0 & a_7 K - a_6 M & a_5 K \end{array}\right) \quad (5)$$

Block Gauss-Seidel Preconditioner:

$$P_{GS} = \left(\begin{array}{cc|cc} a_1 K & a_2 M & 0 & 0 \\ -a_2 M & a_1 K & 0 & 0 \\ \hline -a_4 K & -a_3 M & a_5 K & a_6 M - a_7 K \\ a_3 M & -a_4 K & a_7 K - a_6 M & a_5 K \end{array}\right) \quad (6)$$

Preconditioning

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

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

Preconditioning

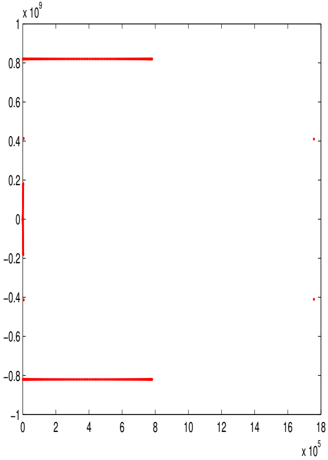
For realistic physical data, $a_1, a_4, a_5 << a_2, a_3, a_6, a_7$. From this realization we propose the following block preconditioner.

$$P = \begin{pmatrix} 0 & a_2 M & 0 & -a_3 M \\ -a_2 M & 0 & a_3 M & 0 \\ 0 & -a_3 M & 0 & a_6 M - a_7 K \\ a_3 M & 0 & a_7 K - a_6 M & 0 \end{pmatrix} \tag{7}$$

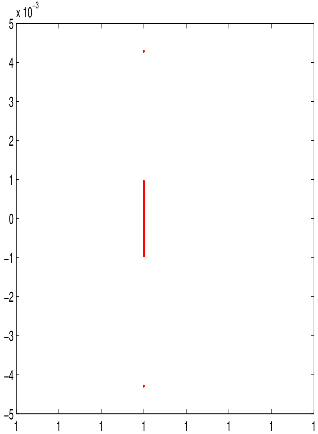
Notice the strong skew-symmetric structure.

Eigenvalues

$\rho(A)$



$\rho(P^{-1}A)$



Preconditioning

N	cond(A)	cond($P_{Jac}^{-1}A$)	cond($P_{GS}^{-1}A$)	cond($P^{-1}A$)
8	1.1135e+05	5.6155e+05	712.6119	1.0072
16	5.2590e+05	6.9769e+07	7.2907e+04	1.0409
32	4.1047e+05	9.6256e+07	1.0562e+05	1.0282

Table: $2-$norm condition numbers of the unpreconditioned and preconditioned matrix for various $N \times N$ meshes.

GMRES preconditioned with P will converge in approximately 5 outer iterations independently of N!

Preconditioning

For each outer GMRES iteration, we must solve the system $P\hat{b} = b$:

$$\left(\begin{array}{cc|cc} 0 & a_2 M & 0 & -a_3 M \\ -a_2 M & 0 & a_3 M & 0 \\ \hline 0 & -a_3 M & 0 & a_6 M - a_7 K \\ a_3 M & 0 & a_7 K - a_6 M & 0 \end{array}\right) \begin{pmatrix} \hat{b_1} \\ \hat{b_2} \\ \hat{b_3} \\ \hat{b_4} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b3 \\ b4 \end{pmatrix}$$

Or by Gaussian elimination:

$$\left(\begin{array}{cc|cc} -a_2 M & 0 & a_3 M & 0 \\ 0 & a_2 M & 0 & -a_3 M \\ \hline 0 & 0 & K - \kappa^2 M & 0 \\ 0 & 0 & 0 & K - \kappa^2 M \end{array}\right) \begin{pmatrix} \hat{b_2} \\ \hat{b_1} \\ \hat{b_4} \\ \hat{b_3} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_1 \\ \frac{1}{a_7}(b_4 + \frac{a_3}{a_2} b_4) \\ -\frac{1}{a_7}(b_3 + \frac{a_3}{a_2} b_1) \end{pmatrix}$$

where $\kappa^2 = \frac{a_6}{a_7} - \frac{a_3^2}{a_2 a_7}$ is the Helmholtz wavenumber.

Preconditioning

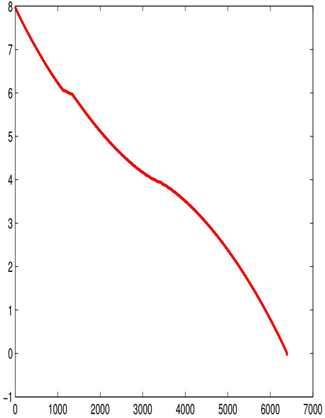
Consider the complex shifted Laplacian matrix $P_H = K - (\alpha + i\beta)\kappa^2 M$ as a ML Helmholtz preconditioner:

(α,β)	$\kappa = 25$	$\kappa = 50$	$\kappa = 100$
(0,0)	11	25	70
(0,0.5)	12	27	91
(0,1)	13	31	103
(0.5,0)	6	19	64
(0.5,0.5)	10	23	77
(1,0)	112	308	1000+
(0.5,1)	12	28	96
(1,0.5)	9	20	56
(1,1)	12	29	92

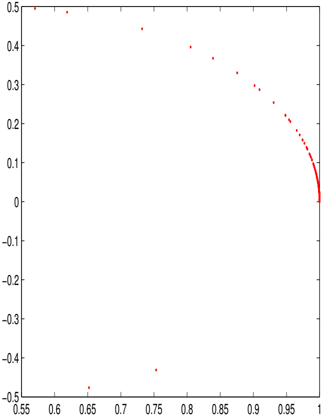
Table: For each test, the number of mesh points per wavelength is kept constant by enforcing $\kappa h \leq \pi/5$.

Helmholtz Eigenvalues

$\rho(H)$



$\rho(P_H^{-1}H)$



Summary and Future Work

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In Summary:

- Initial numerical tests validate the model for plane wave solutions.
- Development of an effective preconditioner.
- Global coupled problem has been reduced to two sub-Helmholtz problems.

Future Work:

- Test other options for solving Helmholtz equation.
- Couple an elasticity model capturing the behaviour of the tuning fork.