Well-Posedness of a Mathematical Model for Trace Gas Sensors

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Introduction to Trace Gas Sensing

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- A *trace gas* is a gas which makes up less than 1% of the Earth's atmosphere.
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- Future Applications:
  1. Non-invasive disease diagnosis

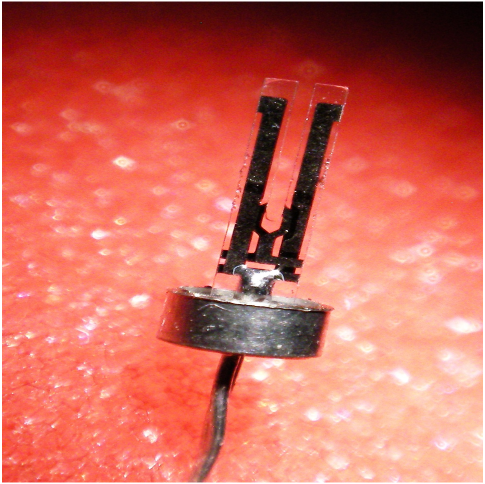

Figure: Trace gas sensor resting on the tip of a finger.

Introduction to Trace Gas Sensing

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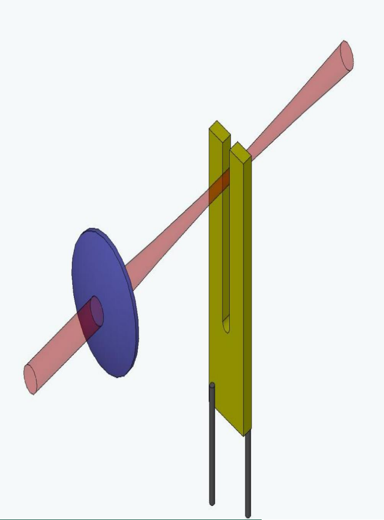

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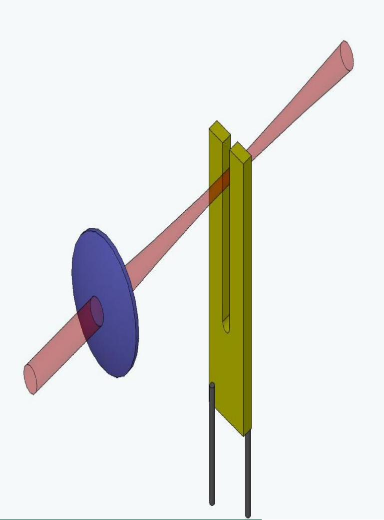

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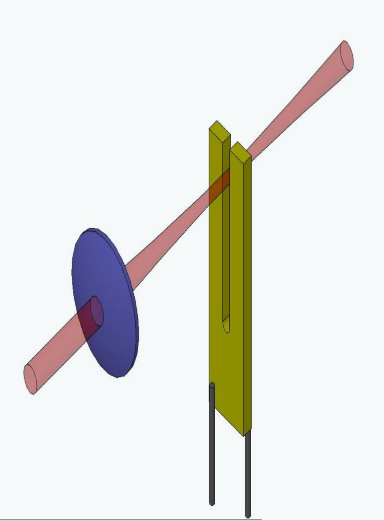

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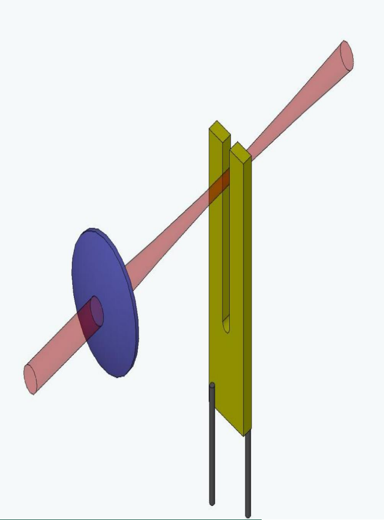

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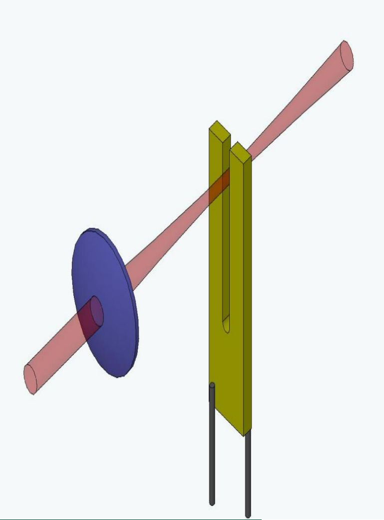

- We fire a modulated laser between the tines of a quartz tuning fork.
- Present gas molecules become excited.
- Thermal and pressure waves are generated.
- Electrodes on the the tuning fork convert waves to electric current.
- The amplitude of the current determines the amount of gas present.

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Current Models:

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

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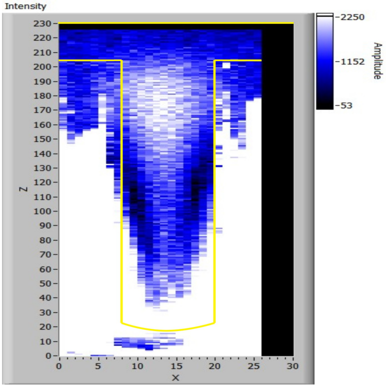

We seek a model which captures both effects simultaneously.

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 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 $b = (S, 0, 0, 0)^T$.

Existence and Uniqueness

Definition

A bilinear form $a(u, v)$ on a normed linear space H is said to be **continuous** on $V \subset H$ if there exists some $M > 0$ such that

$$|a(u,v)| \leq M \|u\|_H \|v\|_H \,, \qquad \text{for all } u, v \in V. \tag{4}$$

and **coercive** on $V \subset H$ if there exists some $C > 0$ such that

$$a(v,v) \geq C \|v\|_H^2 \,, \qquad \text{for all } v \in V. \tag{5}$$

Existence and Uniqueness

Lemma (Lax-Milgram)

Given a Hilbert space V, a continuous and coercive bilinear form $a(\cdot, \cdot)$ and a continuous linear functional $F \in V'$, there exists a unique $u \in V$ such that $a(u, v) = F(v)$, for all $v \in V$.

We will show existence and uniqueness using the Lax-Milgram lemma.

Existence and Uniqueness

For $u = (T_1, T_2, P_1, P_2)$, the bilinear form corresponding to (2) is

$$\begin{aligned} a(u,v) = {} & \frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1}\langle\nabla T_1, \nabla v_1\rangle - \frac{\alpha^2\gamma^2\omega^2}{\gamma-1}\langle T_2, v_1\rangle + \alpha\gamma\omega^2\langle P_2, v_1\rangle \\ & + \frac{\alpha^2\gamma^2\omega^2}{\gamma-1}\langle T_1, v_2\rangle + \frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1}\langle\nabla T_2, \nabla v_2\rangle - \alpha\gamma\omega^2\langle P_1, v_2\rangle \\ & - \alpha\gamma\ell_v c\omega\langle\nabla T_1, \nabla v_3\rangle + \alpha\gamma\omega^2\langle T_2, v_3\rangle + \gamma\ell_v c\omega\langle\nabla P_1, \nabla v_3\rangle \\ & - \gamma\omega^2\langle P_2, v_3\rangle + c^2\langle\nabla P_2, \nabla v_3\rangle - \alpha\gamma\omega^2\langle T_1, v_4\rangle - \alpha\gamma\ell_v c\omega\langle\nabla T_2, \nabla v_4\rangle \\ & + \gamma\omega^2\langle P_1, v_4\rangle - c^2\langle\nabla P_1, \nabla v_4\rangle + \gamma\ell_v c\omega\langle\nabla P_2, \nabla v_4\rangle \end{aligned} \tag{6}$$

Existence and Uniqueness

Now, through repeated use of the Cauchy-Schwarz inequality we can show

$$a(u, v) \leq \left(\frac{\alpha^2\gamma^2\omega^2}{\gamma - 1} + \alpha\gamma\omega^2 + \gamma\omega^2 \right) \|u\| \, \|v\| + \left(\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma - 1} + \alpha\gamma\ell_v c\omega + \gamma\ell_v c\omega + c^2 \right) \|\nabla u\| \, \|\nabla v\| \, .$$

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Using the Friedrichs inequality, we have a bound in the H_0^1 norm.

$$\begin{aligned} a(u,v) &\leq s^2 \left(\frac{\alpha^2\gamma^2\omega^2}{\gamma - 1} + \alpha\gamma\omega^2 + \gamma\omega^2 \right) \|\nabla u\| \, \|\nabla v\| \\ &\quad + \left(\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma - 1} + \alpha\gamma\ell_v c\omega + \gamma\ell_v c\omega + c^2 \right) \|\nabla u\| \, \|\nabla v\| \\ &= M \|u\|_{H_0^1} \|v\|_{H_0^1} . \end{aligned}$$

Existence and Uniqueness

Theorem (Continuity)

For all positive constants $c, \ell_h, \ell_v, \alpha, \gamma$ and ω such that $\gamma > 1$, the rescaled bilinear form (6) is continuous with constant

$$M = s^2\left(\frac{\alpha^2\gamma^2\omega^2}{\gamma-1} + \alpha\gamma\omega^2 + \gamma\omega^2\right) + \left(\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1} + \alpha\gamma\ell_v c\omega + \gamma\ell_v c\omega + c^2\right)$$

This implies well-posedness of the original problem in weak formulation.

Existence and Uniqueness

Our choice of β simplifies our bilinear form in the coercivity estimate:

$$\begin{aligned} a(u,u) &= \frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1}\left(\|\nabla T_1\|^2+\|\nabla T_2\|^2\right)+\gamma\ell_v c\omega\left(\|\nabla P_1\|^2+\|\nabla P_2\|^2\right) \\ &\quad -\alpha\gamma\ell_v c\omega\langle\nabla T_1,\nabla P_1\rangle-\alpha\gamma\ell_v c\omega\langle\nabla T_2,\nabla P_2\rangle. \end{aligned}$$

Our choice of β simplifies our bilinear form in the coercivity definition:

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Now, the generalized Young's inequality gives us that for any $\epsilon>0$

$$\begin{aligned} a(u,u) &\geq \left(\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1}-\frac{\alpha\gamma\ell_v c\omega}{2\epsilon}\right)\left(\|\nabla T_1\|^2+\|\nabla T_2\|^2\right) \\ &\quad +\left(\gamma\ell_v c\omega-\frac{1}{2}\epsilon\alpha\gamma\ell_v c\omega\right)\left(\|\nabla P_1\|^2+\|\nabla P_2\|^2\right) \\ &= C\,\|u\|_{H_0^1}^2 \end{aligned}$$

for $C=\min\left\{\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1}-\frac{\alpha\gamma\ell_v c\omega}{2\epsilon},\ \gamma\ell_v c\omega-\frac{1}{2}\epsilon\alpha\gamma\ell_v c\omega\right\}$.

Existence and Uniqueness

Remember that we must choose ϵ such that $C > 0$ in the previous result. Enforcing this, gives the following result.

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Theorem (Coercivity)

Suppose $\frac{\ell_v(\gamma-1)}{2\gamma\ell_h} < 2$. *Then for all positive constants* $c, \ell_h, \ell_v, \alpha, \gamma$ *and* ω *such that* $\gamma > 1$ *and*

$$\frac{\ell_v(\gamma - 1)}{2\alpha\gamma\ell_h} < \epsilon < \frac{2}{\alpha}.$$

the rescaled bilinear form is coercive with constant

$$C = \min\left\{\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma - 1} - \frac{\alpha\gamma\ell_v c\omega}{2\epsilon},\ \gamma\ell_v c\omega - \frac{1}{2}\epsilon\alpha\gamma\ell_v c\omega\right\}.$$

Error Estimates

Error Estimates

Our previous theorems immediately give us error estimates in H^1.

Lemma (Cea's Lemma)

Let $a : V \times V \to \mathbb{R}$ be a continuous and coercive bilinear form. For a continuous linear functional $F \in V'$, consider the problem of finding an element $u \in V$ such that

$$a(u, v) = F(v), \quad \text{for all } v \in V.$$

Now, consider the same problem on a finite dimensional subspace V_h of V such that $u_h \in V_h$ satisfies

$$a(u_h, v) = F(v), \quad \text{for all } v \in V_h.$$

*By the Lax-Milgram Lemma, this problem has a unique solution and **Cea's Lemma** states that*

$$\|u - u_h\|_V \leq \frac{M}{C} \|u - v\|_V, \quad \text{for all } v \in V_h$$

where M and C are the continuity and coercivity constants respectively.

Error Estimates

L^2 estimates are also of interest. For these need the following assumptions:

Proposition

Given a global interpolator $\mathcal{I}^h u$ on the finite element space, the corresponding shape functions have an approximation order, m, if

$$\left\| u - \mathcal{I}^h u \right\|_{H_0^1} \leq C_{\mathcal{I}^h} h^{m-1} \left\| u \right\|_{H^m} \tag{7}$$

where $C_{\mathcal{I}^h}$ is independent of u and h.

Error Estimates

Proposition (H^2 Regularity)

Suppose that $u \in H^1(U)$ is a weak solution of the elliptic PDE

$$Lu = f, \qquad \textit{in } U$$

with homogeneous Dirichlet boundary conditions. Then $u \in H^2_{loc}(U)$ and for any open subset $V \subset U$

$$\|u\|_{H^2} \leq C_R \|f\|_{L^2}.$$

Error Estimates

To find L^2 estimates, we consider the dual problem in terms of $e = u - u_h$

$$\begin{cases} -\frac{\alpha^2\gamma^2\ell_h c\omega}{\gamma-1}\Delta\phi_T - i\frac{\alpha^2\gamma^2\omega^2}{\gamma-1}\phi_T + \alpha\gamma\ell_v c\omega\Delta\phi_P + i\alpha\gamma\omega^2\phi_P = e_T \\ i\alpha\gamma\omega^2\phi_T - \gamma\ell_v c\omega\Delta z_P - i(\gamma\omega^2 + c^2\Delta)z_P = e_P \end{cases}$$

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This problem has the crucial property

$$a(e, \phi) = \langle e, e\rangle \quad (8)$$

in terms of the original bilinear form $a(\cdot, \cdot)$.

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Notice the solution ϕ also satisfies

$$\|\phi\|_{H^2} \leq C_R \|e\|_{L^2}.$$

Error Estimates

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\begin{aligned}
\|e\|_{L^2}^2 &= \langle e, e\rangle \\
&= a(e,\phi), && \text{(by duality)} \\
&= a(e,\phi - \mathcal{I}^h\phi) && \text{(by Galerkin Orthogonality)} \\
&\le M\|e\|_{H_0^1}\left\|\phi - \mathcal{I}^h\phi\right\|_{H_0^1} && \text{(by continuity)} \\
&\le MC_{\mathcal{I}^h} h\|e\|_{H_0^1}\|\phi\|_{H^2}. && \text{(Approximation estimate)} \\
&\le Kh\|e\|_{H_0^1} && \text{(Regularity)} \\
&\le Kh^2\|u\|_{H^2} && \text{(Approximation estimate).}
\end{aligned}
$$

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&\leq M \|e\|_{H_0^1} \left\| \phi - \mathcal{I}^h \phi \right\|_{H_0^1} && \text{(by continuity)} \\
&\leq M C_{\mathcal{I}^h} h \|e\|_{H_0^1} \|\phi\|_{H^2}. && \text{(Approximation estimate)} \\
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&\leq K h^2 \|u\|_{H^2} && \text{(Approximation estimate).}
\end{aligned}
$$

Theorem (L^2 Error Estimate)

The FEM error in the L^2 norm is of size $\mathcal{O}(h^2)$.

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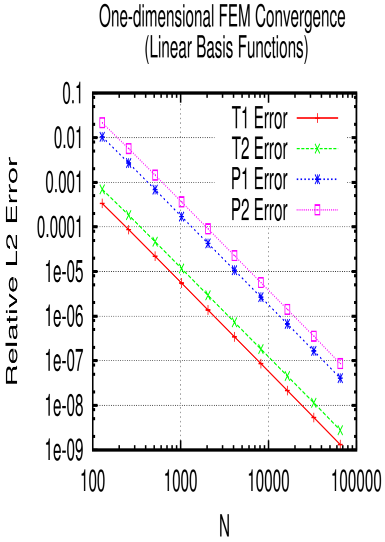
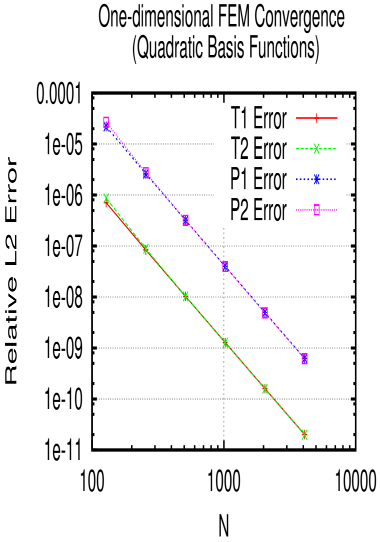
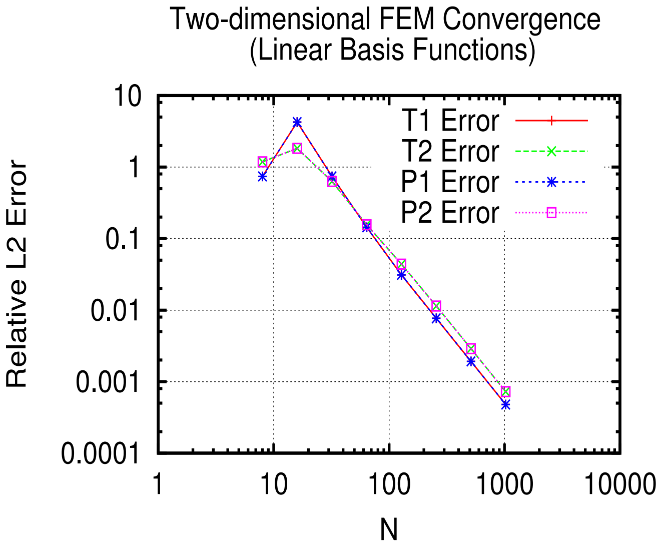
First, we check that our method is converging at the expected rate for order p basis funtions:

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

Numerical Results



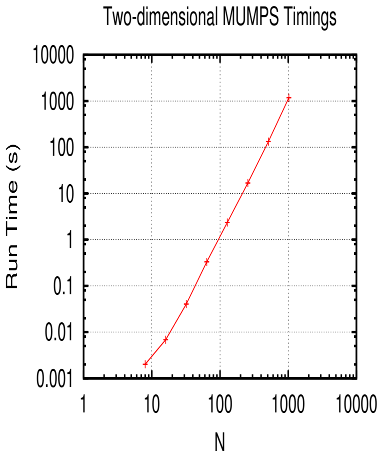


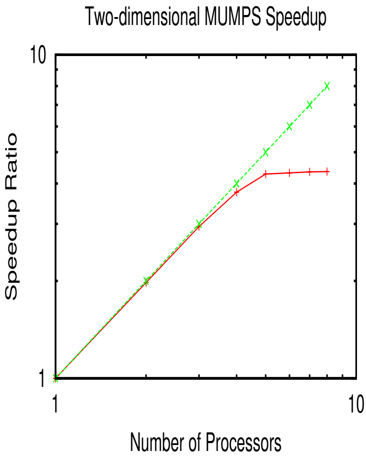

Two-dimensional FEM Convergence
(Linear Basis Functions)
Relative L2 Error
N
10
1
0.1
0.01
0.001
0.0001
1
10
100
1000
10000
T1 Error
T2 Error
P1 Error
P2 Error

Numerical Results

MUMPS Performance:

16 Core Workstation





128 Node Cluster

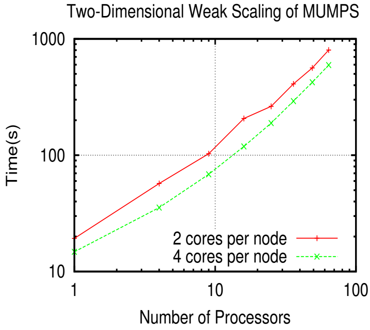


Figure: Weak scaling with a fixed 256×256 problem size per processor.

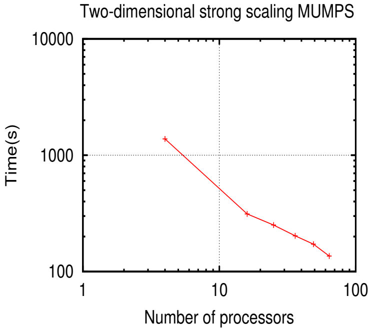


Figure: Strong scaling for a fixed problem size of 1024×1024.

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Future Work:

- Couple an elasticity model capturing the behaviour of the tuning fork.
- Standard linear solvers do not scale well to multi-core machines.
  - → Hermitian-Skew Symmetric (HSS) splitting methods may help.


ANY
QUESTIONS
?