Fast Iterative Solution of the Time-Harmonic Elastic Wave Equation at Multiple Frequencies

Manuel M. Baumann

January 10, 2018
Question you have asked me today...

- Are you nervous? → Yes!

Questions you have asked me during the last years...

- What is your PhD project about?
- What is numerical linear algebra?
- What have you been doing all day? (The German word for this is: rumdoktorn)
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What is applied mathematics?

"Applied maths is about using mathematics to solve real world problems neither seeking nor avoiding mathematical difficulties."

–Lord Rayleigh
What is applied mathematics?

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–Lord Rayleigh
Seismic Full-Waveform Inversion

Interplay of...
- measurements,

Solve the linear systems of equations,

\[
(K + i\omega k C - \omega^2 k M) x_k = b,
\]
efficiently (= fast and at low memory) for multiple frequencies.
Seismic Full-Waveform Inversion

Interplay of...
- measurements,
Seismic Full-Waveform Inversion

Interplay of...
- measurements,
- seismology,

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Seismic Full-Waveform Inversion

Interplay of...
- measurements,
- seismology,
Seismic Full-Waveform Inversion

Interplay of...
- measurements,
- seismology,
- computer simulations
  $\rightarrow$ matrix computations

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(K + i\omega k C - \omega^2 k M)x_k = b
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Efficiently (= fast and at low memory) for multiple frequencies.
Seismic Full-Waveform Inversion

Interplay of...
- measurements,
- seismology,
- computer simulations → matrix computations

"Solve the linear systems of equations,

\[(K + i\omega_k C - \omega_k^2 M)x_k = b,\]

efficiently (= fast and at low memory) for multiple frequencies. “
Seismic Full-Waveform Inversion

Interplay of...
- measurements,
- seismology,
- computer simulations
  \[ \omega_k \xrightarrow{\text{matrix computations}} x_k = \text{oil} = \$ \]

Density distribution

Simulations

\[ \omega_1 \ldots \omega_N \]
Seismic Full-Waveform Inversion

Interplay of...
- measurements,
- seismology,
- computer simulations

$\omega_k \cdot \omega_k = \text{oil} = \$\Rightarrow \text{matrix computations}$

Density distribution

Simulations $\omega_1 \ldots \omega_N$
Numerical Linear Algebra

A very classical linear algebra problem,

\[
\begin{align*}
\text{bike} + \text{soccer} &= 1500 \\
\text{bike} + \text{tea} &= 7.5 \\
\text{beer} - \text{tea} &= 160
\end{align*}
\]

A more formal way of writing this,

\[
\begin{bmatrix}
1 & 1 & 0 \\
1 & 0 & 2 \\
0 & 2 & -3
\end{bmatrix}
\begin{bmatrix}
\text{bike} \\
\text{soccer} \\
\text{tea}
\end{bmatrix}
= 
\begin{bmatrix}
1500 \\
7.5 \\
160
\end{bmatrix}
\]
A very classical linear algebra problem,

\[
\begin{align*}
\text{BIKE} + \text{FOOTBALL} &= 1500 \\
\text{BIKE} + \text{TEA} &= 7.5 \quad \text{(123)} \\
\text{FOOTBALL} - \text{TEA} &= 160
\end{align*}
\]

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\]
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\text{coffee}
\end{bmatrix} =
\begin{bmatrix}
1500 \\
7.5 \\
160
\end{bmatrix}
\]

\[=: A \quad =: x \quad =: b\]
A very classical linear algebra problem,

\[
\begin{align*}
\text{🚲} + \text{⚽} &= 1500 \\
\text{🚲} + \text{☕️} &= 7.5 \\
\text{⚽️} - \text{☕️} &= 160
\end{align*}
\]

A more formal way of writing this,

\[
\begin{bmatrix}
1 & 1 & 0 \\
1 & 0 & 2 \\
0 & 2 & -3
\end{bmatrix}
\begin{bmatrix}
\text{🚲} \\
\text{⚽️} \\
\text{☕️}
\end{bmatrix}
= \begin{bmatrix}
1500 \\
7.5 \\
160
\end{bmatrix}
\]

The matrix \( A \) is symmetric
A very classical linear algebra problem,

\[
\begin{align*}
\text{\(\text{\textbullet}\) + \(\text{\textbullet}\)} & = 1500 \\
\text{\(\text{\textbullet}\)} & \quad + \quad \text{\(\text{\textbullet\textbullet}\)} = 7.5 \\
\text{\(\text{\textbullet\textbullet\textbullet}\)} & \quad - \quad \text{\(\text{\textbullet\textbullet\textbullet}\)} = 160
\end{align*}
\]

A more formal way of writing this,

\[
\begin{align*}
\begin{bmatrix}
* & * \\
* & * \\
* & *
\end{bmatrix}
\begin{bmatrix}
\text{\(\text{\textbullet}\)} \\
\text{\(\text{\textbullet}\textbullet\)} \\
\text{\(\text{\textbullet\textbullet\textbullet}\)}
\end{bmatrix}
& =
\begin{bmatrix}
1500 \\
7.5 \\
160
\end{bmatrix}
\end{align*}
\]

The matrix \(A\) is symmetric and sparse.
A very classical linear algebra problem,

\[
\begin{align*}
\text{bike} + \text{soccer} &= 1500 \\
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\end{align*}
\]

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\[
\begin{align*}
\begin{bmatrix}
* & * \\
* & * \\
\end{bmatrix}
\begin{bmatrix}
\text{bike} \\
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\end{bmatrix}
&= 
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7.5 \\
160
\end{bmatrix}
\end{align*}
\]

The matrix \(A\) is symmetric and sparse.
Numerical Linear Algebra

The matrix $A$ can be...
Numerical Linear Algebra

The matrix $A$ can be...

- symmetric
- skew-symmetric
- positive (semi-)definite
- indefinite
- square
- rectangular
- sparse
- dense
- Port-Hamiltonian
- nilpotent
- low-rank
- diagonalizable
- upper Hessenberg
- block tri-diagonal
- sequentially semi-separable
- SPD
- Hermitian
- ill-conditioned
- invertible
The matrix $A$ can be...

- sequentially semi-separable
- symmetric
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- positive (semi-)definite
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- dense
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- ill-conditioned
Shifted systems vs. matrix equation

Two main approaches for solving,

\[(K + i\omega_k C - \omega_k^2 M)x_k = b, \quad k > 1.\]
Shifted systems vs. matrix equation

Two main approaches for solving,

\[(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}, \quad k > 1.\]

**Shifted systems**

\[
\begin{bmatrix}
  iC & K \\
  I & 0
\end{bmatrix} - \omega_k
\begin{bmatrix}
  M & 0 \\
  0 & I
\end{bmatrix}
\begin{bmatrix}
  \omega_k \mathbf{x}_k \\
  \mathbf{x}_k
\end{bmatrix} =
\begin{bmatrix}
  \mathbf{b} \\
  0
\end{bmatrix}
\]

- Most work for \(\mathbf{x}_0\) (at \(\omega = 0\))
- Requires preconditioning
Shifted systems vs. matrix equation

Two main approaches for solving,

\[(K + i\omega_k C - \omega_k^2 M)x_k = b, \quad k > 1.\]

**Shifted systems**

\[
\begin{pmatrix}
iC & K \\
I & 0
\end{pmatrix} - \omega_k \begin{pmatrix} M & 0 \\
0 & I
\end{pmatrix} \begin{pmatrix} \omega_k x_k \\
x_k
\end{pmatrix} = \begin{pmatrix} b \\
0
\end{pmatrix}
\]

- Most work for \(x_0\) (at \(\omega = 0\))
- Requires preconditioning

**Matrix equation**

\[KX + iCX\Omega - MX\Omega^2 = B\]

- Solve for \(X = [x_1, ..., x_N]\) all-at-once
- Requires preconditioning
Shifted systems vs. matrix equation

Two main approaches for solving,

\[(K + i\omega_k C - \omega_k^2 M)x_k = b, \quad k > 1.\]

**Shifted systems**

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\begin{bmatrix}
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- Most work for \(x_0\) (at \(\omega = 0\))
- Requires **preconditioning**

**Matrix equation**

\[KX + iCX\Omega - MX\Omega^2 = B\]

- Solve for \(X = [x_1, \ldots, x_N]\)
- **all-at-once**
- Requires **preconditioning**

Manuel Baumann
PhD Defense Talk
Preconditioning

Let \( A := K + i\omega C - \omega^2 M \)

Solve large-scale linear system,

\[ Ax = b, \quad \text{with} \quad A \in \mathbb{C}^{N \times N}, \quad N \gg 1 \]  

with an iterative method, i.e. compute \( x_i \) with \( x_i \to x \) as \( i \to \infty \).

Instead of \((*)\), solve the system

\[ P^{-1}Ax = P^{-1}b, \]

where \( P \) is a preconditioner.
Preconditioning

However, it’s often not that simple!

\[
\begin{bmatrix}
iC & K \\
I & 0
\end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\
0 & I
\end{bmatrix} \begin{bmatrix} \omega_k x_k \\
x_k
\end{bmatrix} = \begin{bmatrix} b \\
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\end{bmatrix}
\]

Main challenges:

- multiple linear systems
- single preconditioner
- wide frequency range
- preserve structure
Preconditioning

However, it’s often not that simple!

\[
\left( \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k x_k \\ x_k \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}
\]

\[\tau^* = ?\]

Main challenges:

- multiple linear systems
- single preconditioner
- wide frequency range
- preserve structure
Spectral analysis
Spectral analysis

\[ \epsilon > 0 \]
Spectral analysis

\[ \epsilon > 0 \]
Spectral analysis
Spectral analysis

\[ \epsilon > 0 \]

\[ c \]

\[ R_k \]

\[ c_{k-1} \]

\[ \varphi_{k-1} \]

\[ C \]

\[ C_1 \]

Manuel Baumann
PhD Defense Talk

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Spectral analysis

**Thm.:** Optimal seed shift for multi-shift GMRES [B/vG, 2016]

(i) For $\lambda \in \Lambda[AB^{-1}]$ it holds $\Im(\lambda) \geq 0$.

(ii) The preconditioned spectra are enclosed by circles of radii $R_k$ and center points $c_k$.

(iii) The points $\{c_k\}_{k=1}^N \subset \mathbb{C}$ described in statement (ii) lie on a circle with center $c$ and radius $R$.

(iv) Consider the preconditioner $\mathcal{P}(\tau^*) = A - \tau^*B$. An optimal seed frequency $\tau^*$ for preconditioned multi-shift GMRES is given by,

$$\tau^*(\epsilon, \omega_1, \omega_N) = \min_{\tau \in \mathbb{C}} \max_{k=1,\ldots,N} \left( \frac{R_k(\tau)}{|c_k|} \right) = \ldots =$$

$$= \frac{2\omega_1\omega_N}{\omega_1 + \omega_N} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_N)^2 + (\omega_N - \omega_1)^2]}}{\omega_1 + \omega_N} \omega_1\omega_N$$
Spectral analysis

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= \frac{2\omega_1\omega_N}{\omega_1 + \omega_N} - i \frac{\sqrt{\epsilon^2(\omega_1 + \omega_N)^2 + (\omega_N - \omega_1)^2}}{\omega_1 + \omega_N} \omega_1\omega_N
$$
Spectral analysis

Proof:
Spectral analysis

**Proof:** Not now.
Spectral analysis

**Proof:** There is an App for that.
Convergence behavior and spectral bounds

For any $\tau$...
Convergence behavior and spectral bounds

For the optimal $\tau^*$...
Lot’s of details...
What happens today?

15:00 – 16:00  Formal PhD defense
16:15 – 17:30  Reception (in this building)
21:00 –  ??    More reception (borrel) at Prinsenkwartier
Thank you all for coming!