

# 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*)

## 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*)

## 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*)

## 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*)

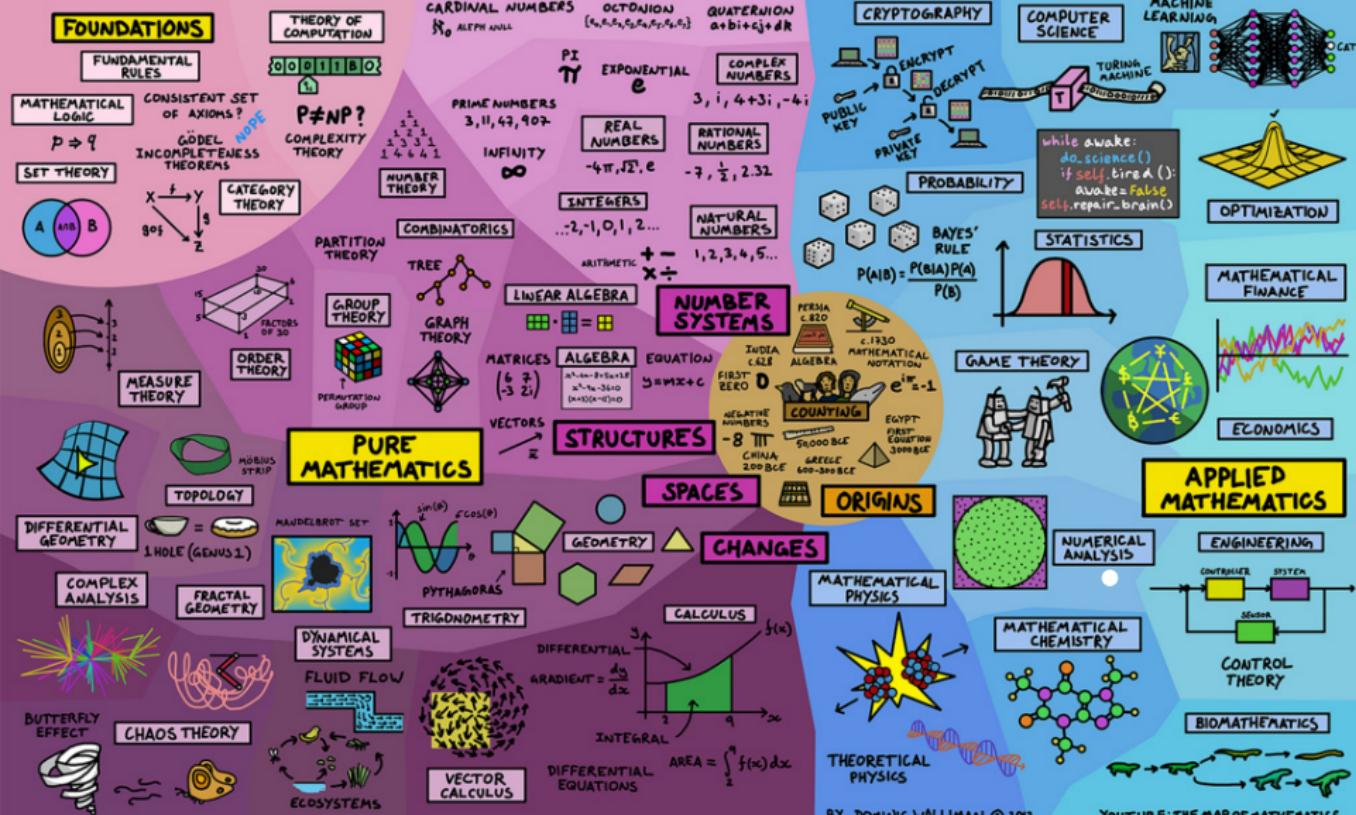
## Question you have asked me today...

- 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*)

# THE MAP OF MATHEMATICS



# THE MAP OF MATHEMATICS



# What is applied mathematics?

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

—Lord Rayleigh



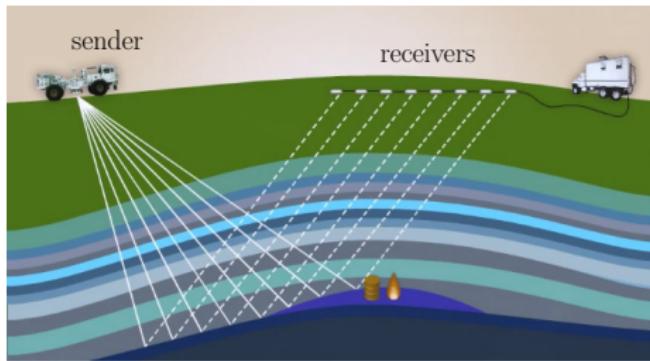
# What is applied mathematics?

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

—Lord Rayleigh



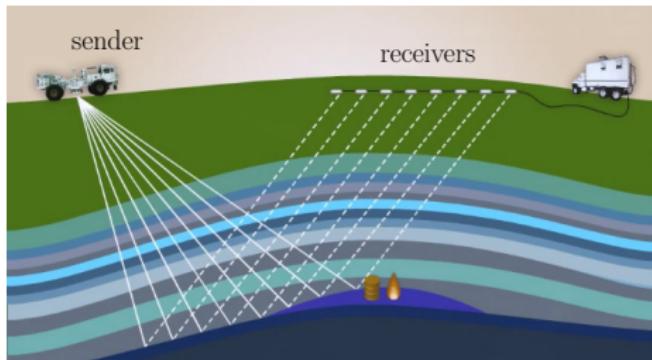
# Seismic Full-Waveform Inversion



Interplay of...

- measurements,

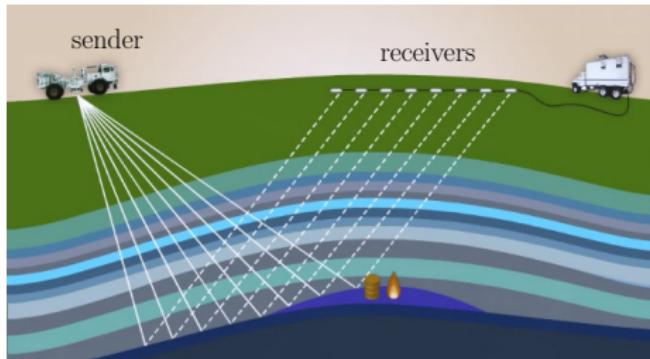
# Seismic Full-Waveform Inversion



Interplay of...

- measurements,

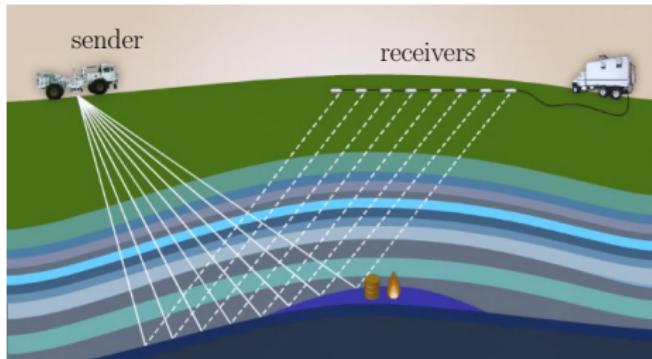
# Seismic Full-Waveform Inversion



Interplay of...

- measurements,
- seismology,

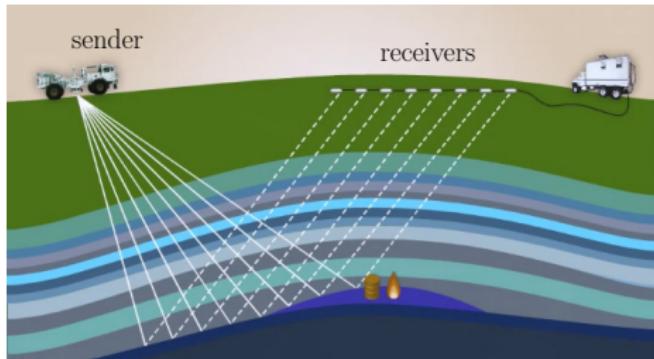
# Seismic Full-Waveform Inversion



Interplay of...

- measurements,
- seismology,

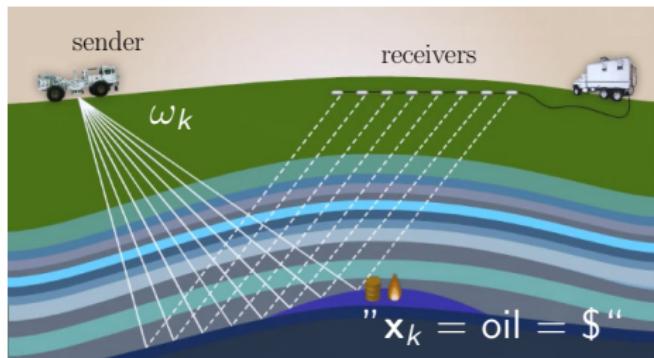
# Seismic Full-Waveform Inversion



Interplay of...

- measurements,
- seismology,
- computer simulations  
    ↪ matrix computations

# Seismic Full-Waveform Inversion



Interplay of...

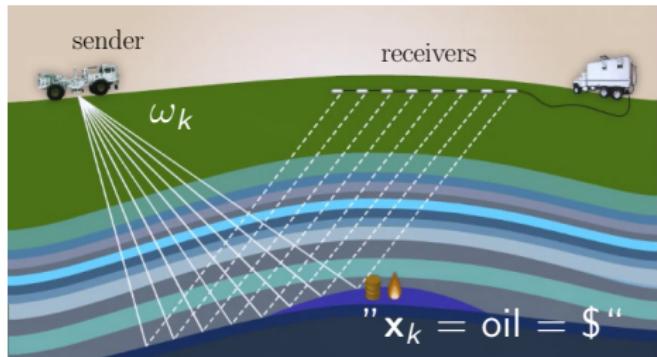
- measurements,
- seismology,
- computer simulations  
     $\hookrightarrow$  matrix computations

"Solve the linear systems of equations,

$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b},$$

efficiently (= fast and at low memory) for multiple frequencies."

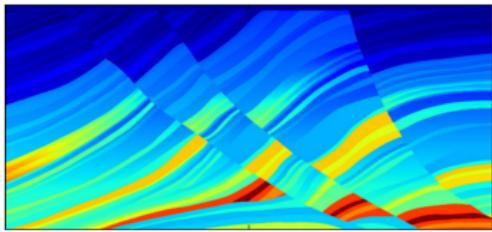
# Seismic Full-Waveform Inversion



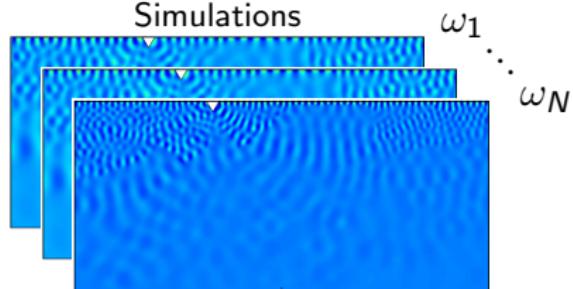
Interplay of...

- measurements,
- seismology,
- computer simulations  
     $\hookrightarrow$  matrix computations

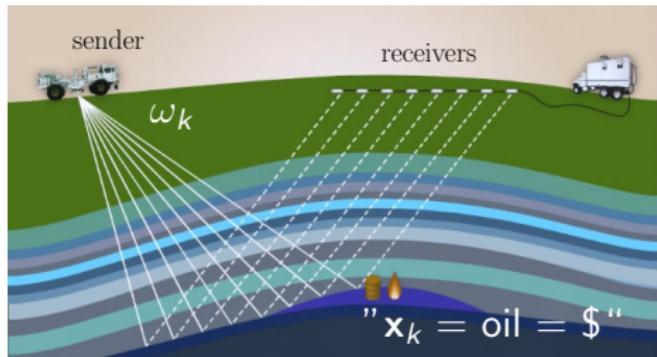
Density distribution



Simulations



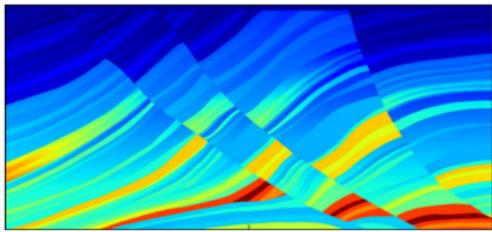
# Seismic Full-Waveform Inversion



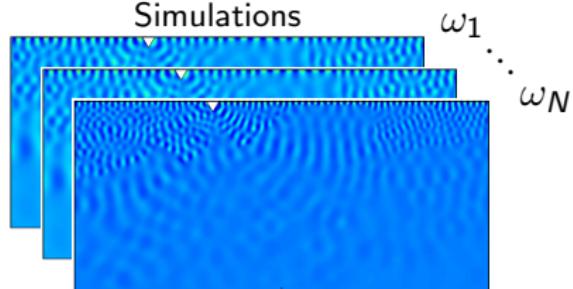
Interplay of...

- measurements,
- seismology,
- computer simulations  
     $\hookrightarrow$  **matrix** computations

Density distribution



Simulations



# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{🚲} + \text{⚽} = 1500$$

$$\text{🚲} + \text{☕☕} = 7.5$$

$$\text{⚽⚽} - \text{☕☕☕} = 160$$

A more formal way of writing this,

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

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{🚲} + \text{⚽} = 1500$$

$$\text{🚲} + \text{☕☕} = 7.5$$

$$\text{⚽⚽} - \text{☕☕☕} = 160$$

A more formal way of writing this,

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

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{🚲} + \text{⚽} = 1500$$

$$\text{🚲} + \text{☕☕} = 7.5$$

$$\text{⚽⚽} - \text{☕☕☕} = 160$$

A more formal way of writing this,

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

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{🚲} + \text{⚽} = 1500$$

$$\text{🚲} + \text{☕☕} = 7.5$$

$$\text{⚽⚽} - \text{☕☕☕} = 160$$

A more formal way of writing this,

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

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{bike} + \text{soccer ball} = 1500$$

$$\text{bike} + \text{cup} = 7.5$$

$$\text{soccer ball} - \text{cup} = 160$$

A more formal way of writing this,

$$\underbrace{\begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & -3 \end{bmatrix}}_{=:A} \underbrace{\begin{bmatrix} \text{bike} \\ \text{soccer ball} \\ \text{cup} \end{bmatrix}}_{=:x} = \underbrace{\begin{bmatrix} 1500 \\ 7.5 \\ 160 \end{bmatrix}}_{=:b}$$

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{bike} + \text{soccer ball} = 1500$$

$$\text{bike} + \text{coffee cup} = 7.5$$

$$\text{soccer ball} - \text{coffee cup} = 160$$

A more formal way of writing this,

$$\underbrace{\begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & -3 \end{bmatrix}}_{=:A} \underbrace{\begin{bmatrix} \text{bike} \\ \text{soccer ball} \\ \text{coffee cup} \end{bmatrix}}_{=:x} = \underbrace{\begin{bmatrix} 1500 \\ 7.5 \\ 160 \end{bmatrix}}_{=:b}$$

The matrix  $A$  is symmetric

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{bike} + \text{soccer ball} = 1500$$

$$\text{bike} + \text{coffee cup} = 7.5$$

$$\text{soccer ball} - \text{coffee cup} = 160$$

A more formal way of writing this,

$$\underbrace{\begin{bmatrix} * & * \\ * & * \\ * & * \end{bmatrix}}_{=:A} \underbrace{\begin{bmatrix} \text{bike} \\ \text{soccer ball} \\ \text{coffee cup} \end{bmatrix}}_{=:x} = \underbrace{\begin{bmatrix} 1500 \\ 7.5 \\ 160 \end{bmatrix}}_{=:b}$$

The matrix  $A$  is symmetric and sparse.

# Numerical Linear Algebra

A very classical linear algebra problem,

$$\text{bike} + \text{soccer ball} = 1500$$

$$\text{bike} + \text{coffee cup} = 7.5$$

$$\text{soccer ball} - \text{coffee cup} = 160$$

A more formal way of writing this,

$$\underbrace{\begin{bmatrix} * & * \\ & * \\ & * \end{bmatrix}}_{=:A} \underbrace{\begin{bmatrix} \text{bike} \\ \text{soccer ball} \\ \text{coffee cup} \end{bmatrix}}_{=:x} = \underbrace{\begin{bmatrix} 1500 \\ 7.5 \\ 160 \end{bmatrix}}_{=:b}$$

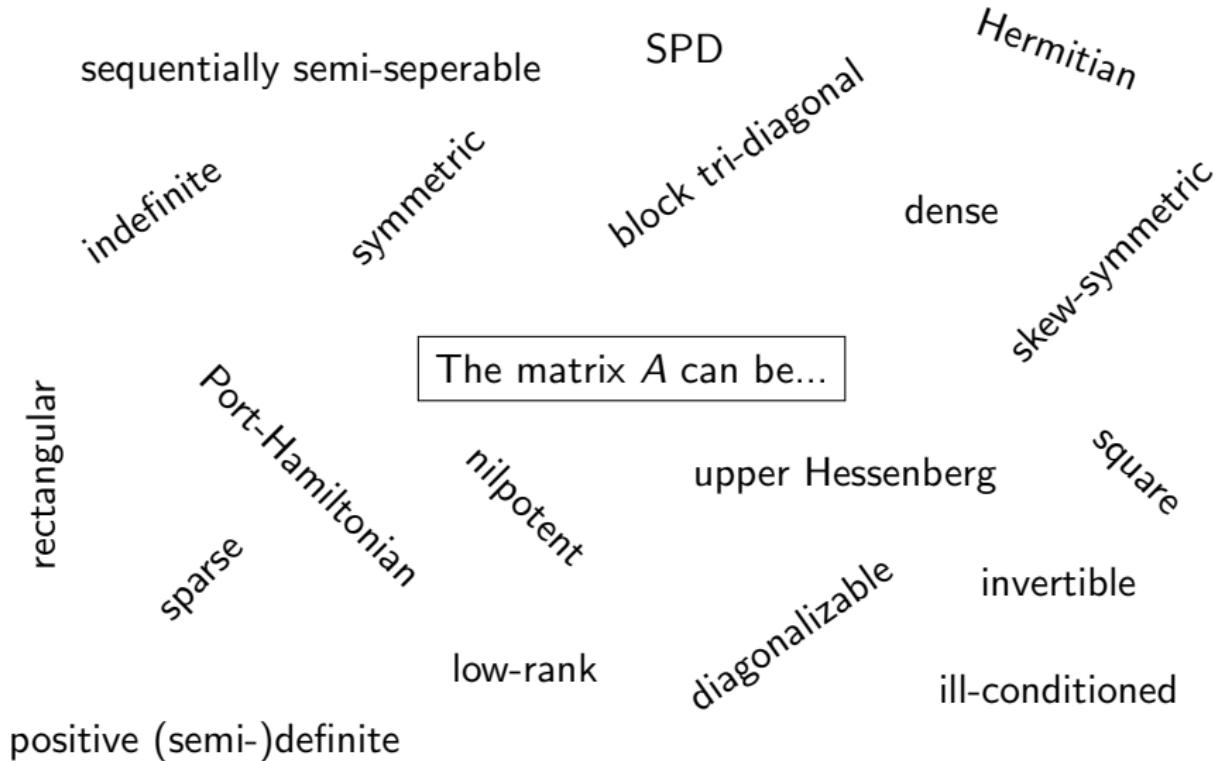
The matrix  $A$  is symmetric and sparse.

# Numerical Linear Algebra

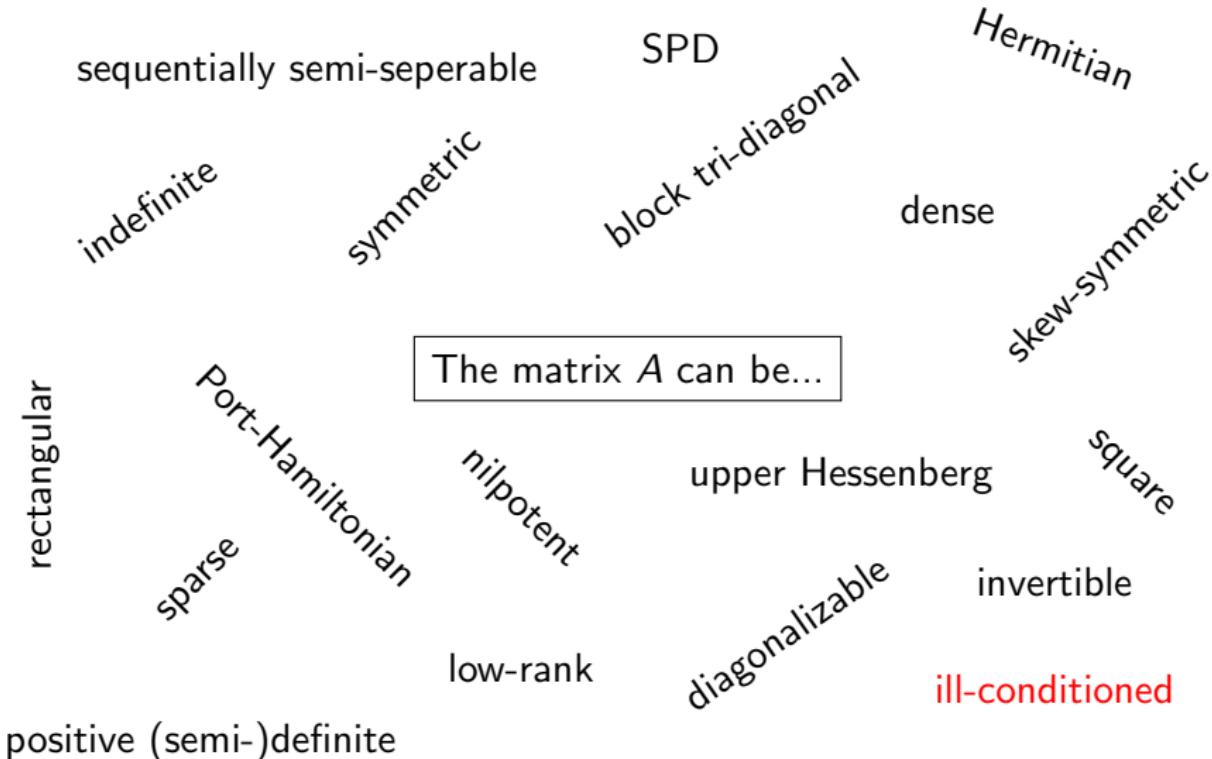
The matrix  $A$  can be...

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

# Numerical Linear Algebra



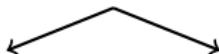
# Numerical Linear Algebra



# Shifted systems vs. matrix equation

Two main approaches for solving,

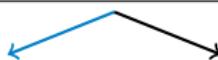
$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}, \quad k > 1.$$



# Shifted systems 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

$$\left( \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

- Most work for  $\mathbf{x}_0$  (at  $\omega = 0$ )
- Requires preconditioning

# Shifted systems vs. matrix equation

Two main approaches for solving,

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



Shifted systems

$$\left( \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

Matrix equation

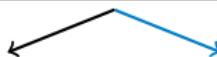
$$K\mathbf{X} + iC\mathbf{X}\Omega - M\mathbf{X}\Omega^2 = \mathbf{B}$$

- Most work for  $\mathbf{x}_0$  (at  $\omega = 0$ )
- Requires preconditioning
- Solve for  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]$  *all-at-once*
- Requires preconditioning

# Shifted systems vs. matrix equation

Two main approaches for solving,

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



Shifted systems

$$\left( \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

Matrix equation

$$K\mathbf{X} + iC\mathbf{X}\Omega - M\mathbf{X}\Omega^2 = \mathbf{B}$$

- Most work for  $\mathbf{x}_0$  (at  $\omega = 0$ )
- Requires **preconditioning**
- Solve for  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]$   
*all-at-once*
- Requires **preconditioning**

Solve large-scale linear system,

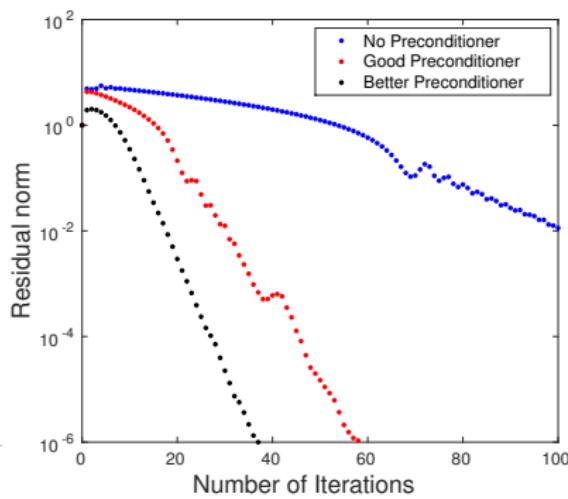
$$A\mathbf{x} = \mathbf{b}, \quad \text{with } A \in \mathbb{C}^{N \times N}, N \gg 1 \quad (*)$$

with an **iterative method**, i.e. compute  $\mathbf{x}_i$  with  $\mathbf{x}_i \rightarrow \mathbf{x}$  as  $i \rightarrow \infty$ .

Instead of (\*), solve the system

$$P^{-1}A\mathbf{x} = P^{-1}\mathbf{b},$$

where  $P$  is a **preconditioner**.



# Preconditioning

*However, it's often not that simple!*

$$\left( \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

Main challenges:

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

# Preconditioning

*However, it's often not that simple!*

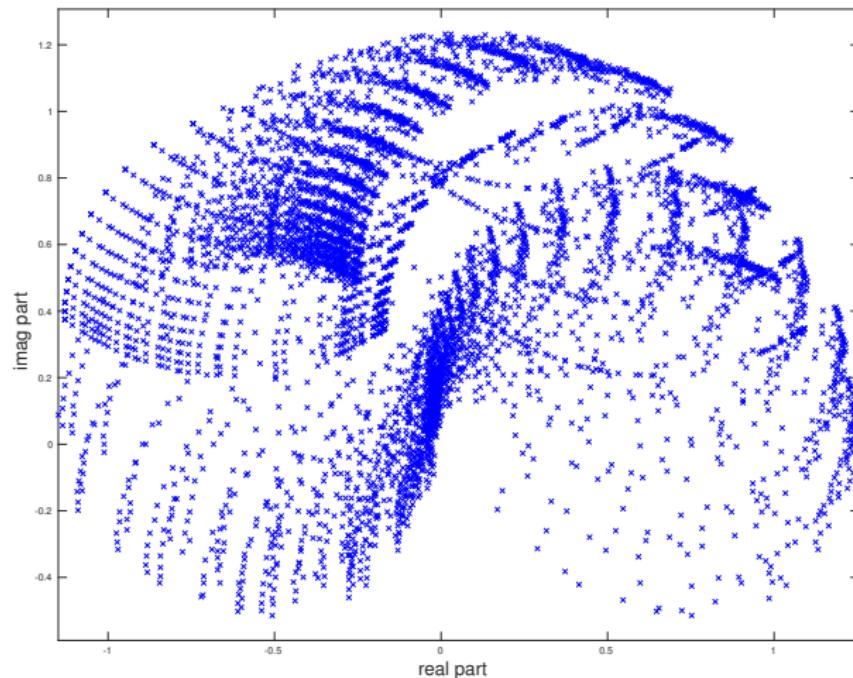
$$\left( \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

$\tau^* = ?$

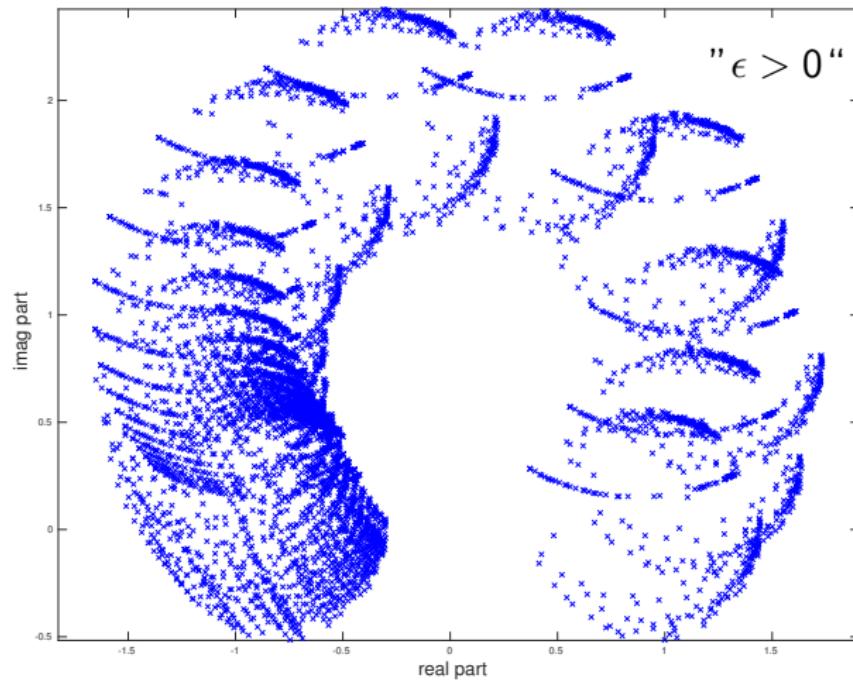
Main challenges:

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

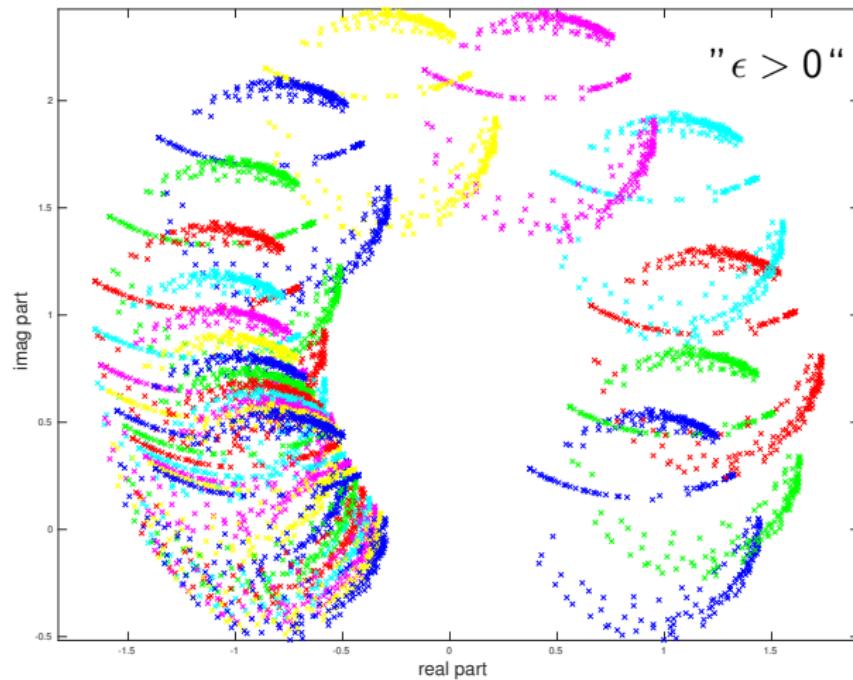
# Spectral analysis



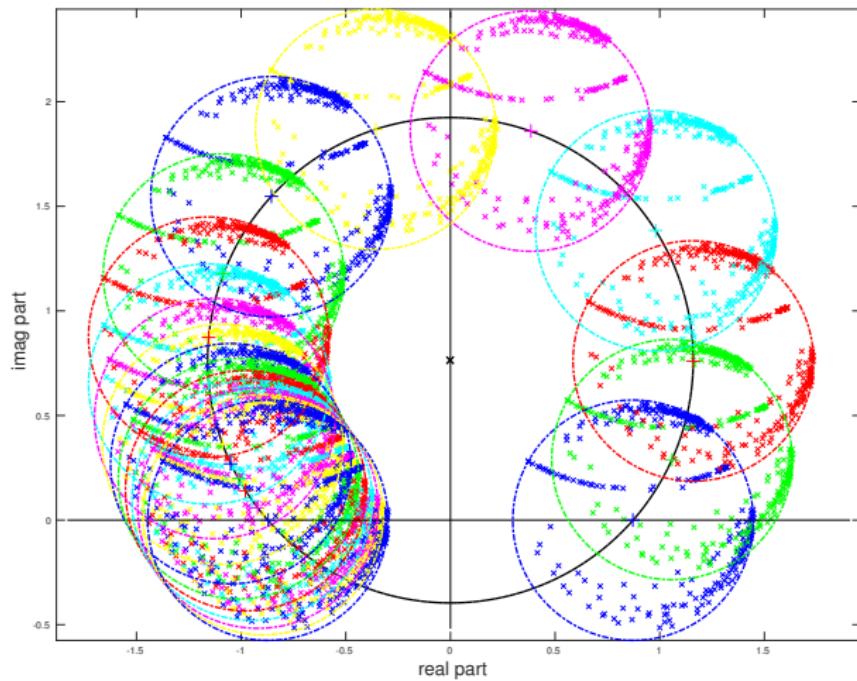
# Spectral analysis



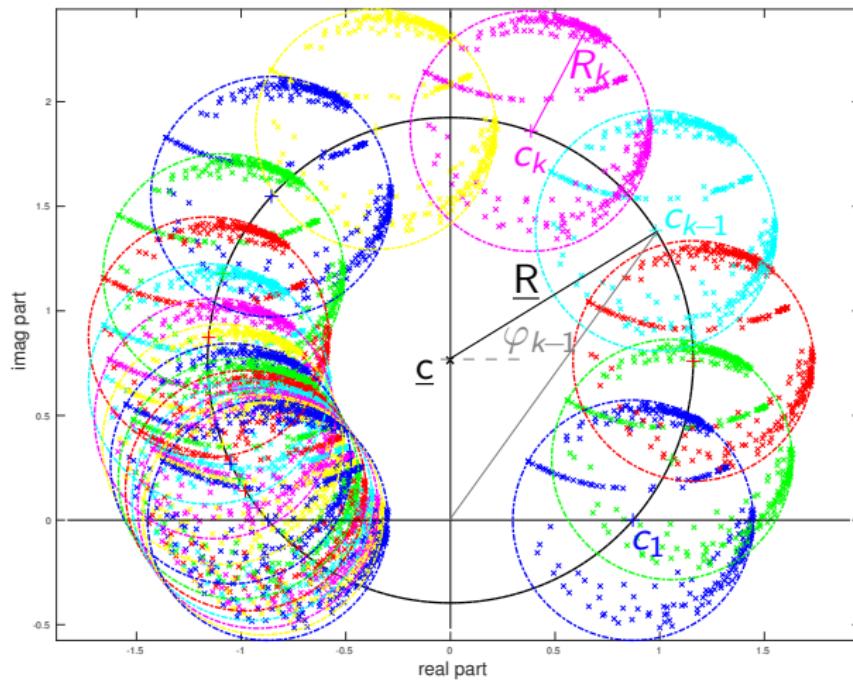
# Spectral analysis



# Spectral analysis



# Spectral analysis



# Spectral analysis

**Thm.:** Optimal seed shift for multi-shift GMRES

[B/vG, 2016]

- (i) For  $\lambda \in \Lambda[\mathcal{A}\mathcal{B}^{-1}]$  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  $\underline{c}$  and radius  $\underline{R}$ .
- (iv) Consider the preconditioner  $\mathcal{P}(\tau^*) = \mathcal{A} - \tau^* \mathcal{B}$ . An optimal seed frequency  $\tau^*$  for preconditioned multi-shift GMRES is given by,

$$\begin{aligned}\tau^*(\epsilon, \omega_1, \omega_N) &= \min_{\tau \in \mathbb{C}} \max_{k=1, \dots, N} \left( \frac{R_k(\tau)}{|c_k|} \right) = \dots = \\ &= \frac{2\omega_1\omega_N}{\omega_1 + \omega_N} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_N)^2 + (\omega_N - \omega_1)^2] \omega_1 \omega_N}}{\omega_1 + \omega_N}\end{aligned}$$

# Spectral analysis

**Thm.:** Optimal seed shift for multi-shift GMRES

[B/vG, 2016]

- (i) For  $\lambda \in \Lambda[\mathcal{A}\mathcal{B}^{-1}]$  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  $\underline{c}$  and radius  $\underline{R}$ .
- (iv) Consider the preconditioner  $\mathcal{P}(\tau^*) = \mathcal{A} - \tau^* \mathcal{B}$ . An optimal seed frequency  $\tau^*$  for preconditioned multi-shift GMRES is given by,

$$\begin{aligned}\tau^*(\epsilon, \omega_1, \omega_N) &= \min_{\tau \in \mathbb{C}} \max_{k=1,\dots,N} \left( \frac{R_k(\tau)}{|c_k|} \right) = \dots = \\ &= \frac{2\omega_1\omega_N}{\omega_1 + \omega_N} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_N)^2 + (\omega_N - \omega_1)^2] \omega_1\omega_N}}{\omega_1 + \omega_N}\end{aligned}$$

# Spectral analysis

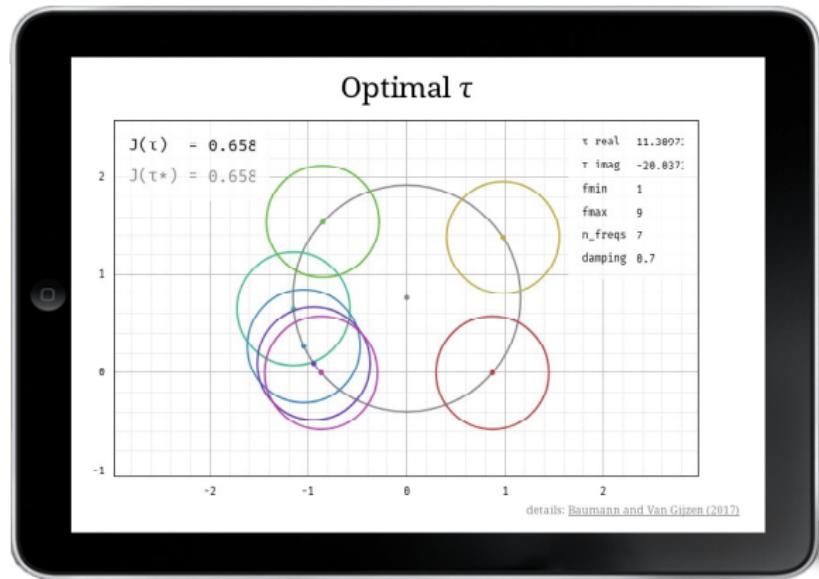
**Proof:**

# Spectral analysis

**Proof:** Not now.

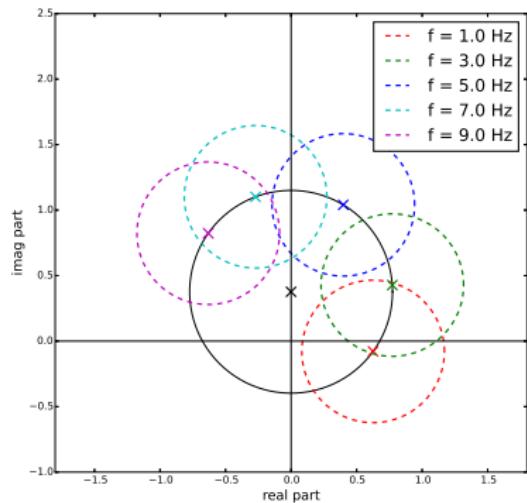
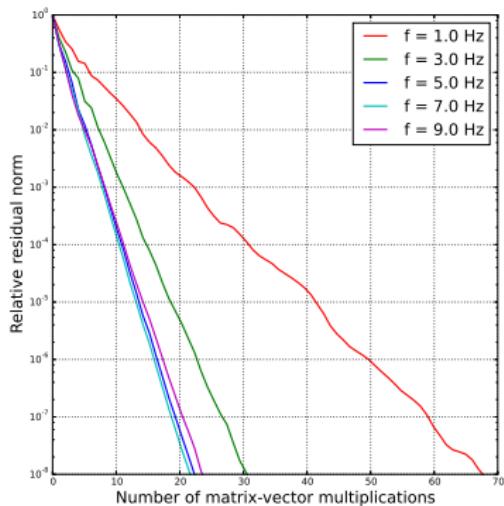
# Spectral analysis

**Proof:** There is an App for that.



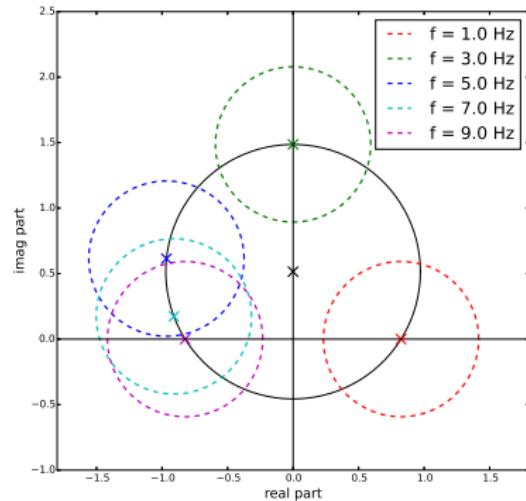
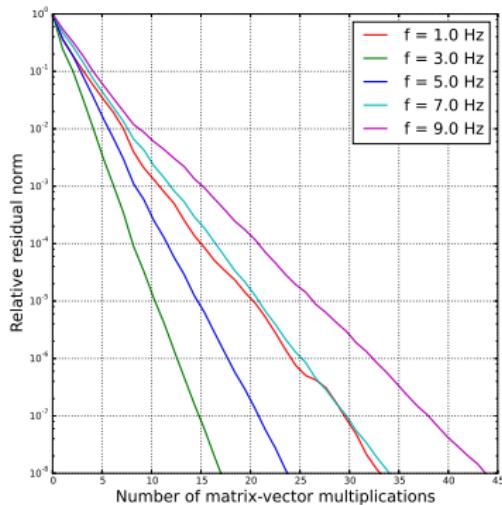
# Convergence behavior and spectral bounds

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!