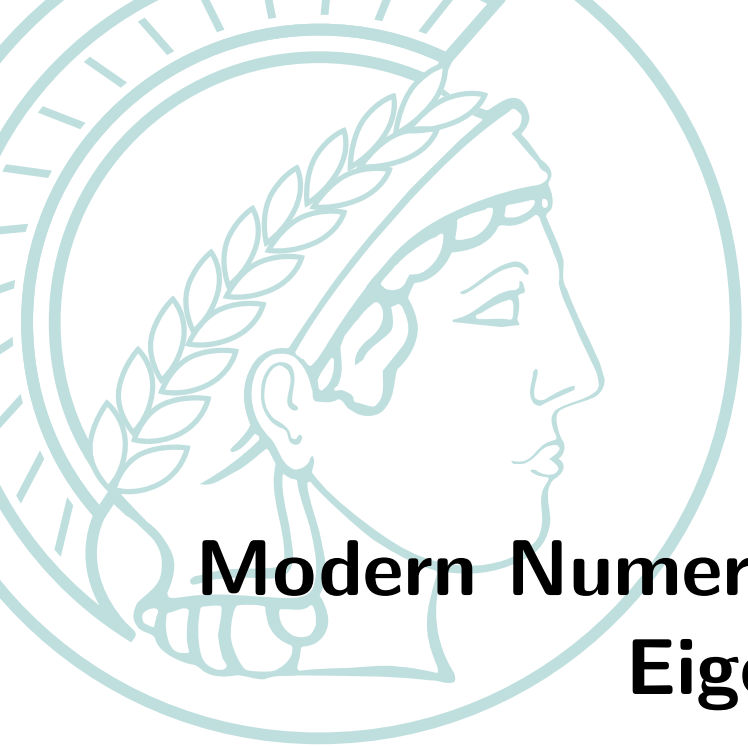
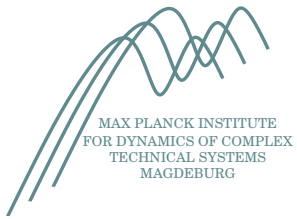


November 5, 2010

Modern Numerical Methods for Large–Scale Eigenvalue Problems

Patrick Kürschner

Max Planck Institute for Dynamics of Complex Dynamical Systems
Computational Methods in Systems and Control Theory



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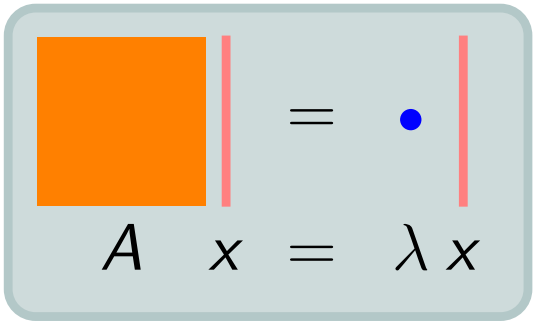
Introduction

What are eigenvalue problems?

Recall the *standard linear eigenvalue problem* from undergraduate linear algebra courses:



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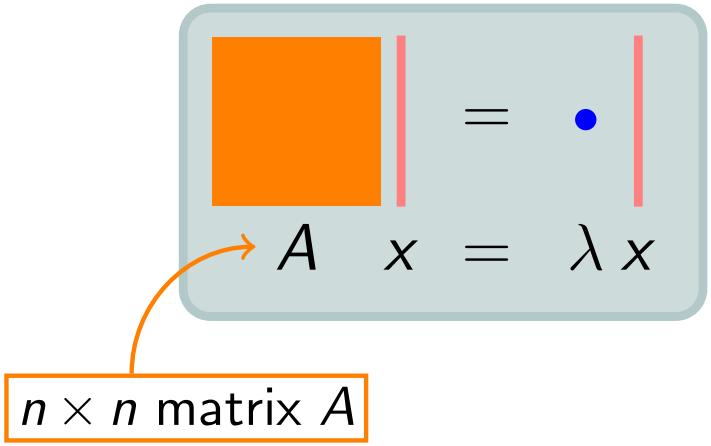

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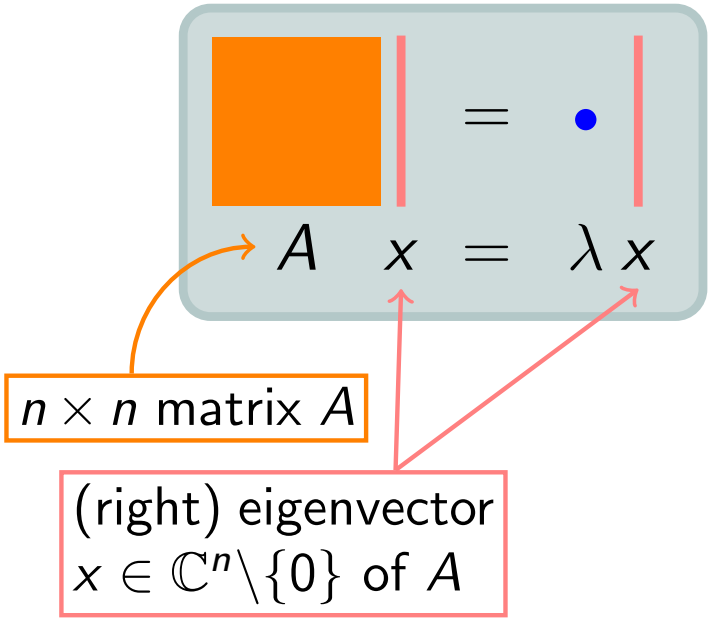

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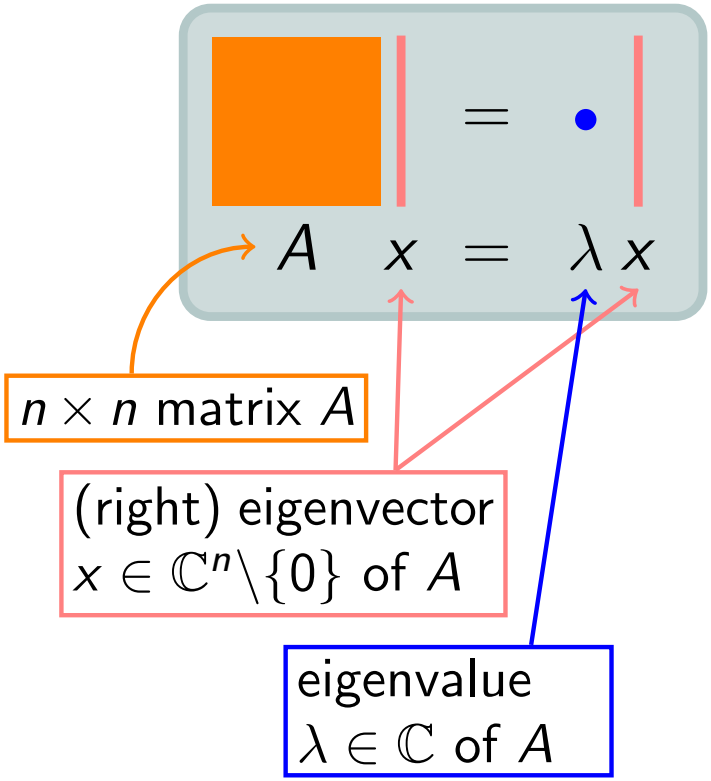

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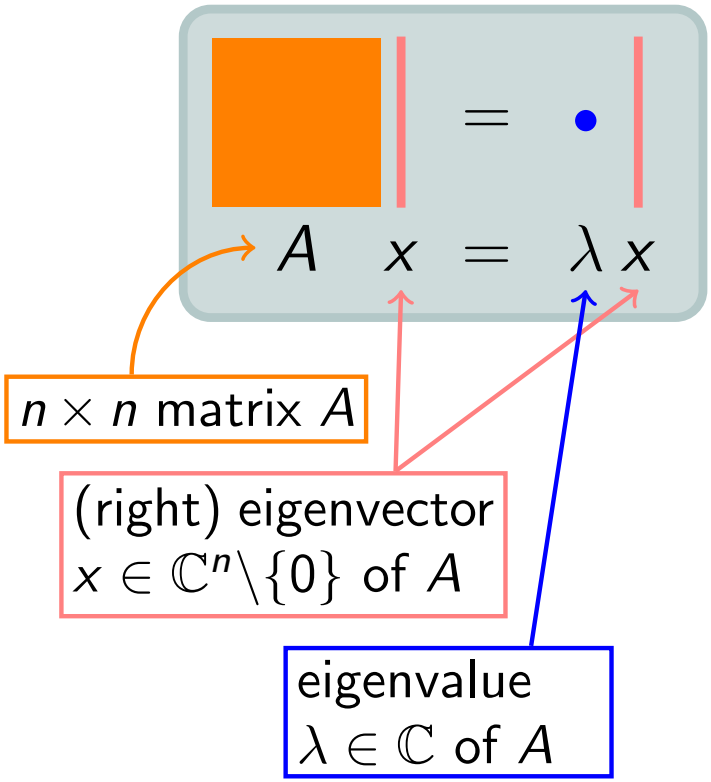

Some facts

- λ is an eigenvalue of A
  - $\Leftrightarrow$ λ is a root of the *characteristic polynomial* $\chi_A(\lambda) := \det(A - \lambda I) = 0$
  - $\Leftrightarrow$ $A - \lambda I$ is singular

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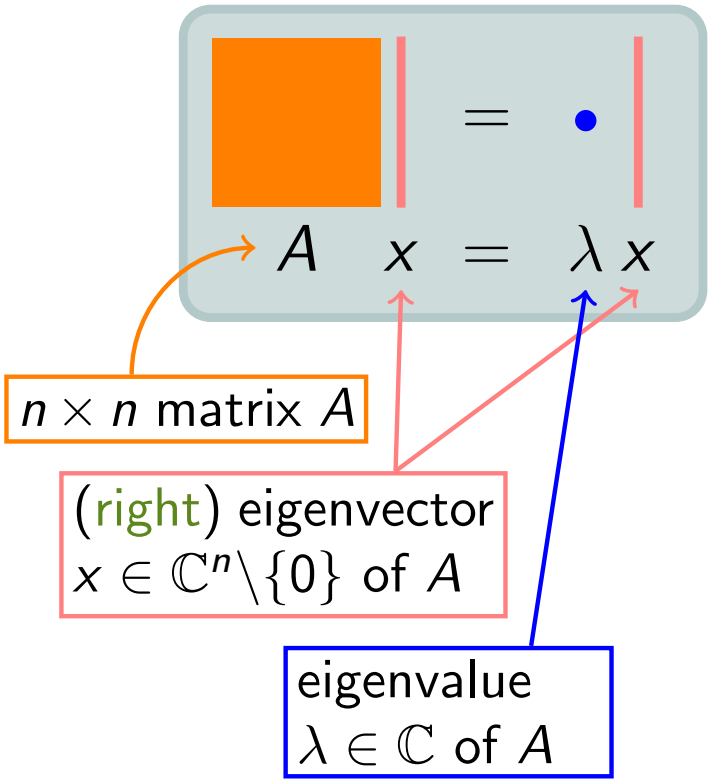

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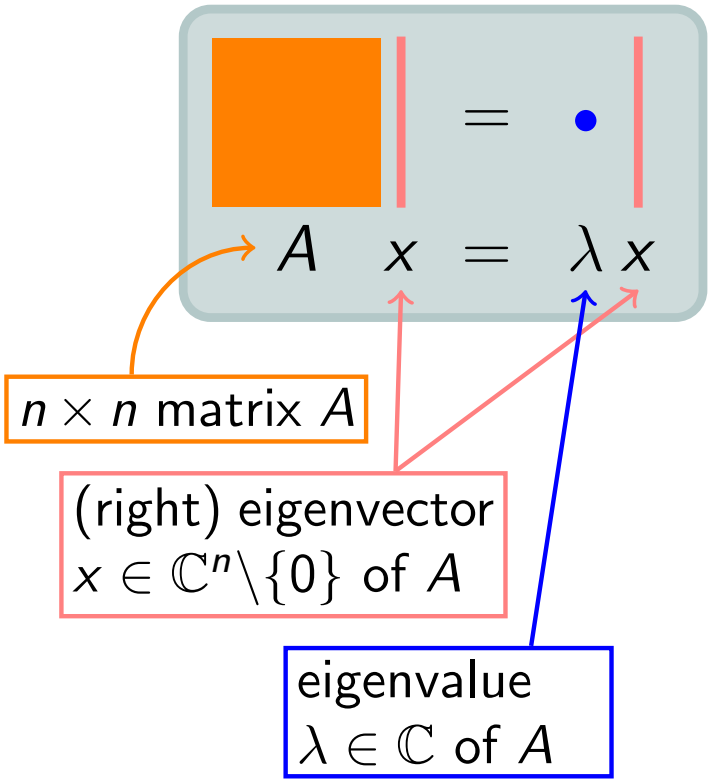

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This is only the beginning!

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Linear eigenvalue problems

standard problems: $Ax = \lambda x$

Different kinds of eigenvalue problems

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$T(\lambda)x = 0$, where $T(\lambda)$ is an arbitrary **nonlinear** matrix-valued operator $T(\cdot) : \mathbb{C} \to \mathbb{C}^{n \times n}$.

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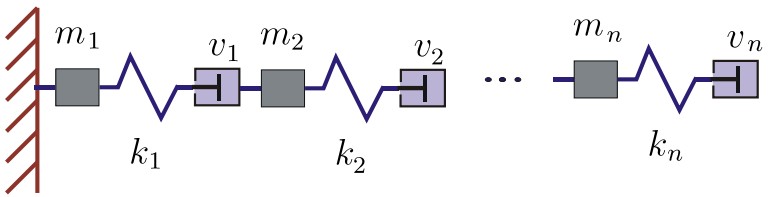
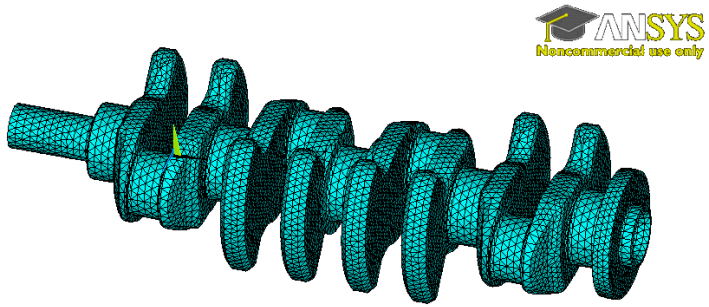
Applications - Linear dynamical systems

Important application: Vibration analysis of mechanical structures



(a) Mass-spring-damper-chain



(b) Structural FE-model of a crankshaft

Description by *second order control system*

$$M\,\ddot{x}(t) + D\,\dot{x}(t) + K\,x(t) = B\,u(t)$$

$$y(t) = C\,x(t)$$

Mass — Damping — Stiffness

large $n \times n$ matrices

output equation

input / control, e.g., excitation by external forces

Introduction

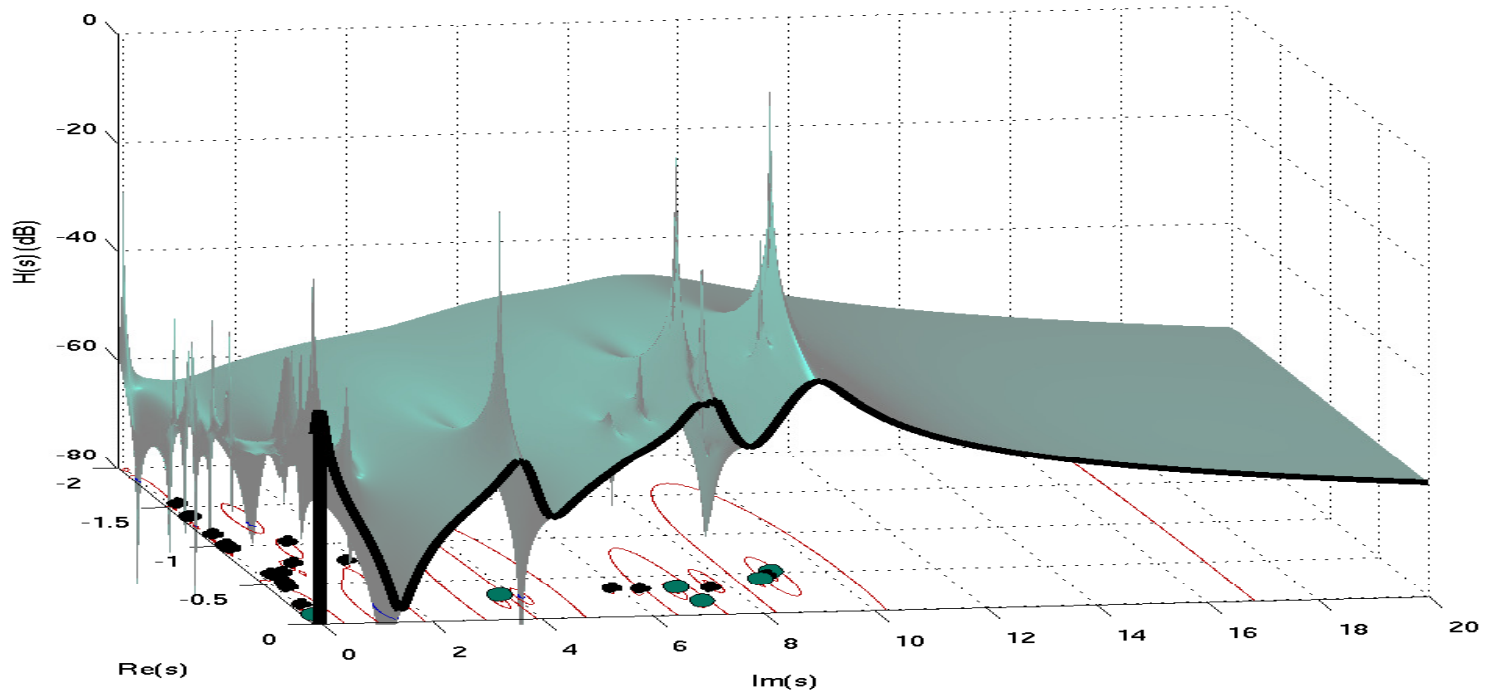
Applications - Linear dynamical systems

Using the Laplace transformation yields the *transfer function* of the control system

$$H(s) = C(s^2M + sD + K)^{-1}B, \ s \in \mathbb{C}.$$

Its poles are the eigenvalues of the quadratic eigenvalue problem

$$T(\lambda)x = (\lambda^2 M + \lambda D + K)x = 0.$$



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Applications - Linear dynamical systems and model order reduction

Original large-scale system

$$M\ddot{x} + D\dot{x} + Kx = Bu$$
$$y = Cx$$

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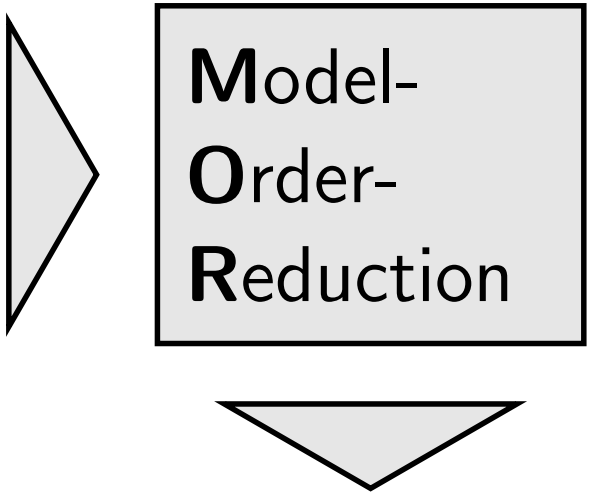

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Model-
Order-
Reduction

Projection of original system

$$W^T M V \ddot{\tilde{x}} + W^T D V \dot{\tilde{x}} + W^T K V \tilde{x} = W^T B u$$
$$\tilde{y} = C V \tilde{x}$$

with $V = \begin{bmatrix} | & & | \\ \cdots & & \cdots \\ | & & | \end{bmatrix}$ right, $W^T = \begin{bmatrix} - & \cdots & - \\ & \vdots & \\ - & \cdots & - \end{bmatrix}$ left

eigenvectors $x,\ y$ of $T(\lambda) = \lambda^2 M + \lambda D + K$

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Model-Order-Reduction

Reduced system

$$\tilde{M}\,\ddot{\tilde{x}} + \tilde{D}\,\dot{\tilde{x}} + \tilde{K}\,\tilde{x} = \tilde{B}\,u$$
$$\tilde{y} = \tilde{C}\,\tilde{x}$$

with $\tilde{M},\ \tilde{D},\ \tilde{K} \in \mathbb{R}^{\mathbf{k}\times\mathbf{k}}$, $\tilde{B} \in \mathbb{R}^{\mathbf{k}\times m}$, $\tilde{C} \in \mathbb{R}^{p\times\mathbf{k}}$ and $\mathbf{k} \ll \mathbf{n}$.

with $V = \begin{bmatrix} | & & | \\ \cdots & & \cdots \\ | & & | \end{bmatrix}$ (right) $W^T = \begin{bmatrix} — \\ \vdots \\ — \end{bmatrix}$ (left)

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Model-Order-Reduction

- see also our poster

  Modal Approximation of Large–Scale Dynamical Systems using Jacobi-Davidson Methods

- other **MOR** techniques in the talks of
  - → Peter Benner (yesterday)
  - → Lihong Feng ($10^{\underline{00}}$)
  - → Tobias Breiten ($10^{\underline{30}}$)

Reduced system

$$\tilde{M}\,\ddot{x} + \tilde{D}\,\dot{x} + \tilde{K}\,x = \tilde{B}\,u, \quad \tilde{M},\ \tilde{D},\ \tilde{K} \in \mathbb{R}^{k\times k}$$
$$y = \tilde{C}\,x, \quad \tilde{B} \in \mathbb{R}^{k\times m},\ \tilde{C} \in \mathbb{R}^{p\times k}$$
$$k \ll n.$$

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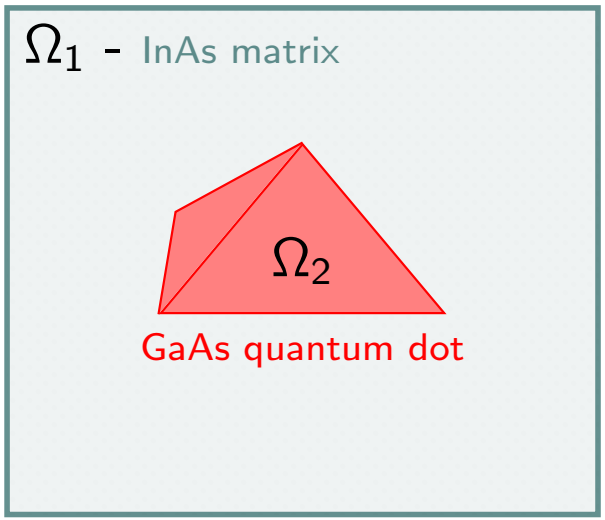
Introduction

Applications – Quantum Mechanics

Another application: semiconductor devices in microelectronics
Consider a so called *quantum dot*, an extremely small semiconductor nanostructure, i.e. its dimensions are smaller than the electron wavelength ($\approx 10^{-12}$ m).
Hence, its electronic states are quantized at discrete energy levels.



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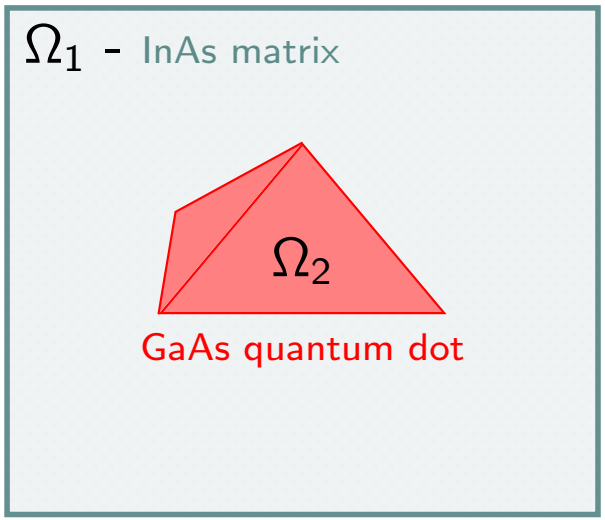

The Schrödinger equation

$$-\nabla \cdot \left(\frac{\hbar^2}{2m_j(\lambda)} \nabla \psi \right) + V_j \psi = \lambda \psi$$

for $j \in \{1, 2\}$ reveals the relevant energy levels λ and wave functions ψ of the electrons.

- $\hbar$ - reduced Planck constant,
- V_j - (constant) confinement potential in Ω_j,
- $m_j(\lambda)$ - effective electron mass in Ω_j ($j \in \{1, 2\}$).

Introduction

Applications – Quantum Mechanics

For this semiconductor setting the *non-parabolic effective mass model*

$$\frac{1}{m_j(\lambda)} = \frac{p_j^2}{\hbar^2}\left(\frac{2}{\lambda + V_j - \tau_j} - \frac{1}{\lambda + V_j - \mu_j}\right), \ \tau_j \neq \mu_j \in \mathbb{R}, \quad j \in \{1, 2\}$$

leads with a discretization of the Schrödinger equation, e.g. by FEM, ..., to a rational eigenvalue problem $T(\lambda)x = 0$, where

$$T(\lambda) = \lambda M - \frac{1}{m_1(\lambda)} N - \frac{1}{m_2(\lambda)} P - Q$$

large, sparse $n \times n$ FE - matrices

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large, sparse $n \times n$ FE - matrices

Solution with *nonlinear Jacobi-Davidson algorithm*:

- multiply by greatest common denominator and solve quintic polynomial problem $T(\lambda) = \lambda^5 A_5 + \lambda^4 A_4 + \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0$

  [Hwang, Lin, Wang, Wang '04/'05]

- directly as rational eigenproblem

  [Voss '06]

Overview

Algorithms for Linear Problems

Small Problems

Back to $Ax = \lambda x$ where A is of small or moderate size.
General procedure:
Transform A via a *similarity transformation* T to an easier form:

such that the eigenvalues appear on the diagonal.

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Algorithms & available software

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MATLAB® (`eig, schur`), LAPACK

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Disadvantage

Similarity / unitary transformations are very expensive (complexity $\mathcal{O}(n^3)$)
$\Rightarrow$ **not** feasible for large-scale problems

Algorithms for Linear Problems

Large-Scale Problems

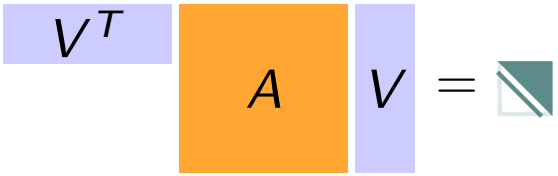
General procedure for large-scale problems		
1.	Project A onto low-dimensional subspace $\mathcal{V} = \mathrm{colspan}(V)$, $V \in \mathbb{R}^{n \times k}$, $k \ll n$ V^T A V $=$ H Similar approach as in MOR with $W = V$.	
2.	Compute eigenvalues θ and eigenvectors q of H using methods for small matrices.	
3.	Approximate eigenpairs of A are $(\theta,\ v := Vq)$, residual $r := Av - \lambda v$.	
4.	If $\|r\|$ is not sufficiently small?	
	YES: converged !	**NO**: expand V by some appropriate new vector t and goto 1.

Algorithms for Linear Problems

Large-Scale Problems I: Krylov–Subspace Methods

Generate $\mathcal{V}$ as *Krylov subspace*
$\mathcal{K}_k(A,\ v) = \operatorname{span}\{v,\ Av,\ A^2v, \ldots,\ A^{k-1}v\}$.

I. Arnoldi method



II. Lanczos method for $A = A^T$

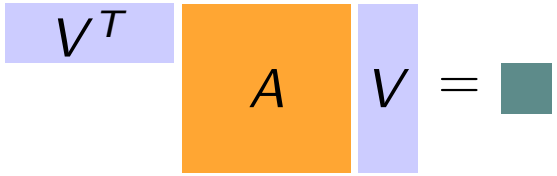
Available software

- `eigs` in MATLAB
- **AR**noldi**PACK**age (ARPACK), Fortran 77 library
- **S**calable **L**ibrary for **E**igenvalue **P**roblem **C**omputations (SLEPc), C++ library for *parallel computers*

Algorithms for Linear Problems

Large-Scale Problems II: Jacobi–Davidson Methods

Jacobi-Davidson methods: Impose no special structure on $\mathcal{V}$



Expand $\mathcal{V}$ orthogonally by $t \perp v$, obtained from the (inexact) solution of the *Jacobi-Davidson correction equation*

$$(I - vv^T)(A - \theta I)(I - vv^T)t = -r.$$

[Sleijpen, Van der Vorst, et al '96/'98/'00]

Available software

- MATLAB routines (JDQR, JDQZ, ...)
  [Sleijpen, Van der Vorst, Fokkema '98]
- SLEPc (since August 2010)
- PRIMME (SLEPc add-on for $A = A^T$) [Stathopoulos '07]

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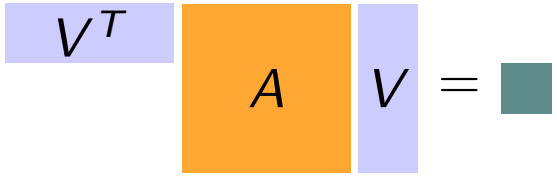

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Preconditioned eigensolver, similar to PINVIT in the talk by

$\rightarrow$ Thomas Mach ($9^{\underline{00}}$)

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Methods for Nonlinear Eigenvalue Problems

Small Problems – Newton's Method

Note that an eigenpair $(\lambda,\ x)$ of $T(\lambda)$ is a root of the function

$$F(x,\ \lambda) = \begin{bmatrix} T(\lambda)x \\ w^H x - 1 \end{bmatrix},\ F : \mathbb{C}^{n+1} \mapsto \mathbb{C}^{n+1}.$$

First idea: apply **Newton's method**.
Initial approximation $(\theta,\ v) \approx (\lambda,\ x)$, Newton system for the next (hopefully better) approximation $(\theta_+,\ v_+)$ is

$$\begin{bmatrix} v_+ \\ \theta_+ \end{bmatrix} = \begin{bmatrix} v \\ \theta \end{bmatrix} - [\partial F(v,\ \theta)]^{-1} F(v,\ \theta).$$

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Drawbacks

- Requires good initial approximations $(\theta,\ v)$
- Matrix inversion infeasible for large problems

Methods for Nonlinear Eigenvalue Problems

Large-Scale Problems - Nonlinear Jacobi-Davidson

Nonlinear Jacobi-Davidson: Project the operator $T(\lambda)$ onto $\mathcal{V}$

$$V^T \; T(\lambda) \; V = H(\lambda)$$

Solve the small problem $H(\theta)q = 0$, e.g., using Newton's method

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Expand $\mathcal{V}$ orthogonally by $t \perp v$, obtained from the (inexact) solution of the *Jacobi-Davidson correction equation for the nonlinear EVP*

$$\left(I - \frac{\dot{T}(\theta)vv^T}{v^T\dot{T}(\theta)v}\right) T(\theta)\left(I - vv^T\right)t = -r = -T(\theta)v.$$

[Betcke, Voss '04, Schreiber, Schwetlick '07/'08]

Methods for Nonlinear Eigenvalue Problems

Large-Scale Problems - Nonlinear Jacobi-Davidson

Nonlinear Jacobi-Davidson: Project the operator $T(\lambda)$ onto $\mathcal{V}$

$$V^T \quad T(\lambda) \quad V = H(\lambda)$$

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[Betcke, Voss '04, Schreiber, Schwetlick '07/'08]

Advantage

Applies only *cheap* operations compared to Newton's method.

Methods for Nonlinear Eigenvalue Problems

Large-Scale Problems - Nonlinear Jacobi-Davidson

Disadvantage

Still highly dependent on good initial approximations!

Methods for Nonlinear Eigenvalue Problems

Large-Scale Problems - Nonlinear Jacobi-Davidson

Disadvantage

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Other methods

- nonlinear Arnoldi
- Rayleigh functional iteration, inverse iteration
- safeguarded iteration, method of successive linear problems
- homotopy methods
- ...

Methods for Nonlinear Eigenvalue Problems

Large-Scale Problems - Nonlinear Jacobi-Davidson

Further Challenges

- efficient treatment of involved linear systems
- stable computation of several eigenvalues and corresponding eigenvectors
- computation of left eigenvectors
- application within MOR for nonlinear systems
- ...

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Thank you for your attention!