Iterative projection methods for general nonlinear eigenproblems

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Outline

- Nonlinear eigenvalue problems

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- Iterative projection methods

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- Minmax characterization for nonlinear eigenproblems
- Numerical examples

Nonlinear eigenvalue problems

Let $D \subset \mathbb{C}$ be an open set (maybe unbounded), and let $T(\lambda) \in \mathbb{C}^{n\times n}$, $\lambda \in D$ be a family of matrices.

Find $\lambda \in D$ and $x \neq 0$ such that

$$T(\lambda)x = 0.$$

Then λ is called an eigenvalue of $T(\cdot)$, and x a corresponding eigenvector.

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Problems of this type arise in vibrations of conservative gyroscopic systems, damped vibrations of structures, problems with retarded argument, lateral buckling problems, fluid-solid vibrations, quantum dot heterostructures, and sandwich plates, e.g.

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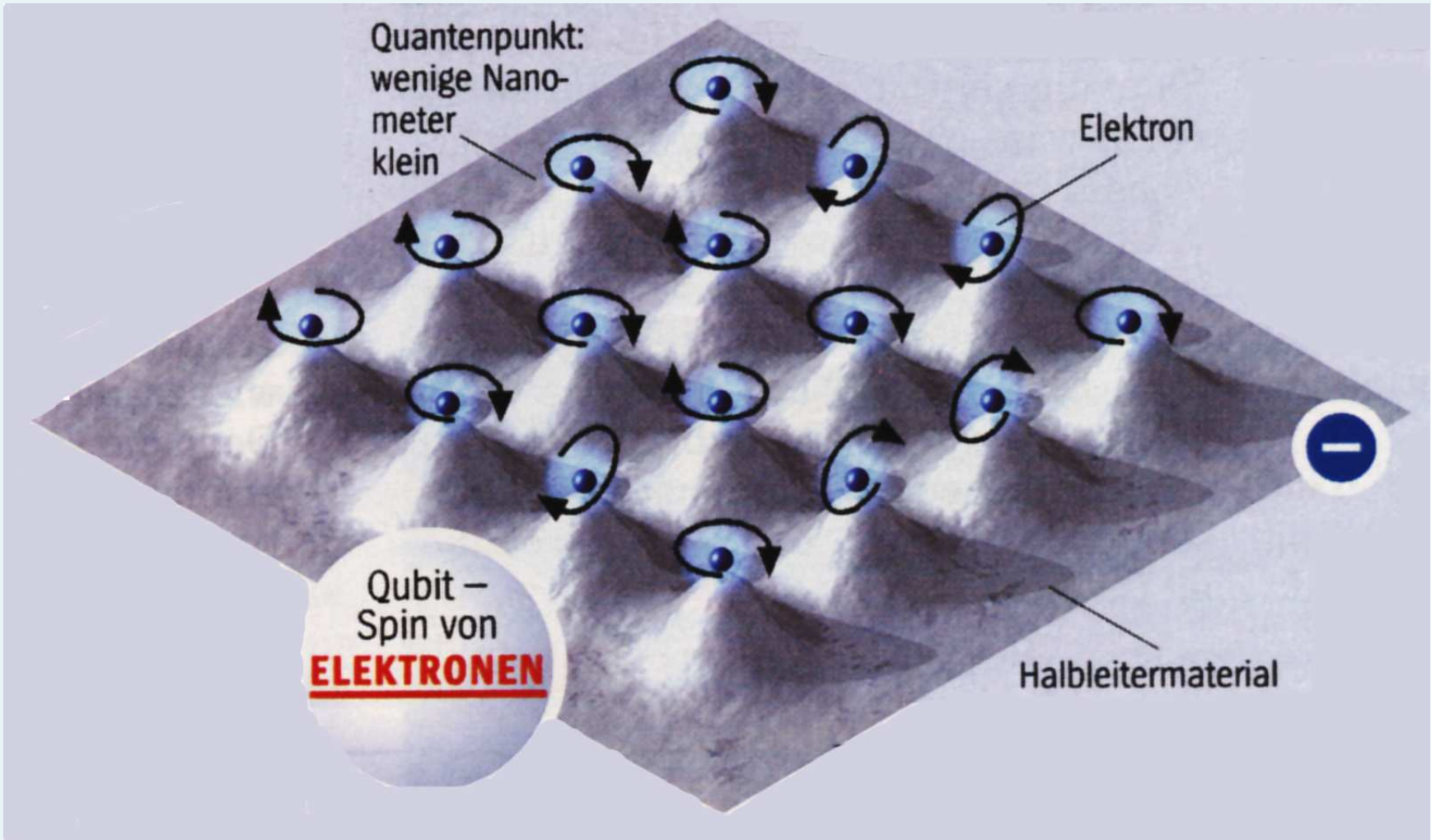
The ultimate limit of low dimensional structures is the quantum dot, in which the carriers are confined in all three directions, thus reducing the degrees of freedom to zero.
Therefore, a quantum dot can be thought of as an artificial atom.

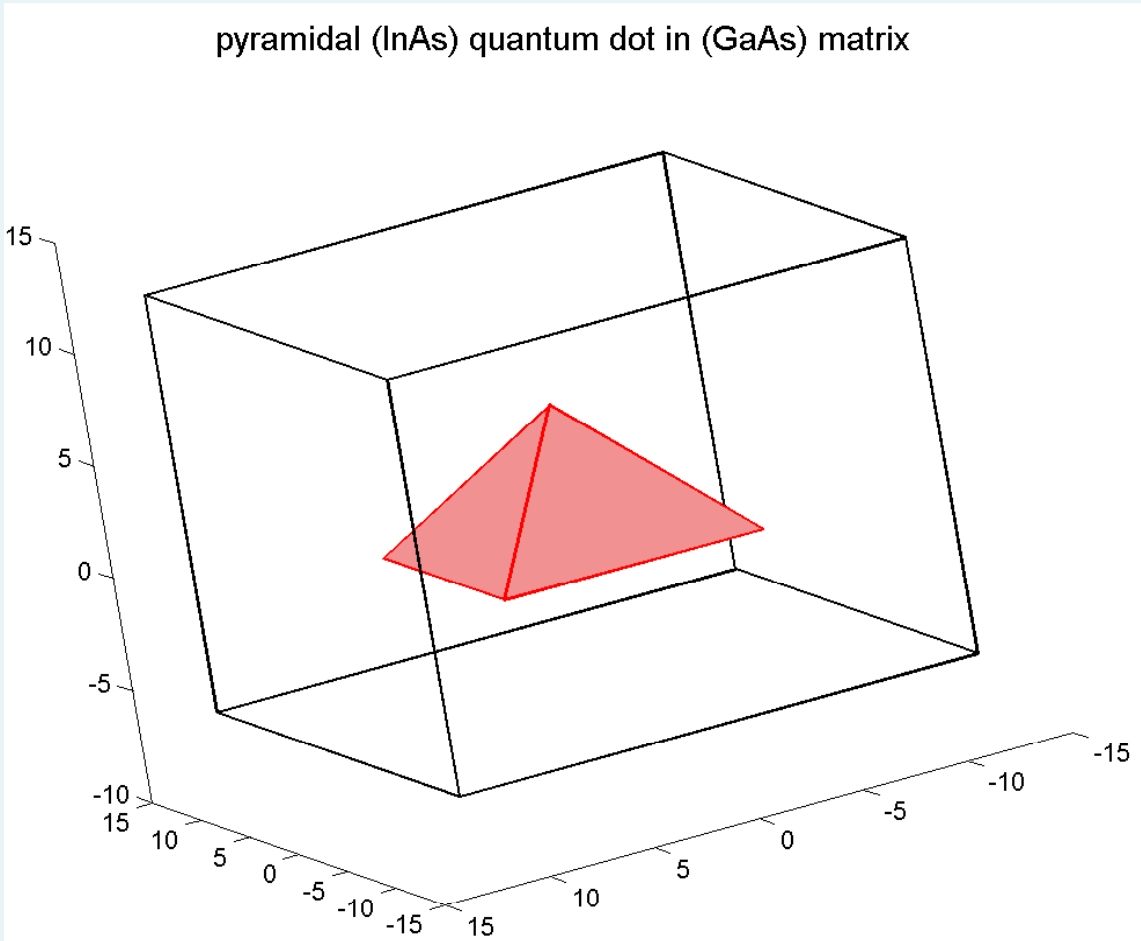
Quantum dots ct.



DER SPIEGEL, March 14, 2005

Quantum dots ct.

Determine relevant energy states (i.e. eigenvalues) and corresponding wave functions (i.e. eigenfunctions) of a three-dimensional quantum dot embedded in a matrix.



Schrödinger equation

$$-\nabla\cdot\left(\frac{\hbar^2}{2m(x,\lambda)}\nabla u\right)+V(x)u=\lambda u,\quad x\in\Omega_1\cup\Omega_2$$

where $\hbar$ is the reduced Planck constant,

$$m(x,\lambda)=\begin{cases}\frac{1}{m_1(\lambda)}, & x\in\Omega_1\\ \frac{1}{m_2(\lambda)}, & x\in\Omega_2\end{cases}\qquad V(x)=\begin{cases}0, & x\in\Omega_1\\ V_2, & x\in\Omega_2\end{cases}$$

$$\frac{1}{m_j(\lambda)}=\frac{P_j^2}{\hbar^2}\left(\frac{2}{\lambda+g_j-V_j}+\frac{1}{\lambda+g_j-V_j+\delta_j}\right)$$

where m_j is the electron effective mass, V_j the confinement potential, P_j the momentum, g_j the main energy gap, and δ_j the spin-orbit splitting in the jth region.

Quantum dot ct.

Boundary and interface conditions

$$u = 0 \quad \text{on outer boundary of matrix } \Omega_1$$

BenDaniel–Duke condition

$$\left.\frac{1}{m_2}\frac{\partial u}{\partial n}\right|_{\partial\Omega_2} = \left.\frac{1}{m_1}\frac{\partial u}{\partial n}\right|_{\partial\Omega_1} \quad \text{on interface}$$

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Variational form

Find $\lambda \in \mathbb{R}$ *and* $u \in H_0^1(\overline{\Omega}_1 \cup \Omega_2)$, $u \neq 0$, *such that*

$$\begin{aligned} a(u,v;\lambda) &:= \frac{1}{m_1(\lambda)}\int_{\Omega_1} \nabla u \nabla v\, dx + \frac{1}{m_2(\lambda)}\int_{\Omega_2} \nabla u \nabla v\, dx + V_2 \int_{\Omega_2} uv\, dx \\ &= \lambda \int_{\Omega_1 \cup \Omega_2} uv\, dx =: \lambda b(u,v) \quad \text{for every } v \in H_0^1(\overline{\Omega}_1 \cup \Omega_2) \end{aligned}$$

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Discretization (FEM, FVM) $\rightarrow$ rational matrix eigenvalue problem

Iterative projection methods

For linear sparse eigenproblems

$$T(\lambda) = \lambda B - A$$

very efficient methods are iterative projection methods (Lanczos, Arnoldi, Jacobi–Davidson method, e.g.), where approximations to the wanted eigenvalues and eigenvectors are obtained from projections of the eigenproblem to subspaces of small dimension which are expanded in the course of the algorithm.

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- methods which project the problem to a sequence of Krylov spaces like Lanczos or Arnoldi, and
- methods which aim at a specific eigenpair like the Jacobi–Davidson method.

Generalizations to nonlinear sparse eigenproblems

- nonlinear rational Krylov: Ruhe (2000,2005), Hager (2001)
  Regula falsi for the nonlinear problem and Arnoldi for the linear problem are knit together to form a sequence of subspaces $V_k \in \mathbb{C}^n$ and corresponding Hessenberg matrices H_k which approximate the projection of $T(\sigma)^{-1}T(\lambda_k)$ on V_k for some shift σ close to the wanted eigenvalues.

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- Arnoldi method: V. (2003, 2004); quadratic probl.: Meerbergen (2001)

- Jacobi-Davidson: Betcke, V. (2002), Schwetlick (2005)
  polynomial problems: Sleijpen, Boten, Fokkema, van der Vorst (1996), Hwang, Lin, Wang, Wang (2003,2004)

Expanding the subspace

Given subspace $V \subset \mathbb{C}^n$. Expand V by a direction with high approximation potential for the next wanted eigenvector.

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BUT: In each step have to solve large linear system with varying matrix

Way out: Residual inverse It.

start with an approximation x_1 to an eigenvector of $T(\lambda)x = 0$
for $\ell = 1, 2, \ldots$ until convergence **do**
    solve $e^H T(\sigma)^{-1} T(\mu_{\ell+1}) x_\ell = 0$ for $\mu_{\ell+1}$
    compute the residual $r_\ell = T(\mu_{\ell+1}) x_\ell$
    solve $T(\sigma) d_\ell = r_\ell$
    set $x_{\ell+1} = x_\ell - d_\ell$, $x_{\ell+1} = x_{\ell+1} / \|x_{\ell+1}\|$
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7: **end for**

Theorem (Neumaier 1985)

Let $T(\lambda)$ be twice continously differentiable. Assume that $\hat{\lambda}$ is a simple eigenvalue of $T(\lambda)x = 0$, and let $\hat{x}$ be a corresponding eigenvector normalized by $\|\hat{x}\| = 1$. Then the residual inverse iteration converges for all σ sufficently close to $\hat{\lambda}$, and it holds

$$\frac{\|x_{\ell+1} - \hat{x}\|}{\|x_\ell - \hat{x}\|} = \mathcal{O}(|\sigma - \hat{\lambda}|), \quad \text{and} \quad |\lambda_{\ell+1} - \hat{\lambda}| = \mathcal{O}(\|x_\ell - \hat{x}\|).$$

Arnoldi method

If θ is an eigenvalue of the projected problem $V^H T(\lambda) V y = 0$ and $\tilde{x} = V\tilde{y}$ is a corresponding Ritz vector, then expand V by new direction

$$v = \tilde{x} - T(\sigma)^{-1} T(\theta)\tilde{x}$$

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If the linear system $T(\sigma)v = T(\theta)\tilde{x}$ is too expensive to solve for v we may choose as new direction $v = MT(\lambda)\tilde{x}$ with $M \approx T(\sigma)^{-1}$, and for the linear problem we obtain the preconditioned Arnoldi method.

Therefore the resulting iterative projection method is called nonlinear Arnoldi method

Nonlinear Arnoldi Method

start with initial basis V, $V^H V = I$; set $k = m = 1$
determine preconditioner $M \approx T(\sigma)^{-1}$, σ close to first wanted eigenvalue
while $m \leq$ number of wanted eigenvalues **do**
  solve $V^H T(\mu) V y = 0$ for (μ, y) and set $u = Vy$, $r_k = T(\mu)u$
  if $\|r_k\|/\|u\| < \epsilon$ **then**
    Accept eigenpair $\lambda_m = \mu$, $x_m = u$,
    if $m ==$ number of wanted eigenvalues **then** STOP **end if**
    $m = m + 1$
    if $(k > 1)$ & $(\|r_{k-1}\|/\|r_k\| >$ tol) **then**
      choose new pole σ, determine preconditioner $M \approx T(\sigma)^{-1}$
    end if
    restart if necessary
    Choose approximations μ and u to next eigenvalue and eigenvector
    determine $r = T(\mu)u$ and set $k = 0$
  end if
  $v = Mr$, $k = k + 1$
  $v = v - VV^H v$,$\tilde{v} = v/\|v\|$, $V = [V, \tilde{v}]$ and reorthogonalize if necessary
end while

Second Way out: Jacobi–Davidson

Solve (approxemately) the correction equation

$$(I - \frac{T'(\theta)xx^T}{x^T T'(\theta)x})T(\theta)(I - xx^T)t = -r, \qquad t \perp x$$

where (x, θ) is the current Ritz pair and $r = T(\theta)x$.

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If the correction equation is solved exactly, then

$$T(\theta)t - \alpha T'(\theta)x = -r$$

where α is chosen such that $t \perp x$. Solving for t yields

$$t = -x + \alpha T(\theta)^{-1}T'(\theta)x.$$

Since $x = Vy$ for some y, and t is orthogonalized against V the expansion by t is equivalent to the expansion by inverse iteration.

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The operator $T(\sigma)$ is restricted to map the subspace $x^{\perp}$ into itself. Hence, if $M \approx T(\sigma)$ is a preconditioner of $T(\sigma)$, $\sigma \approx \theta$, then a preconditioner for an iterativ solver of the correction equation should be modified correspondingly to

$$\tilde{M} := (I - \frac{T'(\theta)uu^H}{x^H T(\theta)u})M(I - \frac{uu^H}{u^H u}).$$

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Taking into account the projectors in the preconditioner, i.e. using $\tilde{M}$ instead of M, raises the cost of the preconditioned Krylov solver only slightly (cf. Sleijpen, van der Vorst). Only one additional linear solve with system matrix M is required.

Variant of Hwang, Lin, Wang, Wang (2004)

Solve

$$\Big(I - \frac{T'(\theta)uu^H}{u^H T'(\theta)u}\Big)T(\theta)\Big(I - \frac{uu^H}{u^H u}\Big)t = -r, \quad t \perp u$$

approximately

Variant of Hwang, Lin, Wang, Wang (2004)

Solve

$$\Big(I - \frac{T'(\theta)uu^H}{u^H T'(\theta)u}\Big)\cancel{T(\theta)}^{M}\Big(I - \frac{uu^H}{u^H u}\Big)t = -r, \quad t \perp u$$

approximately by computing

$$t = M^{-1}r + \alpha M^{-1}T'(\theta)u \quad \text{with } \alpha := \frac{u^H M^{-1} r}{u^H M^{-1} T'(\theta) u}$$

where M is a preconditioner of $T(\theta)$.

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Method combines preconditioned Arnoldi method ($M^{-1}r$) and simplified inverse iteration ($M^{-1}T'(\theta)u$)

Primal-Dual JD Update: Schwetlick (2005)

Given: triplet (u, v, θ), s.t. $\|u\| = \|v\| = 1$, $v^H T(\theta) u = 0$

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- solve $(I - vv^H) T(\theta)(I - uu^H)s = -T(\theta)u,\ u^H s = 0$
- solve $(I - uu^H) T(\theta)^H (I - vv^H)t = -T(\theta)^H v,\ v^H t = 0$
- set $u_+ = (u + s)/\|u + s\|$, $v_+ = (v + t)/\|v + t\|$
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Experience of Schwetlick: If Standard JD works, then it is faster than P-D JD; if $v^H T'(\theta)u$ is small then P-D JD is more robust than Standard JD

Primal-Dual JD

Given orthogonal bases V and U of left and right search spaces, and left and right approximate eigenvectors $v \in \mathrm{span}(V)$ and $u \in \mathrm{span}(U)$, and approximate eigenvalue θ s.t. $v^H T(\theta) u = 0$

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Solve

$$V^H T(\theta)Us = 0 \quad \text{and} \quad U^H T(\theta)^H Vt = 0 \quad \text{for } (s, t, \theta)$$

and set

$$u = Us \quad \text{and} \quad v = Vt.$$

Locking of converged eigenvectors

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- Approach of Hwang et al. can be generalized directly to general problems if all eigenvalues of projected problems are determined
- for Hermitean problems one can often take advantage of a variational characterization of eigenvalues

Nonlinear minmax theory

Let $T(\lambda) \in \mathbb{C}^{n\times n}$, $T(\lambda) = T(\lambda)^H$, $\lambda \in J \subset \mathbb{R}$ an open interval. Assume that

$$f : \begin{cases} J \times \mathbb{C}^n & \to & \mathbb{R} \\ (\lambda, x) & \mapsto & x^H T(\lambda) x \end{cases}$$

is continuously differentiable, and that for every fixed $x \in \mathbb{C}^n$, $x \neq 0$ the real equation

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Then equation $f(\lambda, x) = 0$ implicitly defines a functional p on some subset D of $\mathbb{C}^n$ which we call the Rayleigh functional. If $D = \mathbb{C}^n \setminus \{0\}$ then $T(\lambda)x = 0$ is called overdamped.

Nonlinear minmax theory

Let $T(\lambda) \in \mathbb{C}^{n\times n}$, $T(\lambda) = T(\lambda)^H$, $\lambda \in J \subset \mathbb{R}$ an open interval. Assume that

$$f : \begin{cases} J \times \mathbb{C}^n & \to & \mathbb{R} \\ (\lambda, x) & \mapsto & x^H T(\lambda) x \end{cases}$$

is continuously differentiable, and that for every fixed $x \in \mathbb{C}^n$, $x \neq 0$ the real equation

$$f(\lambda, x) = 0$$

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Suppose that

$$x^H T'(p(x))x > 0 \quad \text{for every } x \in D.$$

which generalizes the definiteness condition for linear eigenproblems.

Enumeration of eigenvalues

If $\lambda \in J$ is an eigenvalue of $T(\cdot)$ then $\theta = 0$ is an eigenvalue of the linear problem $T(\lambda)y = \theta y$, and therefore there exists $\ell \in \mathbb{N}$ such that

$$0 = \max_{V \in H_\ell} \min_{v \in V \setminus \{0\}} \frac{v^H T(\lambda) v}{\|v\|^2}$$

where H_ℓ denotes the set of all ℓ–dimensional subspaces of $\mathbb{R}^n$.

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In this case λ is called an ℓ-th eigenvalue of $T(\cdot)$.

Minmax characterization

Under the conditions given above it holds:

(i) For every $\ell \in \mathbb{N}$ there is at most one ℓ-th eigenvalue of $T(\cdot)$ which can be characterized by

$$\lambda_\ell = \min_{\substack{V \in H_\ell \\ V \cap D \neq \emptyset}} \sup_{v \in V \cap D} p(v). \qquad (*)$$

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(iii) If for $\mu < \nu$ there exist a μ-th and a ν-th eigenvalue of $T(\cdot)$ in J, then for $\ell = \mu, \mu+1, \ldots, \nu$ there is an ℓ-th eigenvalue $\lambda_\ell \in J$, and $\lambda_\mu \leq \lambda_{\mu+1} \leq \cdots \leq \lambda_\nu$.

Safeguarded iteration

The minimum in

$$\lambda_\ell = \min_{\substack{V \in H_\ell \\ V \cap D \neq \emptyset}} \sup_{v \in V \cap D} p(v)$$

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2: **for** $k = 1, 2, \ldots$ until convergence **do**
3: determine eigenvector u corresponding to the ℓ-largest eigenvalue of $T(\mu_k)$
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Convergence quadratic; global to the first eigenvalue, local to further eigenvalues.

Computing several eigenvalues

If $T(\lambda)$ is a family of Hermitean matrices allowing a minmax characterization of its eigenvalues in an open interval J, and if the columns of $V \in \mathbb{C}^{n\times k}$ form a basis of the current search space $\mathcal{V}$, then the projeceted problem

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Usually, while computing the m-th eigenvalue λ_m the algorithm gathers enough information in the search space $\mathcal{V}$ about the next eigenvector to compute λ_{m+1} safely, and the eigenvalues in J can be computed one after the other without determining the same eigenvalue repeatedly.

Numerical example

pyramidal quantum dot:	baselength: 12.4 nm,	height: 6.2 nm
cubic matrix:	$24.8 \times 24.8 \times 18.6$ nm^3	

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$$P_1 = 0.8503, \quad g_1 = 0.42, \quad \delta_1 = 0.48, \quad V_1 = 0.0$$
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Discretization by FEM or FVM yields rational eigenproblem

$$T(\lambda)x = \lambda Mx - \frac{1}{m_1(\lambda)}A_1x - \frac{1}{m_2(\lambda)}A_2x - Bx = 0$$

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All timings for MATLAB 7.0.4 on AMD Opteron Processor 248 $\times$ 860_64 with 2.2 GHz and 4 GB RAM

Numerical example ct.

FVM: Hwang, Lin, Wang, Wang (2004)

dim	λ_1	$\lambda_{2/3}$	λ_4	λ_5	CPU time
$2'475$	0.41195	0.58350	0.67945	0.70478	0.7 s
$22'103$	0.40166	0.57668	0.68418	0.69922	8.1 s
$186'543$	0.39878	0.57477	0.68516	0.69767	150.9 s
$1'532'255$	0.39804	0.57427	0.68539	0.69727	4017.7 s
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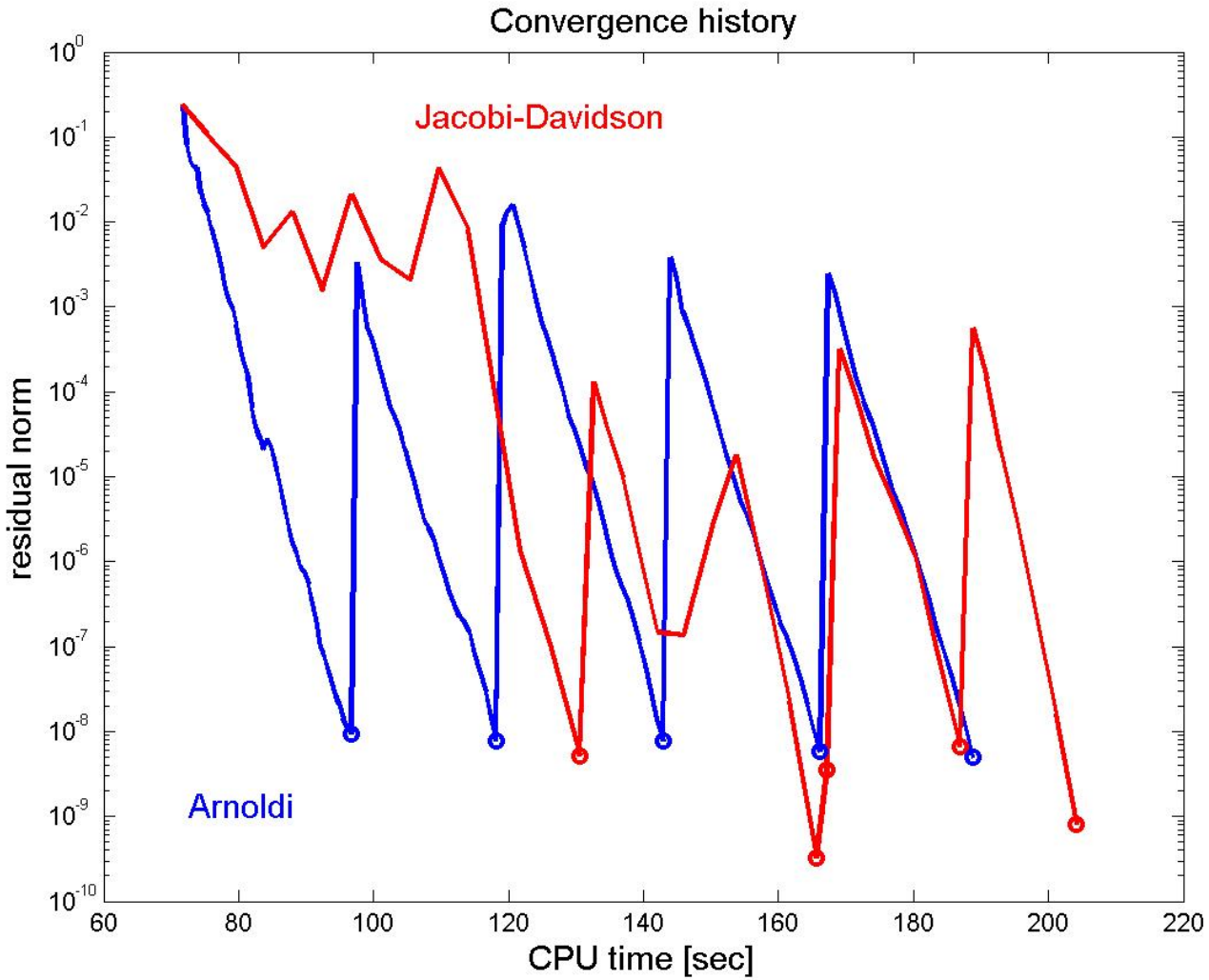
FEM: Cubic Lagrangian elements on tetrahedal grid

dimension: 96'640 $((\mathrm{Dof}_{\mathrm{QD}}, \mathrm{Dof}_{\mathrm{mat}}, \mathrm{Dof}_{\mathrm{interf}}) = (43'615, 43'897, 9'128)$

dim	λ_1	λ_2	λ_3	λ_4	λ_5	CPU time
$96'640$	0.39779	0.57411	0.57411	0.68547	0.69714	
Arnoldi	44 it.	29 it.	29 it.	24 it.	21 it.	188.8 s
JD	15 it.	9 it.	1 it.	7 it.	7 it.	204.4 s
HLWW	45 it.	49 it.	5 it.	24 it.	21 it.	226.7 s

Convergence history



Preconditioning

incomplete LU with cut-off threshold τ

τ	JD	Arnoldi	HLWW	precond.
0.1	261.4	1084.1	1212.4	3.4
0.01	132.7	117.1	155.7	71.7
0.001	118.9	61.2	96.0	246.6
0.0001	155.6	46.6	71.1	665.6

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Eigenfunctions

Example 2: Damped vibrations of a solid

Using a viscoelastic constitutive relation to describe the material behaviour in the equations of motion yields a rational eigenvalue problem in the case of free vibrations.

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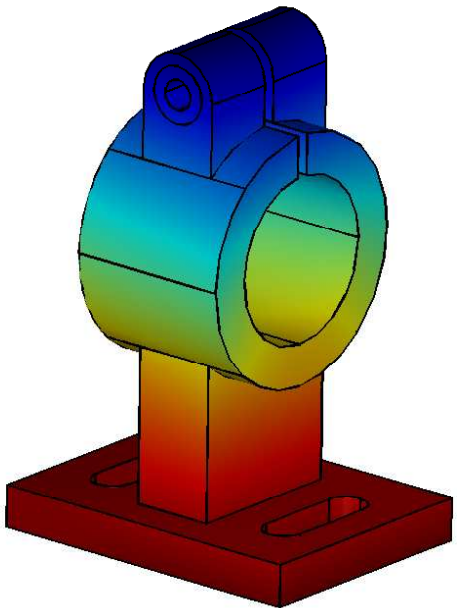
Discretizing by finite elements yields

$$T(\omega)x := \left(\omega^2 M + K - \sum_{j=1}^{k} \frac{1}{1+b_j\omega}\Delta K_j\right)x = 0$$

where M is the consistent mass matrix, K is the stiffness matrix with the instantaneous elastic material parameters used in Hooke's law, and ΔK_j collects the contributions of damping from elements with relaxation parameter b_j.

Nonproportional damping



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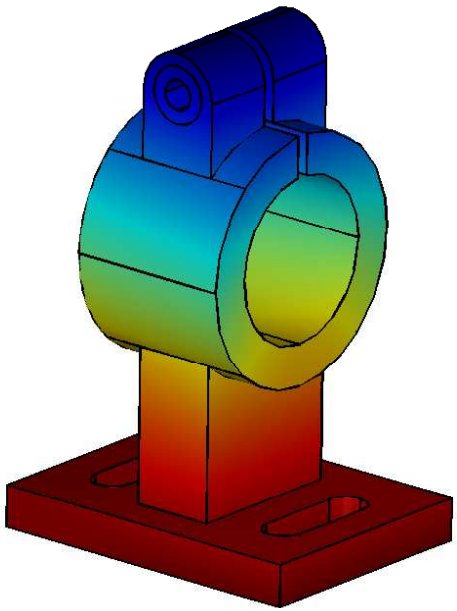

FE model of feeder clamp

linear Lagrangean elements on tetrahedal grid

dimension	193′617
nnz(K)	7′670′533
nnz(M)	2′557′851

Determine 30 eigenvalues with maximal negative imaginary part.

Nonproportional damping ct.

Iterative projection methods

τ	JD	Arnoldi	HLWW	precond.
0.01	3276.6	no conv.	no conv.	49.0
0.001	2077.5	5240.4	5559.9	141.4
0.0001	2067.5	945.4	1452.7	356.3

Conclusions

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- The Arnoldi method seems to be faster than the Jacobi–Davidson method, if accurat preconditioners are available.
- The Jacobi–Davidson method seems to be more robust concerning only coarse preconditioners