November 5, 2010

Hierarchical Matrices:

Concept, Applications and Eigenvalues

Thomas Mach

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

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Householder Notation

Scalar

$$\lambda \in \mathbb{R}$$

Householder Notation

Vector

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n$$

Householder Notation

Matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Dense Matrix Format

Store n vectors (Fortran):

$$\begin{bmatrix} \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ \vdots \\ a_{n1} \end{bmatrix} & \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ \vdots \\ a_{n2} \end{bmatrix} & \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \\ \vdots \\ a_{n3} \end{bmatrix} & \dots & \begin{bmatrix} a_{1n} \\ a_{2n} \\ a_{3n} \\ \vdots \\ a_{nn} \end{bmatrix} \end{bmatrix}$$

- n^2 entries in the storage
- Ax costs $\mathcal{O}(n^2)$ flops
- AB costs $\mathcal{O}(n^\delta)$ flops, $\delta \geq 2.376$ usually $\delta = 3$
- A^{-1} costs $\mathcal{O}(n^3)$ flops

Dense Matrix Format

Store n ...

Landau Symbol

There is a constant c, so that Ax costs not more than cn^2 flops

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & & a_{1n} \\ a_{21} & a_{22} & a_{23} & & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & a_{n3} & & a_{nn} \end{bmatrix}$$

Flops

$1 \text{ flop} = (\alpha\beta + \gamma \rightarrow \gamma)$

- n^2 entries in the storage
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- A^{-1} costs $\mathcal{O}(n^3)$ flops

expensive!

Sparse Matrix Format

$$\begin{bmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{bmatrix}$$

Sparse Matrix Format

$$\begin{bmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{bmatrix}$$

non-zero entries per row/column $= c \leq 5$

Sparse Matrix Format

$$\begin{bmatrix} 4 & -1 & -1 & -1 \\ -1 & -1 & -1 & 4 \\ -1 & 4 & -1 & -1 \\ -1 & -1 & 4 & -1 \\ 4 & -1 & -1 & -1 \\ -1 & -1 & -1 & 4 \\ -1 & -1 & 4 & \\ -1 & 4 & -1 & \\ 4 & -1 & -1 & \end{bmatrix}$$

non-zero entries per row/column $= c \leq 5$

Sparse Matrix Format (Matlab)

Store vector of tripel:

$$\begin{bmatrix} (1,1,\ \ 4) \\ (2,1,-1) \\ (4,1,-1) \\ (1,2,-1) \\ \vdots \end{bmatrix}$$

- $\mathcal{O}(n)$ entries in the storage (if #non-zeros/column $< c \ll n$)
- Ax costs $\mathcal{O}(n)$ flops
- AB may be much denser $\Rightarrow$ better use $A(Bx)$
- A^{-1} not possible, only solve $Ax = b$

Is there something in between?

Yes, e.g.

- Low rank matrices and Tucker tensor format
- Toeplitz/Hankel matrices
- Semiseparable matrices [Gantmacher, Krein 1937]
- Cauchy matrices
- Fast Multipole Method (FMM) [Greengard, Rokhlin '87]
- Mosaic-skeleton matrices [Tyrtyshnikov '96]
- ...

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- Mosaic-skeleton matrices [Tyrtyshnikov '96]
- Hierarchical ($\mathcal{H}$-) Matrices [Hackbusch '98]

Integral Equation

Fredholm equation of first kind:

$$\int_\Omega g(x,y)u(y)dy = f(x)$$

Integral Equation

unknown

Fredholm equation of first kind:

$$\int_\Omega g(x,y)u(y)dy = f(x)$$

Integral Equation

Fredholm equation of first kind:

$$\int_\Omega g(x,y)u(y)dy = f(x)$$

- electrostatic problem:
  - $g(x,y) = \frac{1}{4\pi\epsilon\|x-y\|}$
  - $u(y)$ charge density
  - $f(x)$ electrostatic potential
- inverse of elliptic differential operators
- population dynamics [Koch, Hackbusch, Sundmacher]

$\mathcal{H}$-Matrices [Hackbusch '98]

$$\int_\Omega g(x,y)u(y)dy = f(x)$$

Ritz-Galerkin method:

$$u(y) = \sum_i u_i\psi_i(y)$$

$$\Rightarrow \sum_i \underbrace{\int_\Omega \int_\Omega g(x,y)\psi_i(y)dy\psi_j(x)dx}_{:=M_{ji}} u_i = \underbrace{\int_\Omega f(x)\psi_j(x)dx}_{=f_j}$$

$\mathcal{H}$-Matrices [Hackbusch '98]

discretization error $\epsilon \sim \frac{1}{n^\kappa}$, $0 < \kappa < 1$

$\int_\Omega g(x,y)u(y)dy = f(x)$

Ritz-Galerkin method:

$u(y) = \sum_i u_i \psi_i(y)$

$$\Rightarrow \sum_i \underbrace{\int_\Omega \int_\Omega g(x,y)\psi_i(y)dy\psi_j(x)dx}_{:=M_{ji}} u_i = \underbrace{\int_\Omega f(x)\psi_j(x)dx}_{=f_j}$$

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$$Mu = f$$

$\mathcal{H}$-Matrices [Hackbusch '98]

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Ritz-Galerkin method:

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$x \in \Omega_s, y \in \Omega_t$: $g(x,y) \approx \sum_{p=1}^k g_p^{x,s}(x) g_p^{y,t}(y)$

$\mathcal{H}$-Matrices [Hackbusch '98]

$$\int_\Omega g(x,y)u(y)dy = f(x)$$

Ritz-Galerkin method:

$$u(y) = \sum_i u_i \psi_i(y)$$

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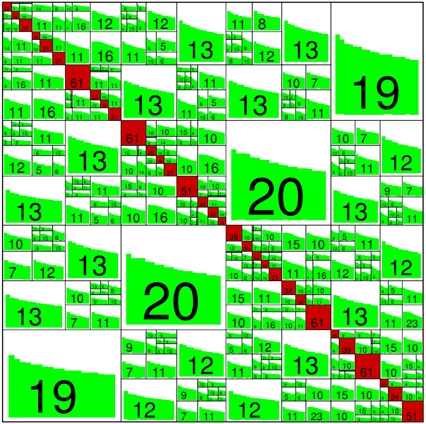
$x \in \Omega_s, y \in \Omega_t$: $g(x,y) \approx \sum_{p=1}^k g_p^{x,s}(x) g_p^{y,t}(y)$

$$M_{ji} = \int_\Omega \int_\Omega g(x,y)\psi_j(x)\psi_i(y)dydx$$

$$\approx \sum_{p=1}^k \int_\Omega g_p^x(x)\psi_j(x)dx \int_\Omega g_p^y(y)\psi_i(y)dy = A_{j\cdot} B_{i\cdot}^T$$

$\mathcal{H}$-Matrices [Hackbusch '98]



$$x \in \Omega_s, y \in \Omega_t : \quad g(x,y) \approx \sum_{p=1}^{k} g_p^{x,s}(x) g_p^{y,t}(y)$$

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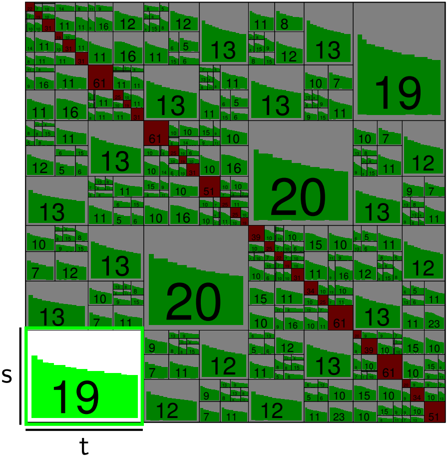
$$\approx \sum_{p=1}^{k} \int_\Omega g_p^x(x)\psi_j(x)dx \int_\Omega g_p^y(y)\psi_i(y)dy = A_{j.} B_{i.}^T$$

$\mathcal{H}$-Matrices [Hackbusch '98]

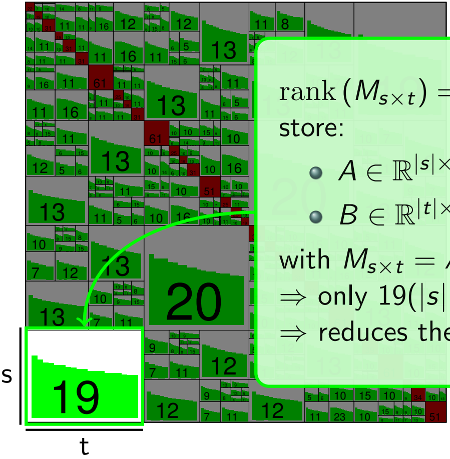


$$x \in \Omega_s, y \in \Omega_t : \quad g(x,y) \approx \sum_{p=1}^{k} g_p^{x,s}(x) g_p^{y,t}(y)$$

$$M_{ji} = \int_\Omega \int_\Omega g(x,y)\psi_j(x)\psi_i(y)\,dy\,dx$$

$$\approx \sum_{p=1}^{k} \int_\Omega g_p^x(x)\psi_j(x)\,dx \int_\Omega g_p^y(y)\psi_i(y)\,dy = A_{j.} B_{i.}^T$$

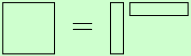
$\mathcal{H}$-Matrices [Hackbusch '98]



$\operatorname{rank}(M_{s\times t}) = 19$

store:

- $A \in \mathbb{R}^{|s|\times 19}$,
- $B \in \mathbb{R}^{|t|\times 19}$



with $M_{s\times t} = AB^T$

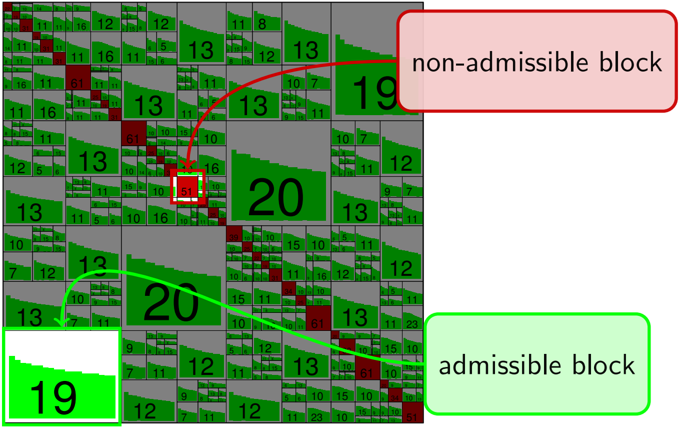
$\Rightarrow$ only $19(|s| + |t|)$ instead of $|s|\,|t|$ storage

$\Rightarrow$ reduces the required storage to 15%

$\mathcal{H}$-Matrices [Hackbusch '98]

if $x \approx y$ then $\frac{1}{\|x-y\|}$ is large
small matrices on the diagonal have no low rank approximation
$\Rightarrow$ use dense matrix format

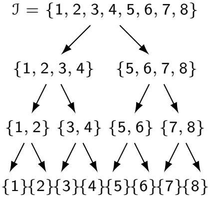
$\mathcal{H}$-Matrices [Hackbusch '98]



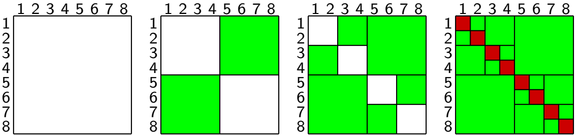
$\mathcal{H}$-Matrices [Hackbusch '98]

rank-k-matrix: $M_{s \times t} = AB^T,\ A \in \mathbb{R}^{n \times k}, B \in \mathbb{R}^{m \times k}\ (k \ll n, m)$

hierarchical tree $T_{\mathcal{I}}$



block $\mathcal{H}$-tree $T_{\mathcal{I} \times \mathcal{I}}$

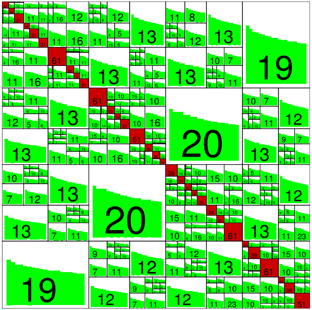


dense matrices, **rank-k-matrices**

$\mathcal{H}$-Matrices [Hackbusch '98]

Hierarchical matrices

$$\mathcal{H}(T_{\mathcal{I}\times\mathcal{I}}, k) = \left\{ M \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}} \middle| \operatorname{rank}(M_{s\times t}) \leq k \ \forall s \times t \text{ admissible} \right\}$$



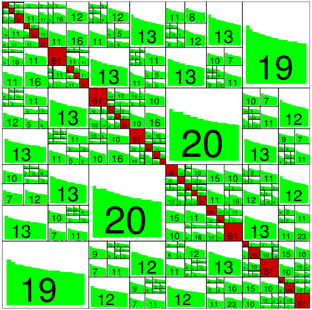
- adaptive rank $k(\varepsilon)$
- storage $N_{St,\mathcal{H}}(T, k) = \mathcal{O}(n \log n \ k(\varepsilon))$
- complexity of approximate arithmetic

$M_{\mathcal{H}} v$	$\mathcal{O}(n \log n \ k(\varepsilon))$
$+_{\mathcal{H}}, -_{\mathcal{H}}$	$\mathcal{O}(n \log n \ k(\varepsilon)^2)$
$*_{\mathcal{H}}, \mathcal{H}LU(\cdot), (\cdot)^{-1}_{\mathcal{H}}$	$\mathcal{O}(n (\log n)^2 \ k(\varepsilon)^2)$

$\mathcal{H}$-Matrices [Hackbusch '98]

Hierarchical matrices

$$\mathcal{H}(T_{\mathcal{I}\times\mathcal{I}}, k) = \left\{ M \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}} \middle| \operatorname{rank}(M_{s\times t}) \leq k \ \forall s \times t \text{ admissible} \right\}$$



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- storage $N_{St,\mathcal{H}}(T, k) = \mathcal{O}(n \log n \; k(\varepsilon))$
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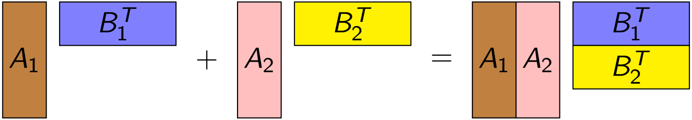


Special Case: $\mathcal{H}_\ell$-Matrices

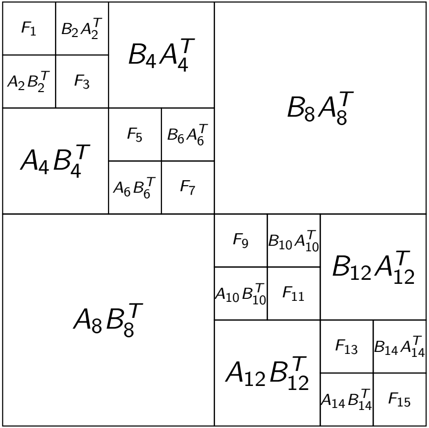


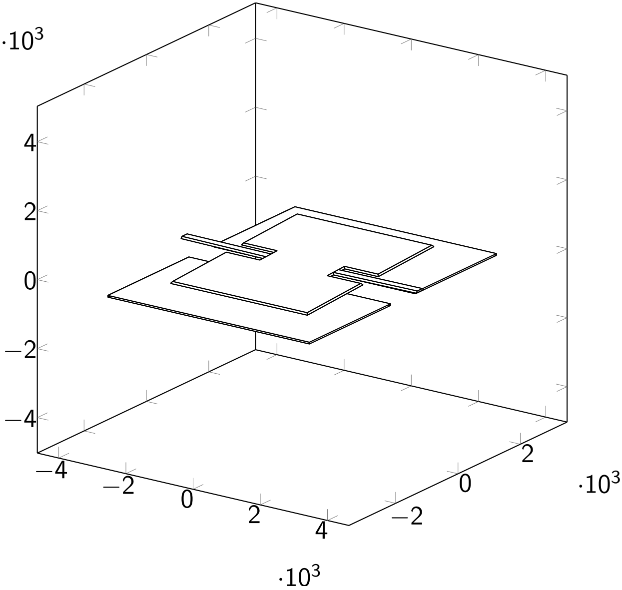
Figure: Structure of an $\mathcal{H}_3(k)$-matrix

Applications

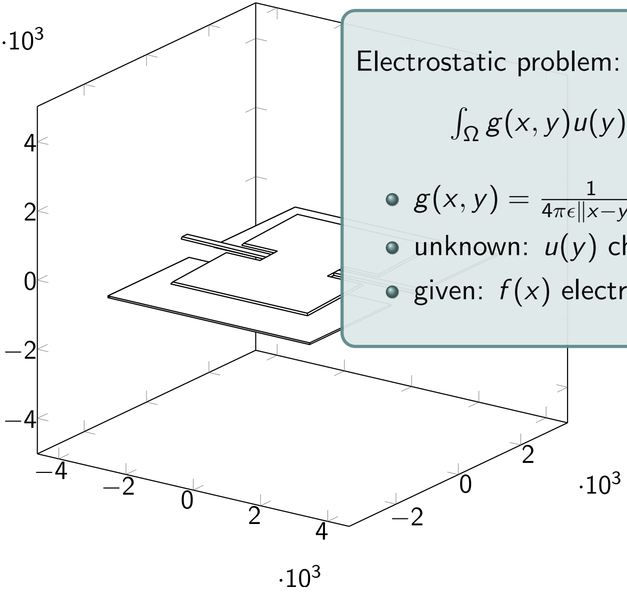
Applications

- Finite-Element-Method (FEM)
  - Inverse of FEM matrices
- Integral equations
- Solving matrix equations for model order reduction
  - $AX + XA^T + BB^T = 0$, $A \in \mathcal{H}, B \in \mathbb{R}^{n \times k}$
  - Sign function iteration
  - [Baur '07, Grasedyck '03, et al.]
- Boundary-Element-Method (BEM)

BEM for Electrostatic Computations



BEM for Electrostatic Computations

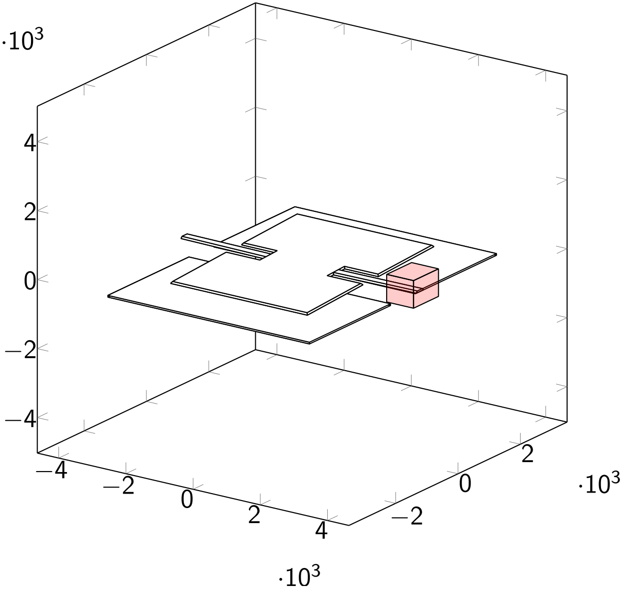


Electrostatic problem:

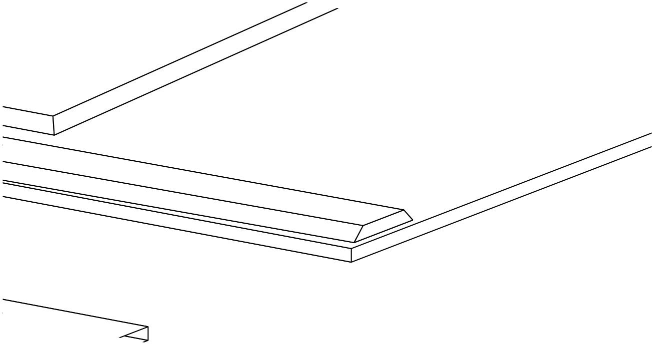
$$\int_\Omega g(x,y)u(y)dy = f(x)$$

- $g(x,y) = \frac{1}{4\pi\epsilon\|x-y\|}$
- unknown: $u(y)$ charge density
- given: $f(x)$ electrostatic potential

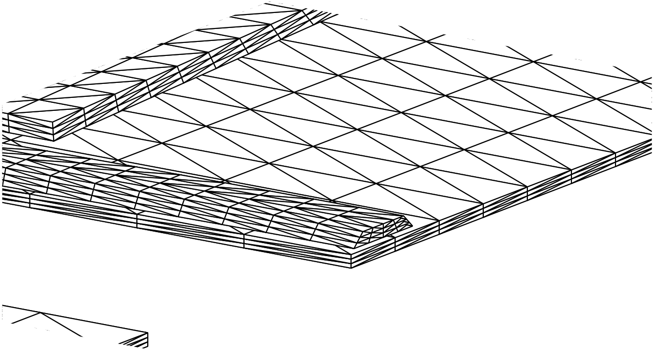
BEM for Electrostatic Computations



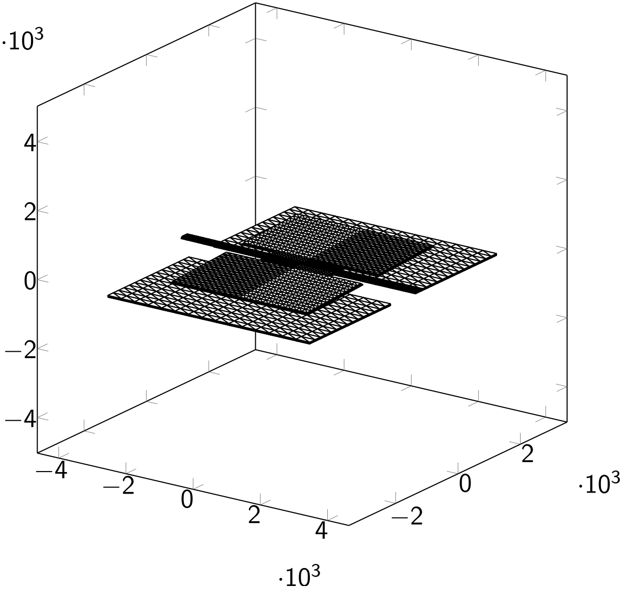
BEM for Electrostatic Computations



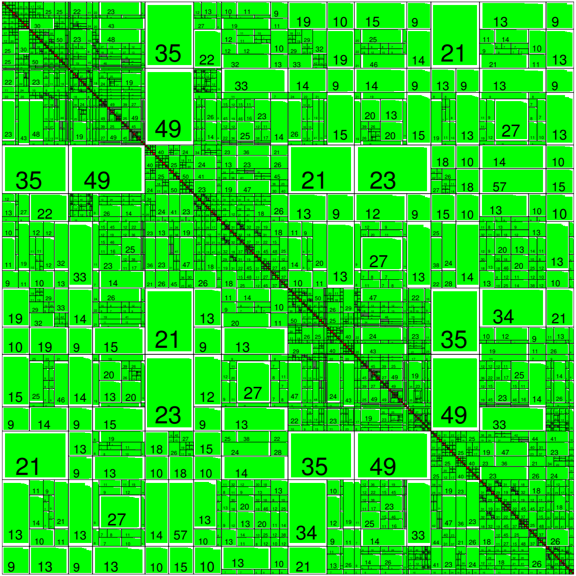
BEM for Electrostatic Computations



BEM for Electrostatic Computations

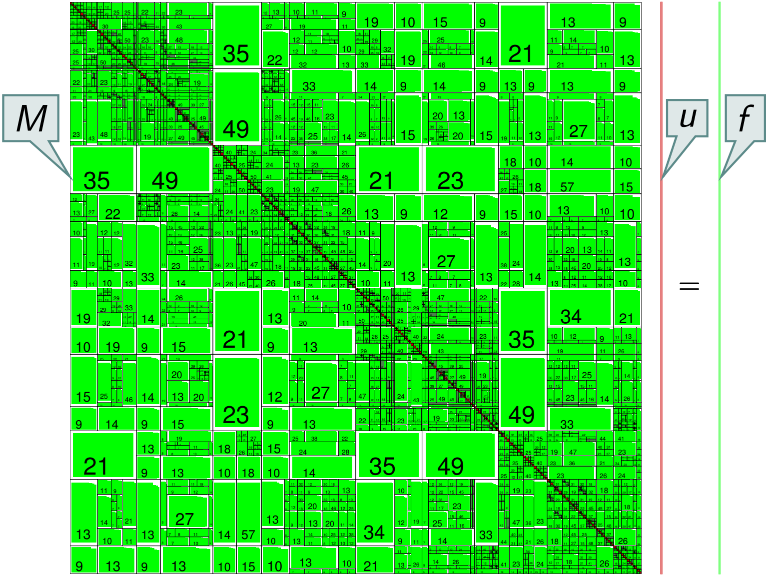


BEM for Electrostatic Computations

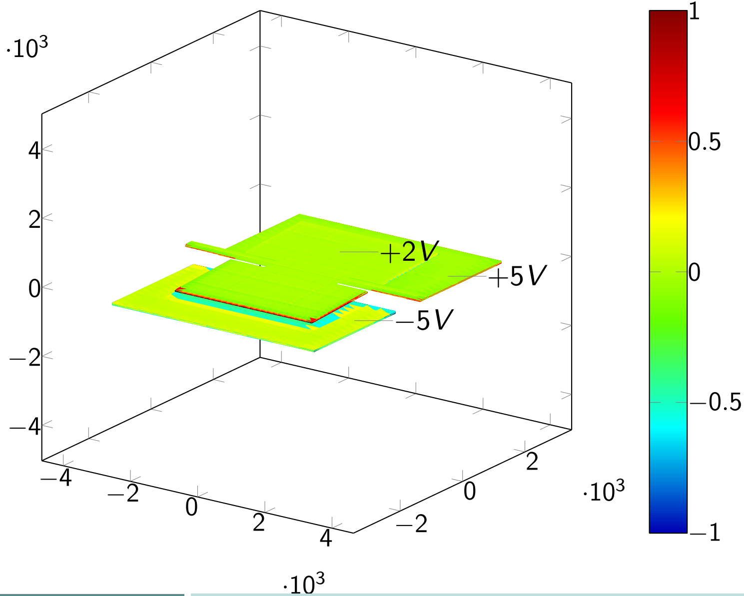


$\in \mathbb{R}^{7416 \times 7416}$

BEM for Electrostatic Computations



BEM for Electrostatic Computations



Eigenvalues

Definition

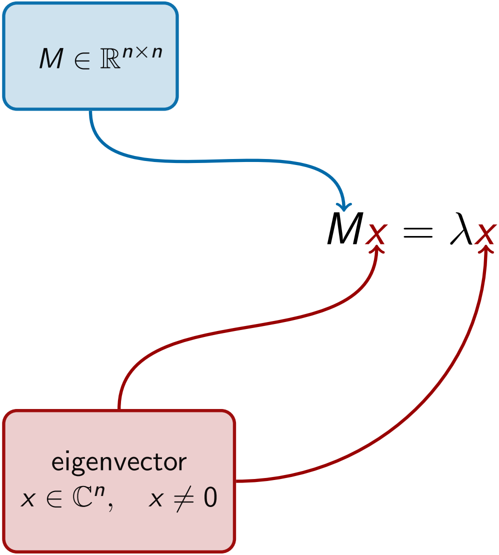
$$Mx = \lambda x$$

Definition

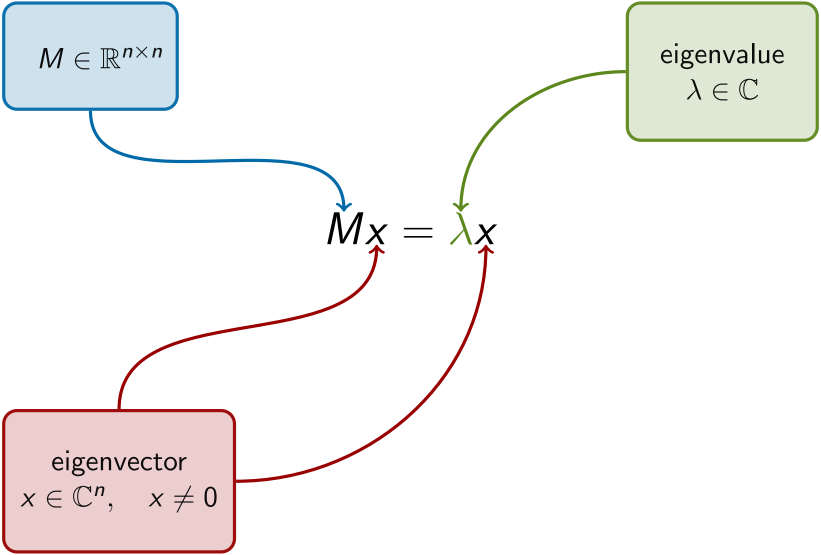
$M \in \mathbb{R}^{n \times n}$

$$Mx = \lambda x$$

Definition


$M \in \mathbb{R}^{n \times n}$
$Mx = \lambda x$
eigenvector
$x \in \mathbb{C}^n, \quad x \neq 0$

Definition


$M \in \mathbb{R}^{n \times n}$
eigenvalue
$\lambda \in \mathbb{C}$
$Mx = \lambda x$
eigenvector
$x \in \mathbb{C}^n, \quad x \neq 0$

Definition

$M = M^T \in \mathbb{R}^{n \times n}$

eigenvalue

$\lambda \in \mathbb{R}$

$$Mx = \lambda x$$

eigenvector

$x \in \mathbb{R}^n, \quad x \neq 0$

Application

Eigenvalue problems occur in many different applications:

- vibration analysis,
- molecular and quantum dynamics (e.g. Schrödinger or Kohn-Sham equations),
- finite state of a Markov chain,
- numerical mathematics (e.g. MOR, e^M, convergence theory),
- ...

Definition

$M = M^T \in \mathcal{H}(T, k)$

eigenvalue
$\lambda \in \mathbb{R}$

$$Mx = \lambda x$$

eigenvector
$x \in \mathbb{R}^n, \quad x \neq 0$

Preconditioned Inverse Iteration

[Knyazev, Neymeyr, et al.]

Definition

The function

$$\mu(x) = \mu(x, M) = \frac{x^T M x}{x^T x}$$

is called the *Rayleigh quotient*.

Preconditioned Inverse Iteration

[Knyazev, Neymeyr, et al.]

Definition

The function

$$\mu(x) = \mu(x, M) = \frac{x^T M x}{x^T x}$$

is called the *Rayleigh quotient*.

Minimize the Rayleigh quotient by a gradient method:

$$x_{i+1} := x_i - \alpha \nabla \mu(x_i), \quad \nabla \mu(x) = \frac{2}{x^T x}(Mx - x\mu(x)),$$

Preconditioned Inverse Iteration

[Knyazev, Neymeyr, et al.]

Residual $r(x) = Mx - x\mu(x)$.

Minimize the Rayleigh quotient by a gradient method:

$$x_{i+1} := x_i - \alpha \nabla \mu(x_i), \quad \nabla \mu(x) = \frac{2}{x^T x}(Mx - x\mu(x)),$$

Preconditioned Inverse Iteration

[Knyazev, Neymeyr, et al.]

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is called the *Rayleigh quotient*.

Minimize the Rayleigh quotient by a gradient method:

$$x_{i+1} := x_i - \alpha \nabla \mu(x_i), \quad \nabla \mu(x) = \frac{2}{x^T x}(Mx - x\mu(x)),$$

$+$ preconditioning $\Rightarrow$ update equation:

$$x_{i+1} := x_i - T^{-1}\,(Mx_i - x_i \mu(x_i)).$$

Preconditioned Inverse Iteration

[Knyazev, Neymeyr '09]

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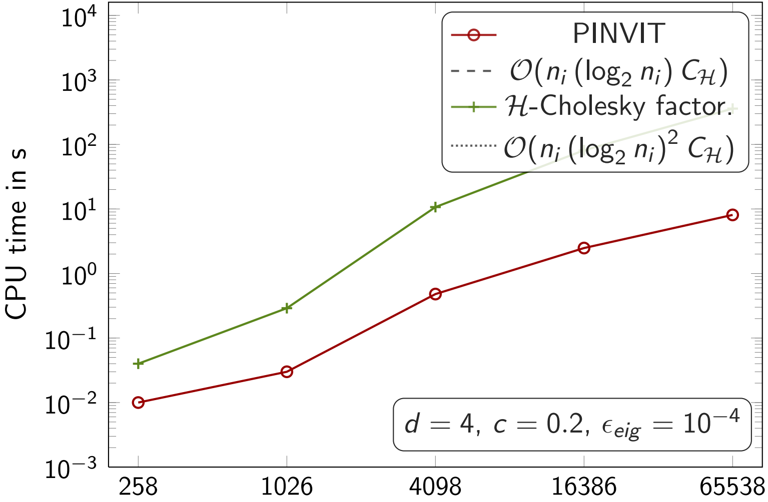
BEM, smallest eigenvalues

dense matrix, but approximable by an $\mathcal{H}$-matrix



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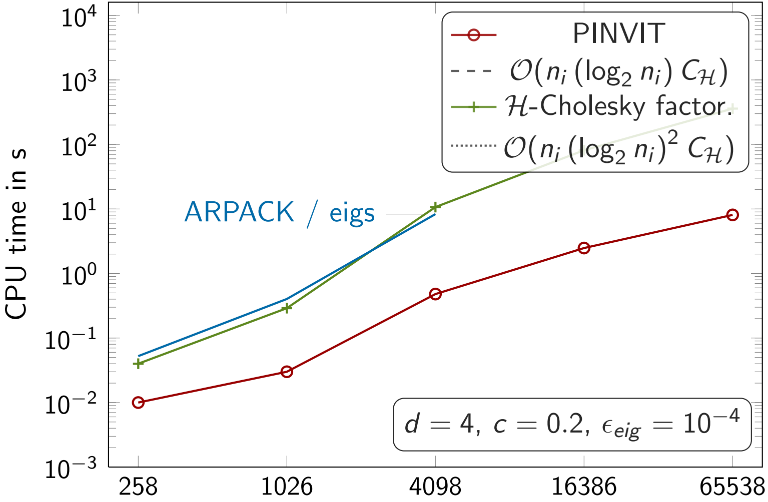

Concluding Remarks

- $\mathcal{H}$-arithmetic is cheap and applicable too many problems.
- Computing eigenvalues of $\mathcal{H}$-matrices in linear-polylogarithmic complexity is possible.
- See poster: *"Slicing the Spectrum of Symmetric $\mathcal{H}_\ell$-Matrices"*.

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Thank you for your attention.

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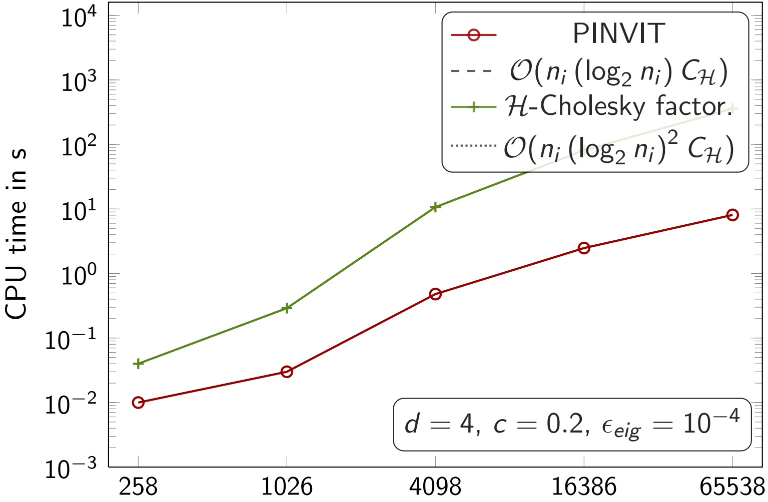

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