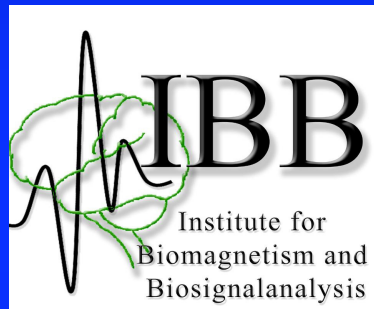


Linear complexity of finite element method based forward modeling in bioelectromagnetism



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Lecture on Nov.26, 2024

Structure of the lecture

- Linear complexity for FEM forward modeling: Transfer matrices
- Fast FE solver methods

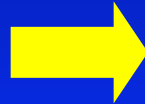
Link to own work for transfer matrices:

The screenshot shows a web browser window with the following elements:

- Address Bar:** <https://campus.uni-muenster.de/fileadmin/einrichtung/biomag/Mitarbeiter/Wolters-Publications.pdf>
- Search Bar:** carsten wolters
- Navigation Bar:** Includes links like 'Erste Schritte', 'Aktuelle Nachric...', 'Apple', 'Amazon', 'Lehre', 'Haus', 'News', 'Wörterbücher', 'Apple-Mac', 'University of Utah', and 'Muenster'.
- Page Information:** Seite: 9 von 30, Automatischer Zoom.
- Content:**
 - [Webversion](#), [pdf](#)
 - 6. Wolters, C.H., Grasedyck, L. and Hackbusch, W., Efficient Computation of Lead Field Bases and Influence Matrix for the FEM-based EEG and MEG
 - Inverse Problem. *Inverse Problems*, 20(4), pp. 1099–1116, (2004).
 - [DOI](#), [Eprint](#), [pdf](#)

EEG transfer matrix

$$\begin{aligned} \nabla \cdot (\sigma \nabla \Phi) &= J_p = \nabla \cdot \vec{j}_p && \text{in } \Omega \\ (\sigma \nabla \Phi) \cdot \vec{n} &= 0 && \text{on } \Gamma = \partial\Omega \\ \Phi|_{\text{Ref}} &= 0 \end{aligned}$$



$$(*) \mathbf{K} \underline{\Phi} = \underline{J}$$

$$\mathbf{K} \in R^{N \times N}$$

$$\begin{aligned} \underline{\Phi}^{EEG} &= \mathbf{R} \underline{\Phi} \\ (*) \\ &= \mathbf{R} (\mathbf{K}^{-1} \underline{J}) \\ &= (\mathbf{R} \mathbf{K}^{-1}) \underline{J} \end{aligned}$$

$$\mathbf{R} = \begin{pmatrix} 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ \vdots & & & & & & \\ 0 & \vdots & 1 & 0 & \dots & \dots & \dots & 0 \\ \vdots & & & & & & & \\ 1 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \end{pmatrix} \in R^{(s^{EEG}-1) \times N}$$

$$T^{EEG} := \mathbf{R} \mathbf{K}^{-1} \in R^{(s^{EEG}-1) \times N}$$

$$s^{EEG} - 1$$



$$T^{EEG} : \underline{J} \rightarrow \underline{\Phi}^{EEG}$$

$$N$$

MEG transfer matrix

$$\underline{\Psi}_i = \underline{\Psi}_i^s + \underline{\Psi}_i^{\text{sek}} = \frac{\mu}{4\pi} \int_{\Omega} \left\langle \vec{j}^s(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y} - \frac{\mu}{4\pi} \int_{\Omega} \left\langle \sigma(\vec{y}) \nabla \Phi(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y}$$

MEG transfer matrix

$$\underline{\Psi}_i = \underline{\Psi}_i^s + \underline{\Psi}_i^{\text{sek}} = \frac{\mu}{4\pi} \int_{\Omega} \left\langle \vec{j}^s(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y} - \frac{\mu}{4\pi} \int_{\Omega} \left\langle \sigma(\vec{y}) \nabla \Phi(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y}$$



$$\nabla \Phi(\vec{y}) \approx \nabla \left(\sum_{j=1}^N \psi_j(\vec{y}) \underline{\Phi}_j \right) = \sum_{j=1}^N \nabla \psi_j(\vec{y}) \underline{\Phi}_j$$

MEG transfer matrix

$$\underline{\Psi}_i = \underline{\Psi}_i^p + \underline{\Psi}_i^{\text{sek}} = \frac{\mu}{4\pi} \int_{\Omega} \left\langle \vec{j}^s(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y} - \frac{\mu}{4\pi} \int_{\Omega} \left\langle \sigma(\vec{y}) \nabla \Phi(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y}$$

$$\mathbf{S}_{ij} := -\frac{\mu}{4\pi} \int_{\Omega} \left\langle \sigma(\vec{y}) \nabla \psi_j(\vec{y}), \oint_{\partial F_i} \frac{1}{|\vec{x} - \vec{y}|} d\vec{x} \right\rangle d\vec{y} \in R^{s^{\text{MEG}} \times N}$$

$$\underline{\Psi}^{\text{sek}} = \mathbf{S} \underline{\Phi} \stackrel{(*)}{=} \mathbf{S} (\mathbf{K}^{-1} \underline{J}) = (\mathbf{S} \mathbf{K}^{-1}) \underline{J}$$

$$\mathbf{T}^{\text{MEG}} := \mathbf{S} \mathbf{K}^{-1} \in R^{s^{\text{MEG}} \times N}$$

$$\mathbf{S}^{\text{MEG}}$$

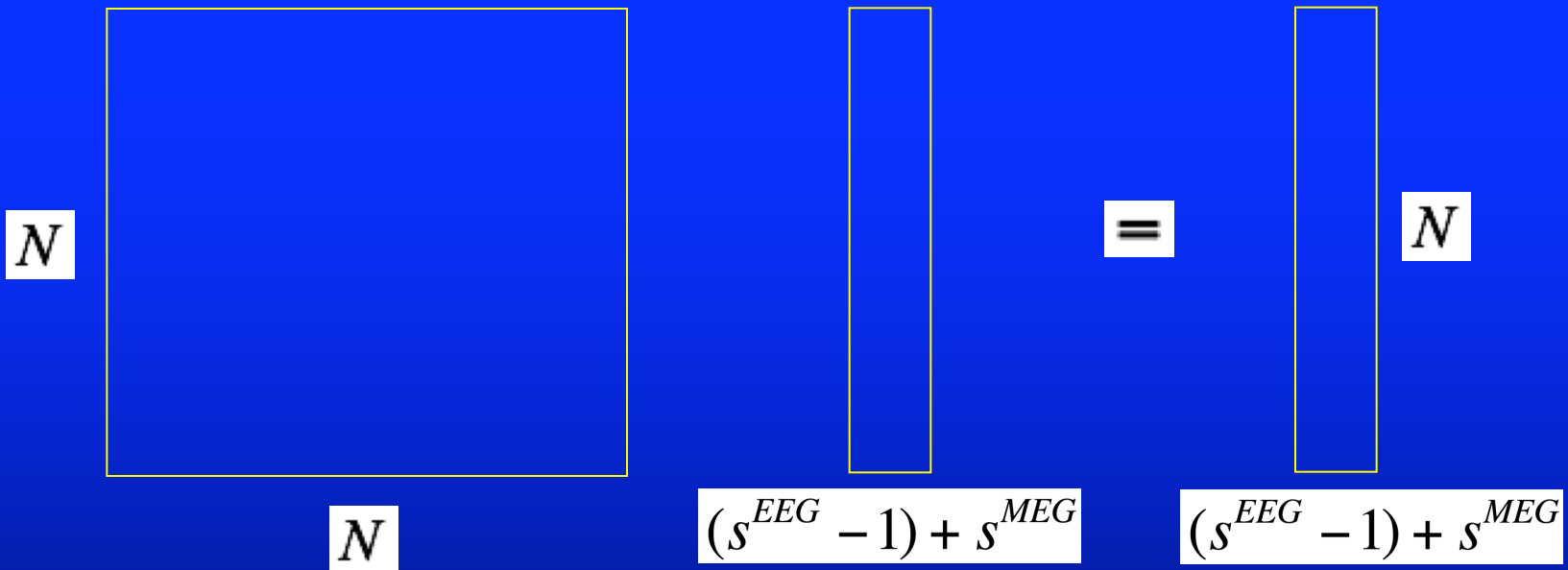
$$\mathbf{T}^{\text{MEG}} : \underline{J} \rightarrow \underline{\Psi}^{\text{sek}}$$

N

Computing the transfer matrices

$$\begin{pmatrix} T^{EEG} \\ T^{MEG} \end{pmatrix} := \begin{pmatrix} \mathbf{R} \\ \mathbf{S} \end{pmatrix} \mathbf{K}^{-1} \Leftrightarrow \begin{pmatrix} T^{EEG} \\ T^{MEG} \end{pmatrix} \mathbf{K} = \begin{pmatrix} \mathbf{R} \\ \mathbf{S} \end{pmatrix}$$

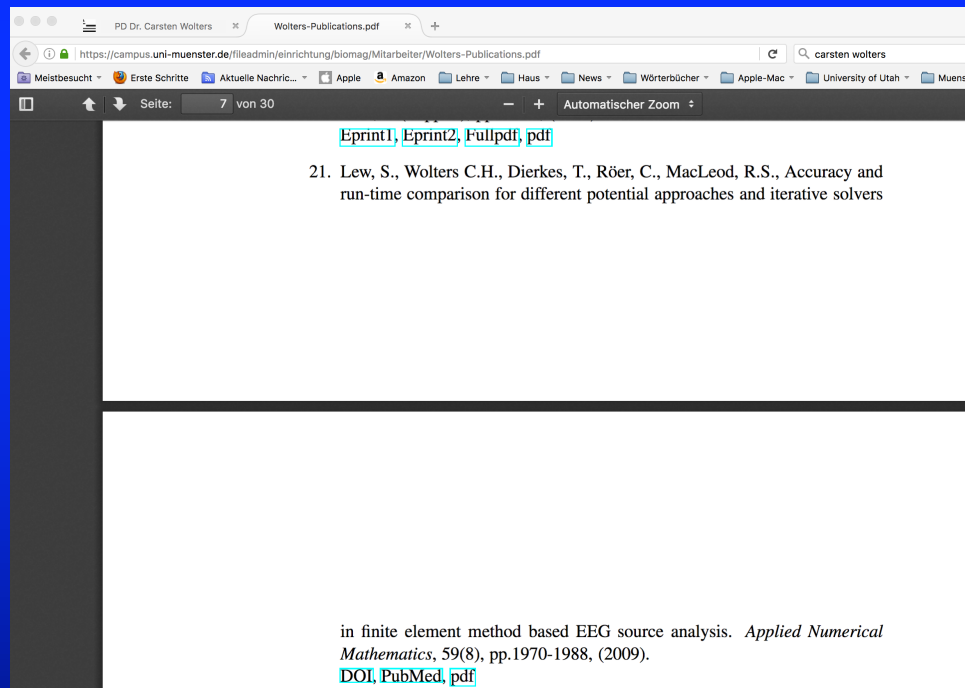
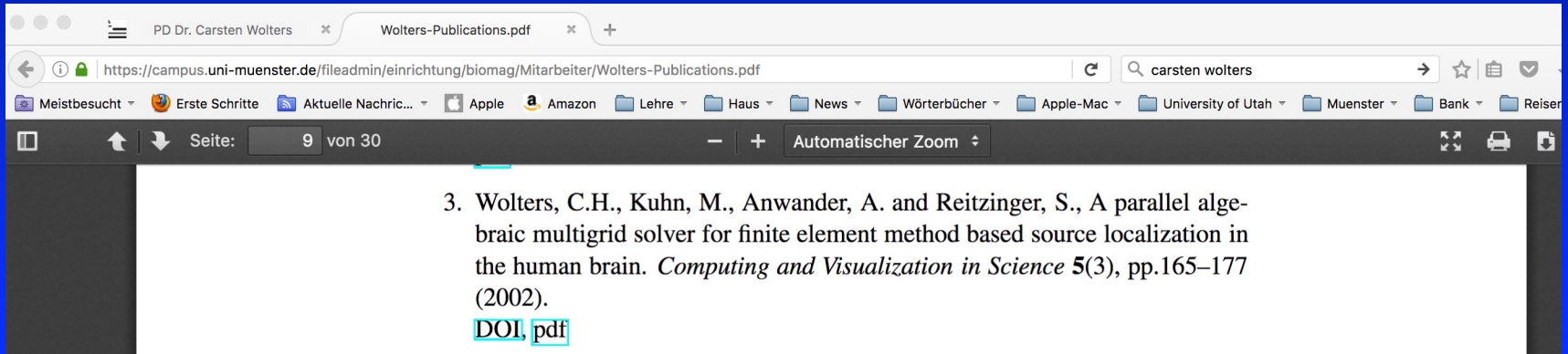
$$\Leftrightarrow \mathbf{K} \begin{pmatrix} (T^{EEG})^{tr} & (T^{MEG})^{tr} \end{pmatrix} = \begin{pmatrix} \mathbf{R}^{tr} & \mathbf{S}^{tr} \end{pmatrix}$$



Outline

- **Linear complexity for FEM forward modeling: Transfer matrices**
- **Fast FE solver methods**

Link to this work:



FEM solver aspects

$$\mathbf{K}_h \underline{u}_h = \underline{j}_h$$

$$\begin{bmatrix} \times & \times & & \times & \times & & \\ \times & \times & \times & & & & \times \\ & \times & \times & & \times & & \\ \times & & & \times & & \times & \times \\ \times & & \times & & \times & & \\ & \times & & & \times & \times & \times \\ & & \times & & & \times & \\ & & & \times & & \times & \\ & & & \times & \times & \times & \end{bmatrix}$$

$$\underline{u}_h = K_h^{-1} \underline{j}_h ??$$

Preconditioned Conjugate Gradient Method

Algorithm 1 PCG : $(K_h, \underline{u}_h, \underline{j}_h, C_h, \text{ACCURACY}) \rightarrow (\underline{u}_h)$

$$\underline{r}_h = \underline{r}_h^0 = \underline{j}_h - K_h \underline{u}_h$$

$$\text{SOLVE } C_h \underline{w}_h = \underline{r}_h$$

$$\underline{s}_h = \underline{w}_h$$

$$\gamma^0 = \gamma = \gamma_{\text{OLD}} = \langle \underline{w}_h, \underline{r}_h \rangle$$

$$\text{while } \left(\gamma / \gamma^0 = \left(\frac{\|\underline{r}_h\|_{C_h^{-1}}}{\|\underline{r}_h^0\|_{C_h^{-1}}} \right)^2 = \left(\frac{\|K_h \underline{e}_h\|_{C_h^{-1}}}{\|K_h \underline{e}_h^0\|_{C_h^{-1}}} \right)^2 = \left(\frac{\|\underline{e}_h^i\|_{K_h C_h^{-1} K_h}}{\|\underline{e}_h^0\|_{K_h C_h^{-1} K_h}} \right)^2 > \text{ACCURACY}^2 \right) \text{ do}$$

$$\underline{v}_h = K_h \underline{s}_h$$

$$\alpha = \gamma / \langle \underline{s}_h, \underline{v}_h \rangle$$

$$\underline{u}_h = \underline{u}_h + \alpha \underline{s}_h$$

$$\underline{r}_h = \underline{r}_h - \alpha \underline{v}_h$$

$$\text{SOLVE } C_h \underline{w}_h = \underline{r}_h$$

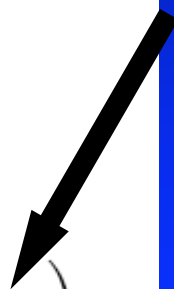
$$\gamma = \langle \underline{w}_h, \underline{r}_h \rangle$$

$$\beta = \gamma / \gamma_{\text{OLD}}, \quad \gamma_{\text{OLD}} = \gamma$$

$$\underline{s}_h = \underline{w}_h + \beta \underline{s}_h$$

end while

**PCG
accuracy**



Iterative solver for FE-equation system

- **FE discretization, meshsize:** h

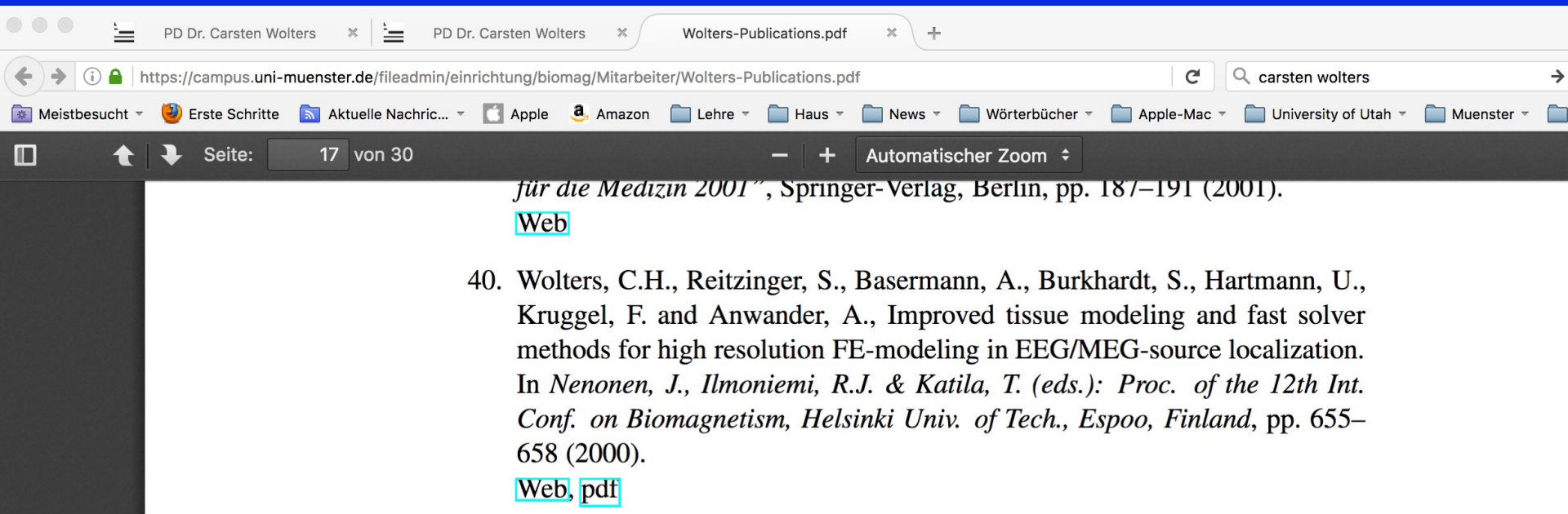
$$\mathbf{K}_h \underline{u}_h = \underline{j}_h$$

with condition number

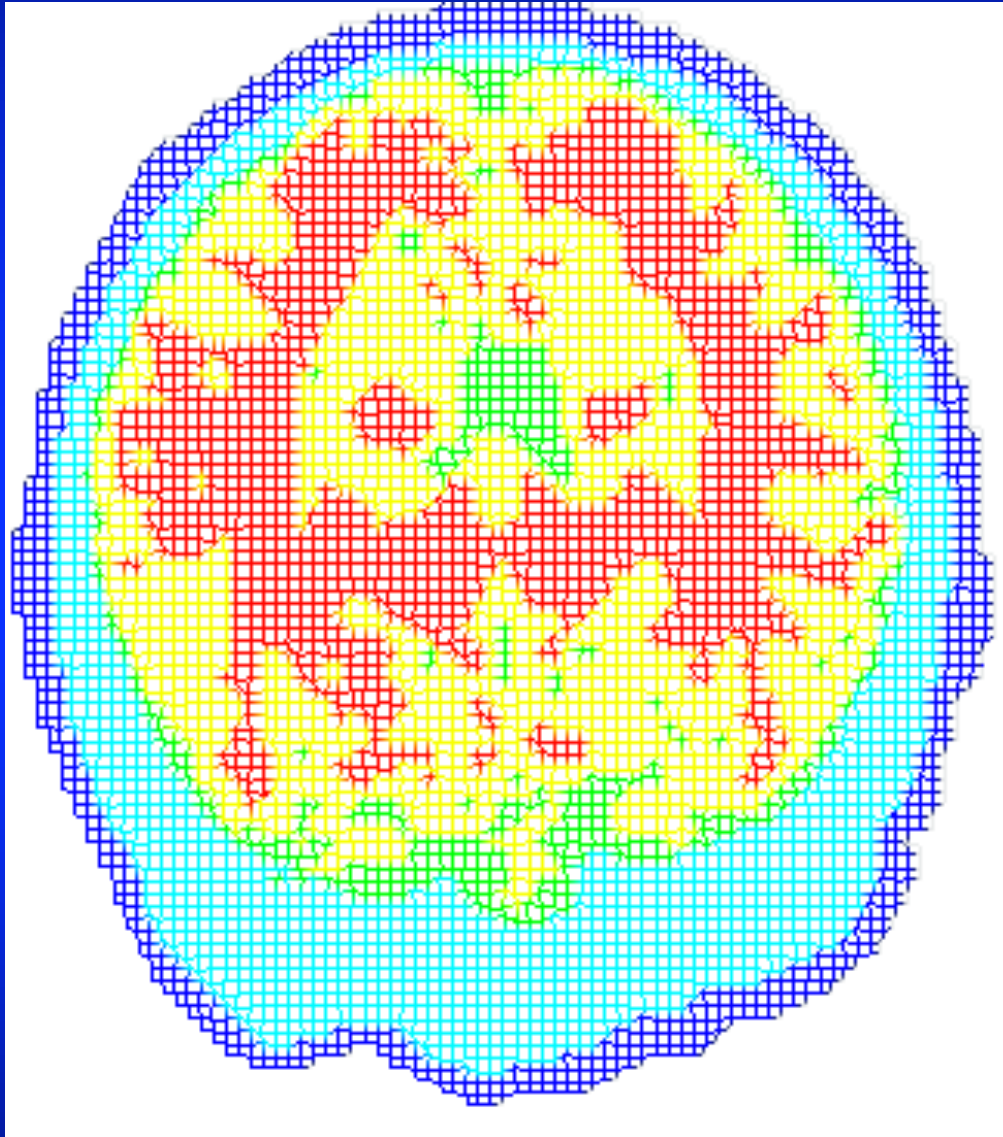
$$\kappa(K_h) = \frac{\lambda_h^{\max}}{\lambda_h^{\min}} = O(h^{-2})$$

- **Example:** $h \approx 2mm$

Link to this work:



Iterative solver for FE-equation system



Iterative solver for FE-equation system

- FE discretization, meshsize: h

$$\mathbf{K}_h \underline{u}_h = \underline{j}_h$$

with condition number

$$\kappa(K_h) = \frac{\lambda_h^{\max}}{\lambda_h^{\min}} = O(h^{-2})$$

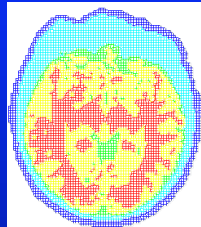
- Convergence of the CG solver:

$$\left\| \underline{u}_h^* - \underline{u}_h^{(i)} \right\|_{K_h} \leq 2c_h^i \left\| \underline{u}_h^* - \underline{u}_h^{(0)} \right\|_{K_h}$$

$$c_h = \frac{\sqrt{\kappa(K_h)} - 1}{\sqrt{\kappa(K_h)} + 1}$$

Example:

$$h \approx 2mm$$



$$\kappa(K_h) \approx 10^7$$

$$c_h = 0.9993$$

Strategy: Preconditioning!

Jacobi preconditioning

Jacobi preconditioning or scaling

The simplest preconditioner is the scaling or Jacobi-preconditioning ([264, pp.265f], [281, pp.257f]), where

$$C_h := D_h^2, \quad D_h := \text{DIAG}(\sqrt{K_h^{[11]}}, \dots, \sqrt{K_h^{[N_h N_h]}}).$$

Theorem 6.5.8. *Let K_h be SPD and $C_h := D_h^2$ the Jacobi-preconditioner. Assume that each row of K_h does not contain more than d nonzero entries. Then, for all diagonal matrices $\tilde{D}_h^{-1}$, it is*

$$\kappa_2(C_h^{-1}K_h) \leq d \kappa_2(\tilde{D}_h^{-1}K_h),$$

Incomplete Cholesky preconditioning

Incomplete Cholesky preconditioning

The SPD stiffness matrix K_h can be decomposed into a left triangular matrix L_h and its transpose using the Cholesky-decomposition, $K_h = L_h L_h^{tr}$ [281, pp.209f]. Algorithm 19 shows the Cholesky-decomposition.

Algorithm 19 Cholesky decomposition $K_h = L_h L_h^{tr}$

```

for  $p = 1, \dots, N_h$  do
     $L_h^{[pp]} = \sqrt{K_h^{[pp]}}$ 
    for  $i = (p + 1), \dots, N_h$  do
         $L_h^{[ip]} = K_h^{[ip]} / L_h^{[pp]}$ 
        for  $k = (p + 1), \dots, i$  do
             $K_h^{[ik]} = K_h^{[ik]} - L_h^{[ip]} / L_h^{[kp]}$ 
        end for
    end for
end for

```

Incomplete Cholesky preconditioning

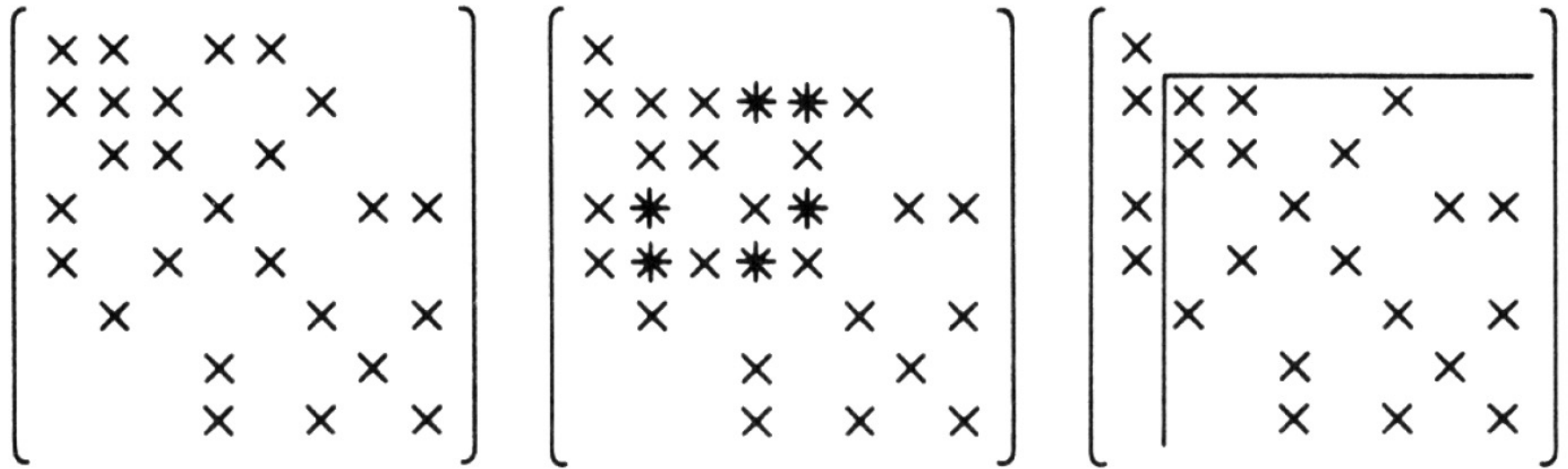


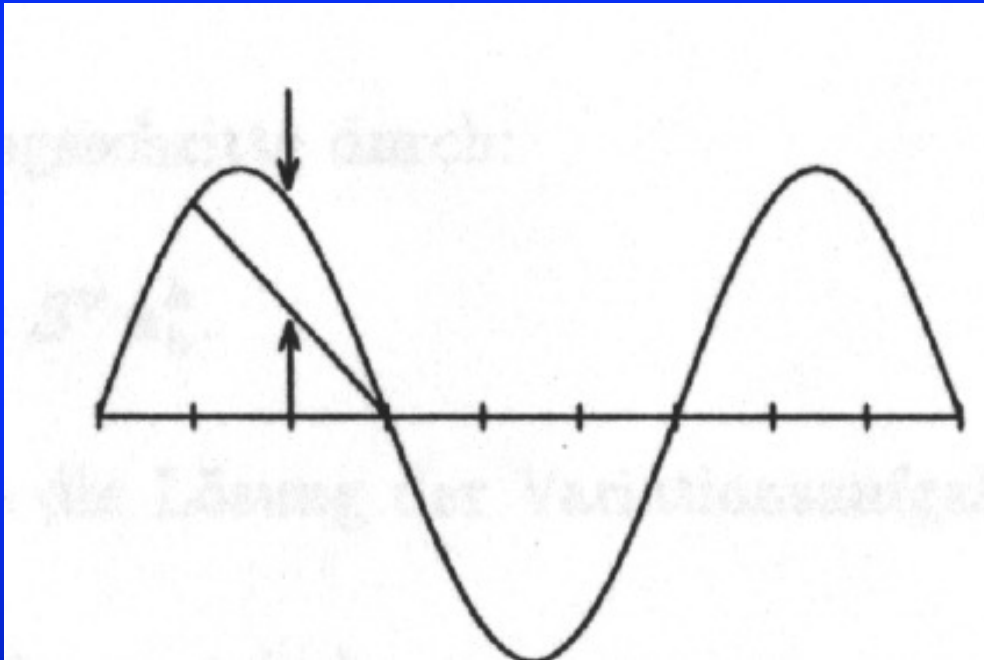
Figure 7.1: *Principle of IC0 (taken from Schwarz [281]): nonzero matrix pattern (left), situation after first step of Algorithm 19 (fill-in is marked with *), situation after the first step of IC0.*

MultiGrid (MG) preconditioning

Principle of MG

- **Smoother** for high-frequency error components is effective

$$\underline{d}_h = K_h \underline{u}_h - \underline{j}_h$$

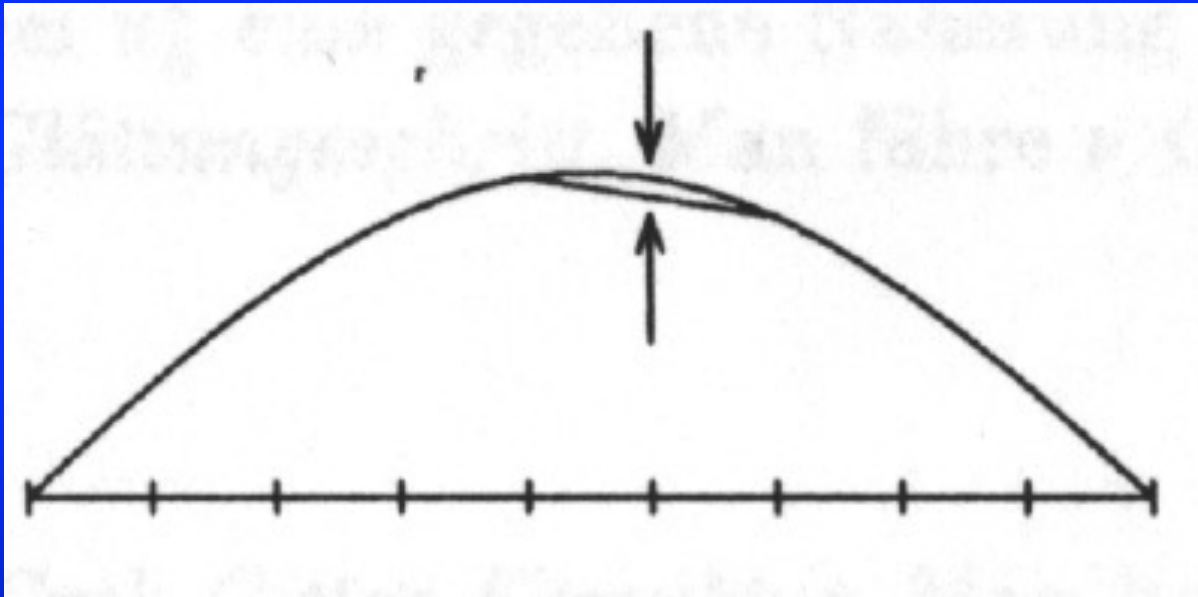


MultiGrid (MG) preconditioning

Principle of MG

- **Smoother** for low-frequency error components not effective

$$\underline{d}_h = K_h \underline{u}_h - \underline{j}_h$$

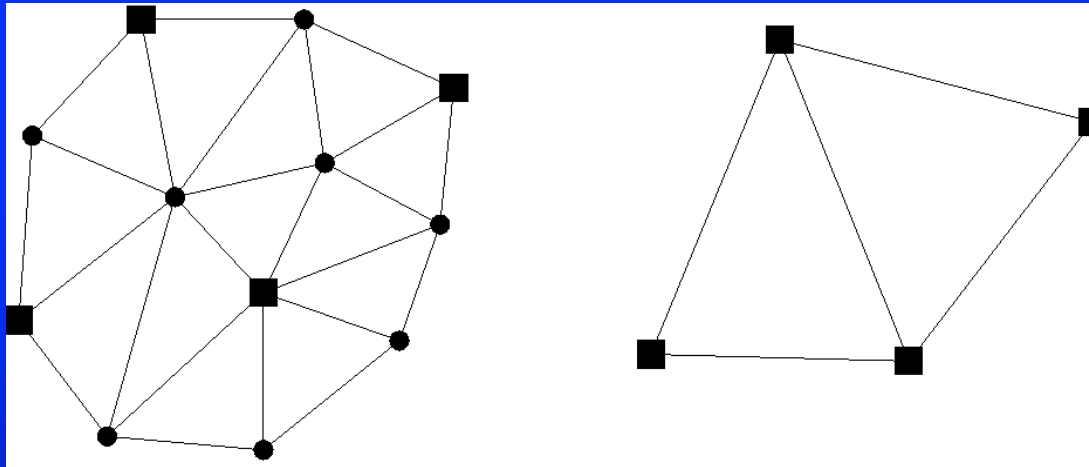


MultiGrid (MG) preconditioning

Principle of the MG

- Smoother for high-frequency error components
- Coarse grid correction for low-frequency error components

$$\underline{d}_H = P_{h,H}^{tr} \underline{d}_h$$



MultiGrid (MG) preconditioning

Algorithm 3 V-cycle MG : $(K_h, \underline{u}_h, \underline{j}_h, \nu_F, \nu_B) \rightarrow (\underline{u}_h)$

if CoarseGrid **then**

$\underline{u}_h \leftarrow \text{DirectSolve}(K_h \underline{u}_h = \underline{j}_h)$

else

$\underline{u}_h \leftarrow \nu_F \text{ TIMES SMOOTH FORWARD}(K_h, \underline{u}_h, \underline{j}_h)$

$\underline{d}_h = K_h \underline{u}_h - \underline{j}_h$

$\underline{d}_H = P_{h,H}^{tr} \underline{d}_h$

$\underline{w}_H = 0$

$\underline{w}_H = \text{MG}(K_H, \underline{w}_H, \underline{d}_H)$

$\underline{w}_h = P_{h,H} \underline{w}_H$

$\underline{u}_h = \underline{u}_h - \underline{w}_h$

$\underline{u}_h \leftarrow \nu_B \text{ TIMES SMOOTH BACKWARD}(K_h, \underline{u}_h, \underline{j}_h)$

end if

Geometric Multigrid

● Geometric MG (GMG)

- Problem-specific smoother for high-frequency error components
- Coarse grid correction for low-frequency error components



Complexity:

- $O(N)$

Convergence rate:

- h-independent
- high

● Problems in our application

- Choice of the smoother is difficult (Inhomogeneities/Anisotropies)
- Generation of the coarse grids difficult



Strategy: Algebraic MG (AMG)!

Algebraic Multigrid

[Ruge and Stüben, *SIAM*, 1986; Stüben, GMD, Tech.Report, 1999]

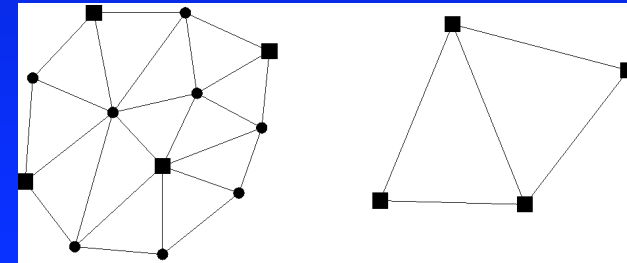
[Wolters, Vorlesungsskriptum, Chapter 7.2]

[Wolters, Kuhn, Anwender & Reitzinger, *Comp. Vis. Sci.*, 2002]

[Lew, Wolters, Dierkes, Roer & MacLeod, *Appl.Num.Math.*, 2009]

● Principle of the AMG:

- Smoother is given (Gauss-Seidel)
- Coarse grids and interpolation matrices are constructed from the entries of K
 - Diagonal entries $\leftrightarrow$ nodes
 - Nondiagonal entries $\leftrightarrow$ edges
- Only one high resolution FE mesh!



● Problems:

- AMG-interpolation non-optimal:
 - Some few error components are not well reduced, i.e., some few eigenvalues of the AMG iteration matrix are close to 1



Strategy: AMG-CG!

Preconditioned Conjugate Gradient Method

Algorithm 1 PCG : $(K_h, \underline{u}_h, \underline{j}_h, C_h, \text{ACCURACY}) \rightarrow (\underline{u}_h)$

$$\underline{r}_h = \underline{r}_h^0 = \underline{j}_h - K_h \underline{u}_h$$

$$\text{SOLVE } C_h \underline{w}_h = \underline{r}_h$$

$$\underline{s}_h = \underline{w}_h$$

$$\gamma^0 = \gamma = \gamma_{\text{OLD}} = \langle \underline{w}_h, \underline{r}_h \rangle$$

$$\text{while } \left(\gamma / \gamma^0 = \left(\frac{\|\underline{r}_h\|_{C_h^{-1}}}{\|\underline{r}_h^0\|_{C_h^{-1}}} \right)^2 = \left(\frac{\|K_h \underline{e}_h\|_{C_h^{-1}}}{\|K_h \underline{e}_h^0\|_{C_h^{-1}}} \right)^2 = \left(\frac{\|\underline{e}_h^i\|_{K_h C_h^{-1} K_h}}{\|\underline{e}_h^0\|_{K_h C_h^{-1} K_h}} \right)^2 > \text{ACCURACY}^2 \right) \text{ do}$$

$$\underline{v}_h = K_h \underline{s}_h$$

$$\alpha = \gamma / \langle \underline{s}_h, \underline{v}_h \rangle$$

$$\underline{u}_h = \underline{u}_h + \alpha \underline{s}_h$$

$$\underline{r}_h = \underline{r}_h - \alpha \underline{v}_h$$

$$\text{SOLVE } C_h \underline{w}_h = \underline{r}_h$$

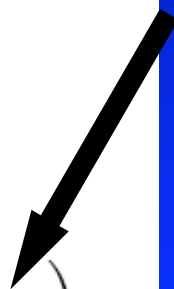
$$\gamma = \langle \underline{w}_h, \underline{r}_h \rangle$$

$$\beta = \gamma / \gamma_{\text{OLD}}, \quad \gamma_{\text{OLD}} = \gamma$$

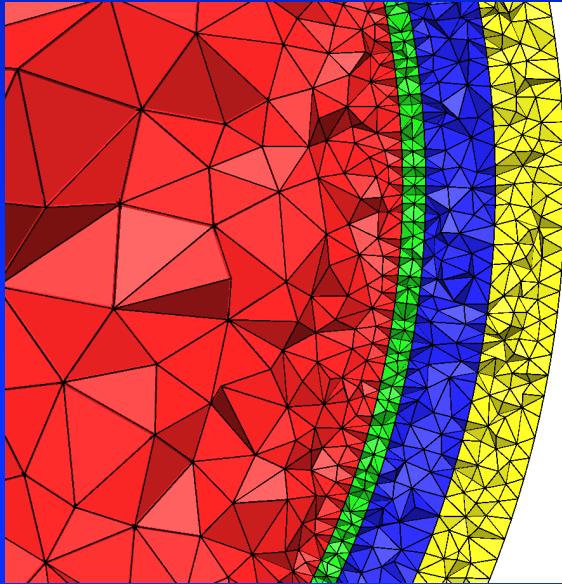
$$\underline{s}_h = \underline{w}_h + \beta \underline{s}_h$$

end while

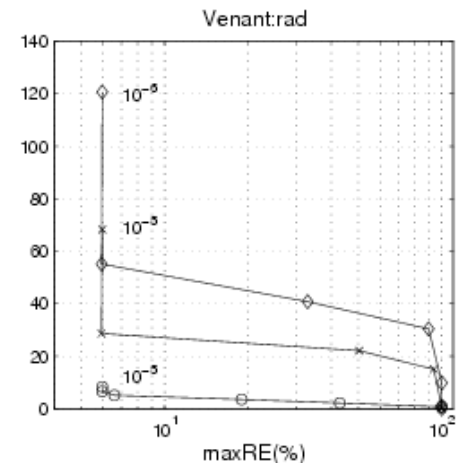
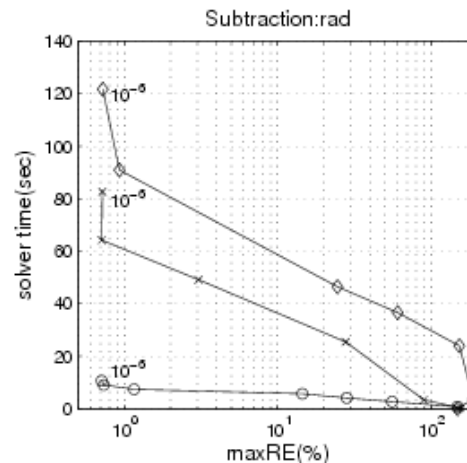
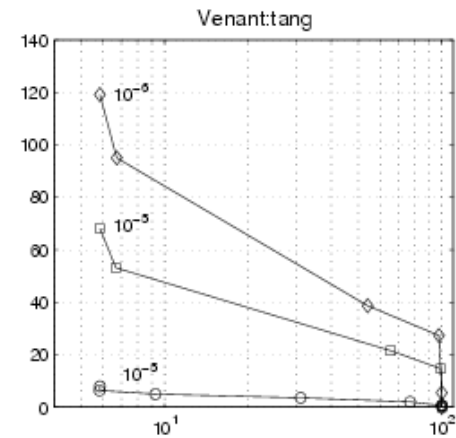
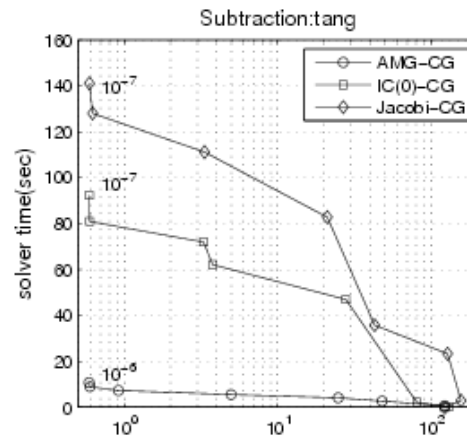
PCG
accuracy



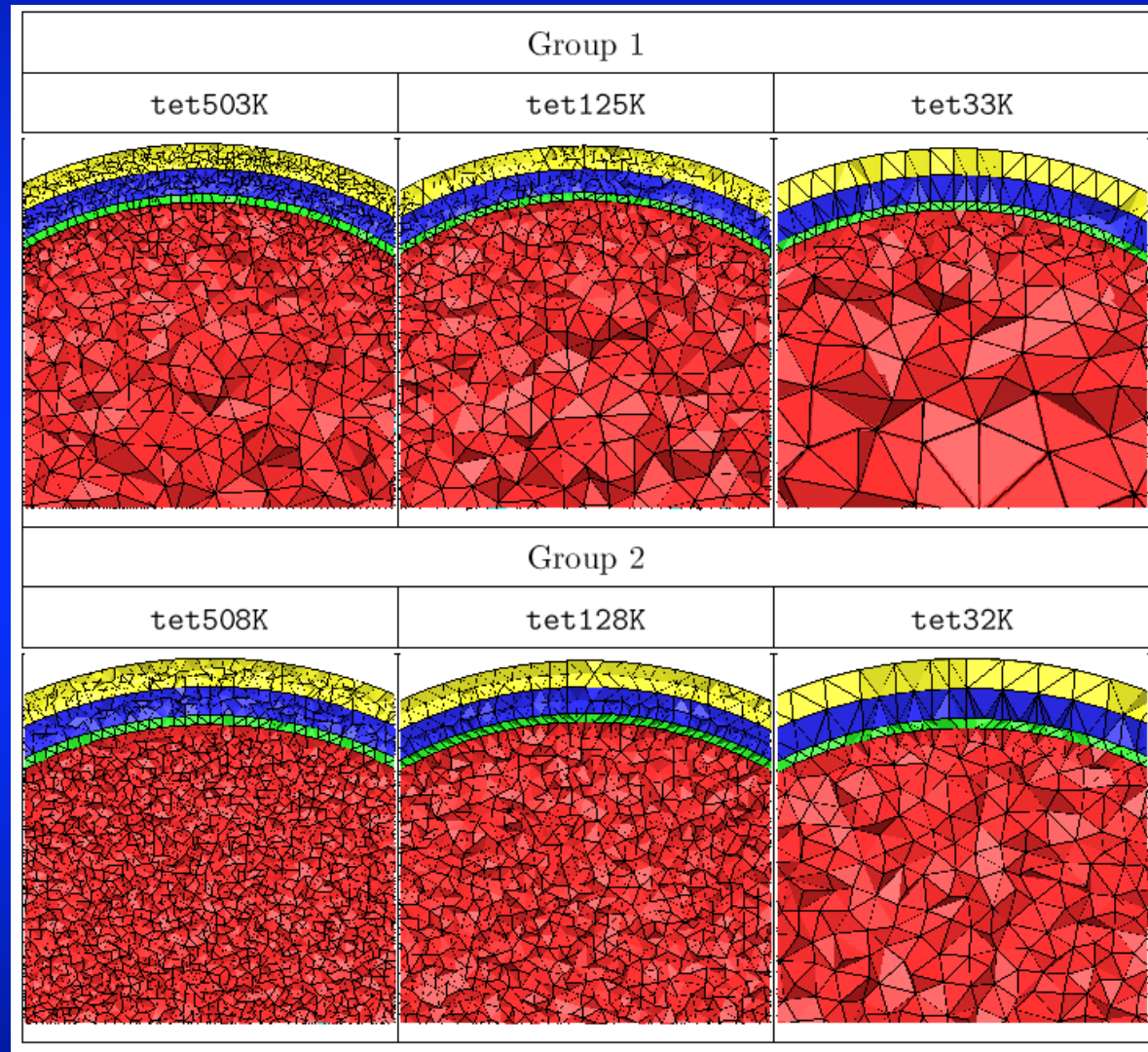
Solver: “Maximal relative error over all eccentricities” versus “solution time”



Nodes: 360,056
Elements: 2,165,281



FE models tuned for subtraction (group 1) and for the direct potential methods (group 2)



Comparison of different preconditioners

	group 1						group 2					
	tet503K		tet125K		tet33K		tet508K		tet128K		tet32K	
solver	time	iter	time	iter	time	iter	time	iter	time	iter	time	iter
AMG-CG	12.25	11.20	1.87	9.04	0.18	5.89	9.18	10.40	1.36	7.27	0.15	5.81
IC(0)-CG	112.03	233.43	8.40	128.39	0.45	72.63	72.41	215.05	5.20	98.96	0.31	52.84
Jacobi-CG	167.82	679.43	16.98	414.00	0.76	229.52	99.60	578.04	9.62	331.15	0.47	161.68
gain factor	13.70	60.66	9.08	45.8	4.22	38.97	10.85	55.58	7.07	45.55	3.13	27.83

Link to this work:

PD Dr. Carsten Wolters x PD Dr. Carsten Wolters x Wolters-Publications.pdf x +

https://campus.uni-muenster.de/fileadmin/einrichtung/biomag/Mitarbeiter/Wolters-Publications.pdf carsten wolters

Meistbesucht Erste Schritte Aktuelle Nachric... Apple Amazon Lehre Haus News Wörterbücher Apple-Mac University of Utah

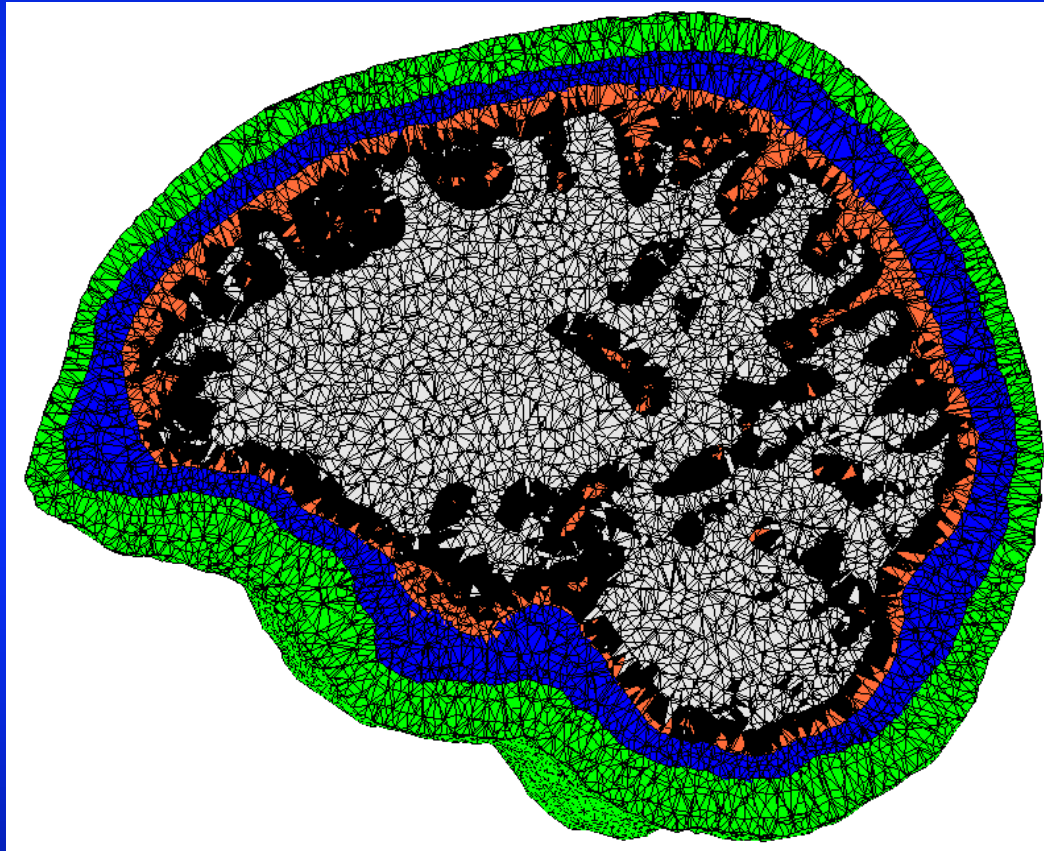
Seite: 16 von 30 Automatischer Zoom

September 26-29, 2 pages (2007).

32. Wolters, C.H., Grasedyck, L., Anwander, A. and Hackbusch, W., Efficient Computation of Lead Field Bases and Influence Matrix for the FEM-based EEG and MEG Inverse Problem. In *Halgren, E., Ahlfors, S., Hämeäläinen, M. and Cohen, D. (eds.): BIOMAG 2004, Proc. of the 14th Int. Conf. on Biomagnetism, Boston, USA*, pp. 104–107 (2004).
[Web](#), [pdf](#).

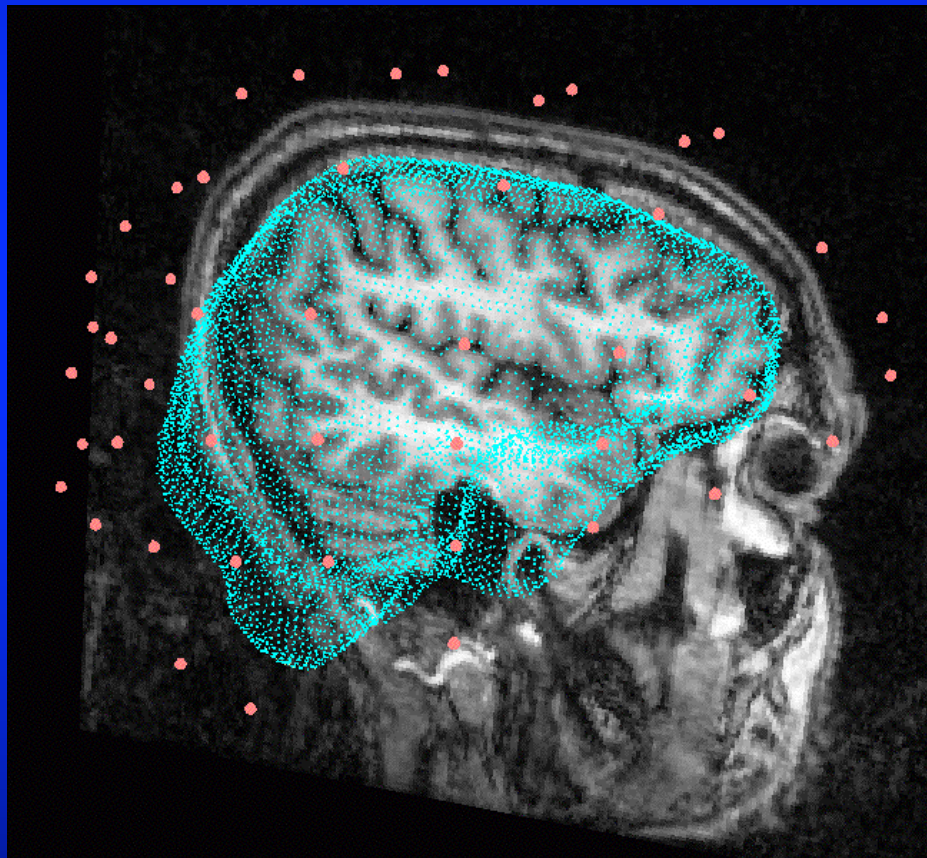
Efficiency of the fast FE transfer matrix approaches

- Head model: Tetrahedral FE, 147,287 nodes, 892,119 elements



Efficiency of the fast FE transfer matrix approaches

- Head model: Tetrahedral FE, 147,287 nodes, 892,119 elements
- Influence space: brain surface mesh, 2mm resolution, 9555 nodes



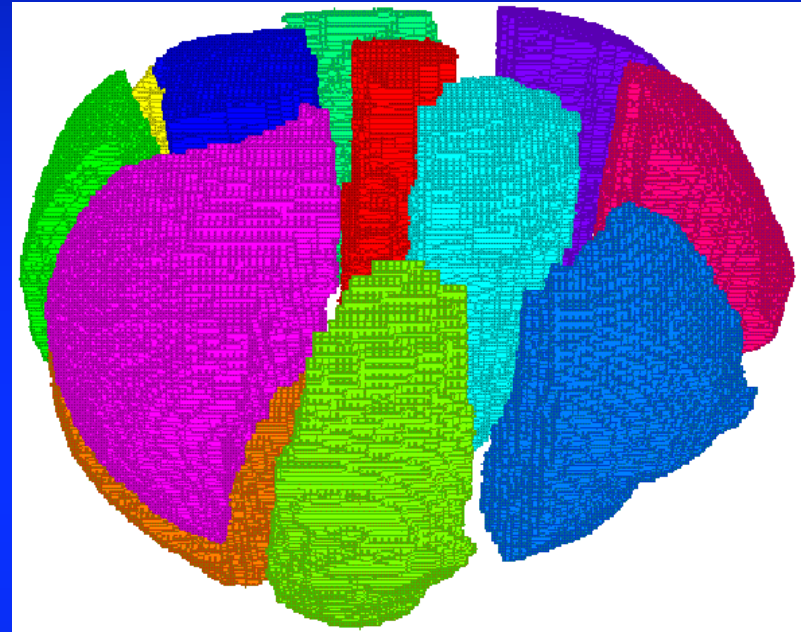
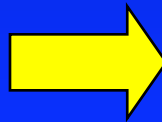
Efficiency of the fast FE transfer matrix approaches

- Head model: Tetrahedral FE, 147,287 nodes, 892,119 elements
- Influence space: brain surface mesh, 2mm resolution, 9555 nodes
- Number of FE forward solutions:
 EEG, 71 electrodes: $9555 * 3 = 28665$
 MEG, 147 channels: $9555 * 2 = 19110$ (tangential constraint)
- FE approach and dipole model: Venant

Platform	Method	Solver method	Setup time		Influence matrix		Max.memory (in MB)	
			MEG	EEG	MEG	EEG	MEG	EEG
Mac G4	New Lead field bases approach	3RHS-AMG-CG	14min	6.5min	63 sec	56 sec	654	405
	Standard	symIC(0)-CG	0.5sec	0.5sec	230 h	302 h	432	219

Parallel AMG-CG on distributed memory computers

“Element-wise”
partitioning into
subdomains

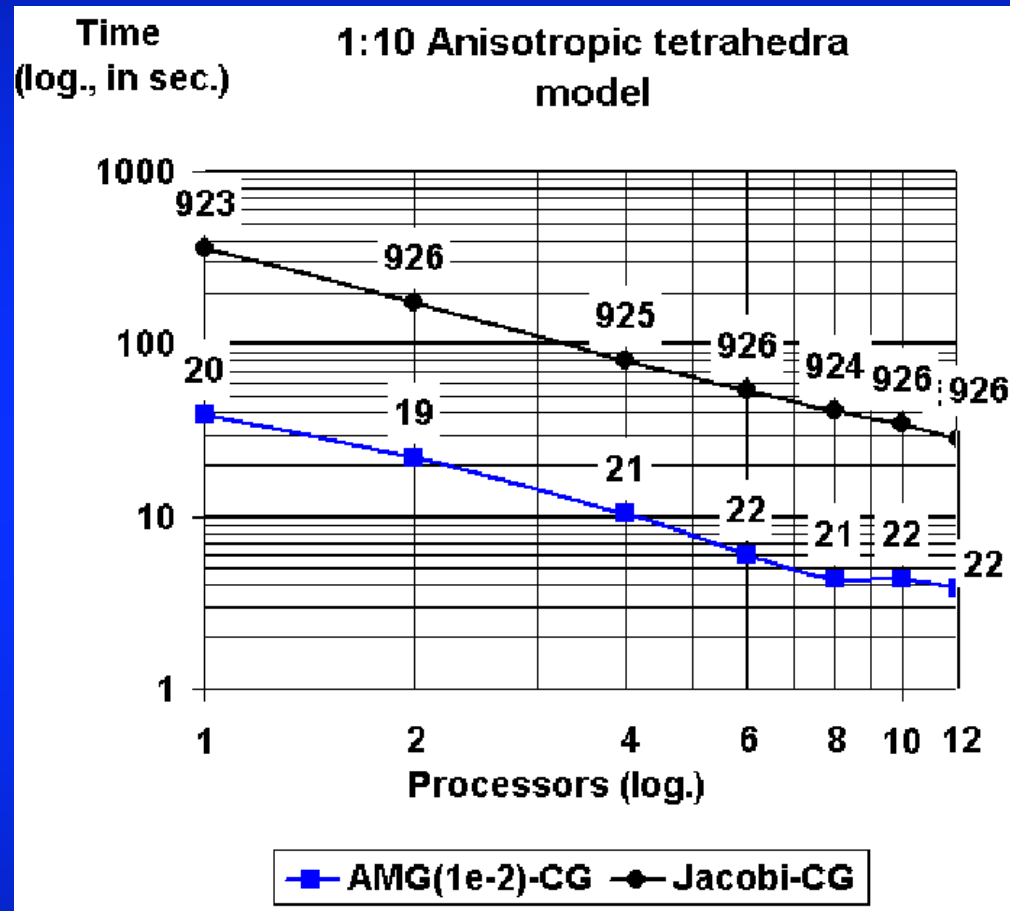


Parallel MultiRHS-AMG-CG: Communication is only necessary for:

- Smoother (ω -Jacobi within interface nodes, Gauss-Seidel between blocks and for inner nodes)
- distribution of coarse grid solution
- inner products within PCG method

Results for parallel solver methods

SGI Origin2000, each processor 195MHz, MIPS 10000



Solver time comparison: Unknowns:147.287

- **Distribution of memory**
- **About a linear speedup for moderate processor number**
- **Jacobi-CG on 1 proc <-> AMG-CG on 8 procs: Speedup factor of about 80 (10 MG, 8 parallel.)**
- **Anisotropy and inhomogeneity does not change performance results**
- **Stable preconditioning for moderate processor numbers**

Thank you for your attention!



SIM-NEURO work-group at IBB

