$\mathcal{H}$-MATRIX BASED PRECONDITIONER FOR THE SKIN PROBLEM

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joint work with

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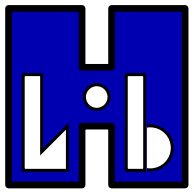

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A skin fragment in 2D

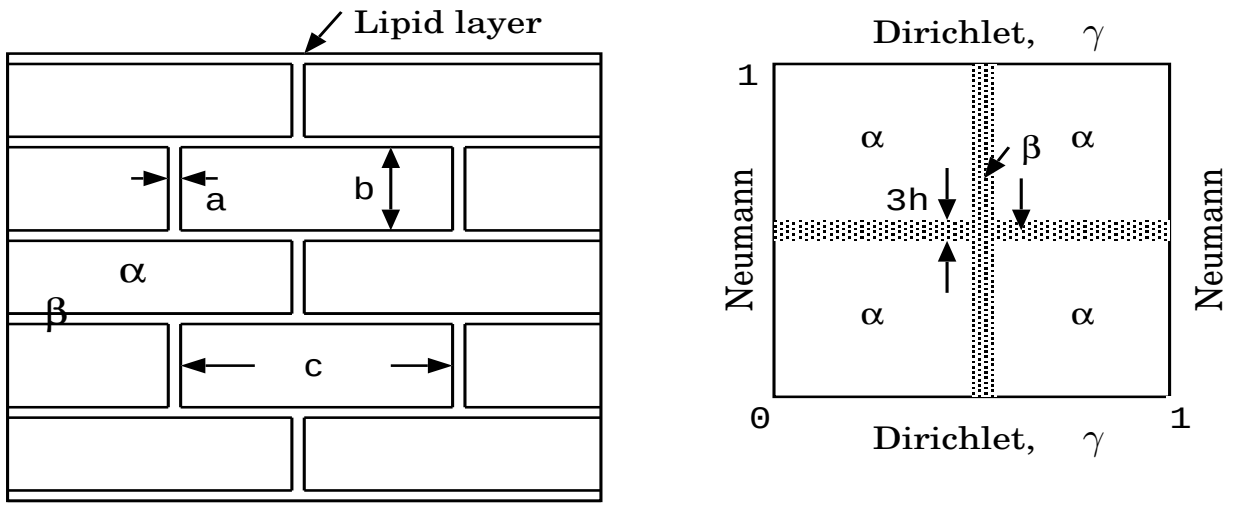


Fig. 1 – **(left)** A skin fragment consists of cells and the lipid layer. The penetration through cells goes very slowly and very fast through the lipid layer. **(right)** The simplified model of a skin fragment in 2D contains 4 cells with the lipid layer between them. $\Omega = [-1, 1]^2$, $\alpha(x) = \varepsilon$ inside cells and $\alpha(x) = \beta = 1$ in the lipid layer.

A skin fragment in 3D

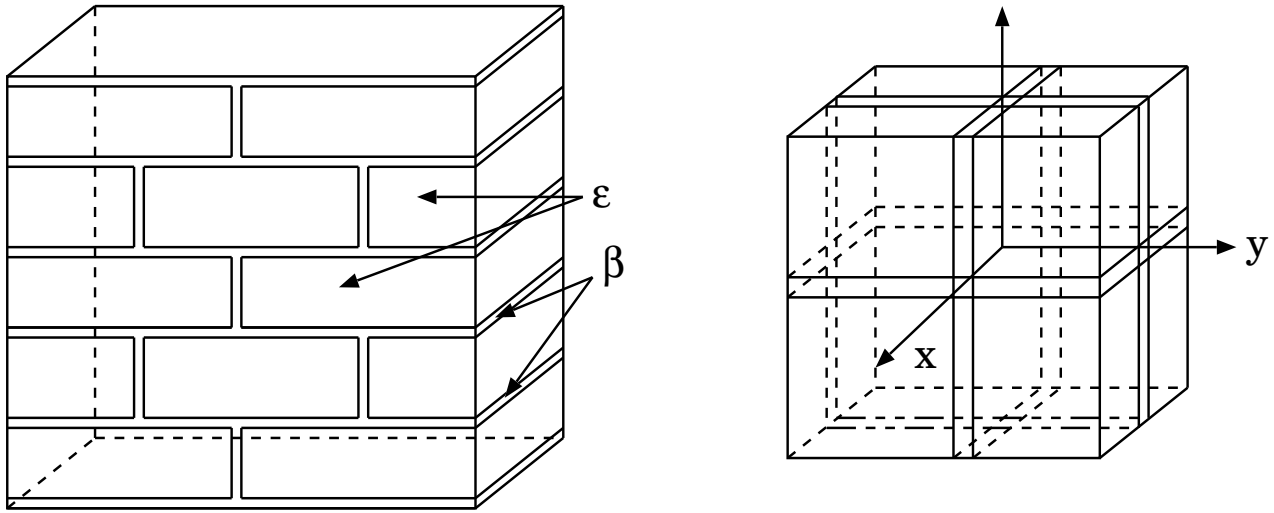


Fig. 2 – **(left)** A skin fragment consists of cells and the lipid layer. The penetration through cells goes very slowly and very fast through the lipid layer. **(right)** The simplified model of a skin fragment in 3D contains 8 cells with the lipid layer between them. $\Omega = [-1, 1]^3$, $\alpha(x) = \varepsilon$ inside cells and $\alpha(x) = \beta = 1$ in the lipid layer.

The Skin Problem Setup

$$\operatorname{div}(\alpha(x,y)\nabla u) = f \quad x \in \Omega \subseteq \mathbb{R}^d,\ d = 2,3$$

$$u = g_0 \qquad x \in \gamma$$

$$\frac{\partial u}{\partial n} = g \qquad x \in \Gamma \setminus \gamma$$

where $\alpha(x,y) = \alpha \ll 1$ in cells
and $\alpha(x,y) = \beta = 1$ in between.

[Khoromskij, Wittum 02]

Discretisation (FEM)

τ_h - triangulation is compatible with the lipid layer. Let $V_h \subset H^1(\Omega)$, $V_h := \{b_j\}_{j=1}^n$, b_j - piecewise linear.
find $u \in H^1_\gamma(\Omega)$:

$$a(u,v) = \int \alpha(\nabla u, \nabla v)dx = c(v) := \int_\Omega fvdx + \int_{\Gamma\setminus\gamma} gvd\Gamma$$

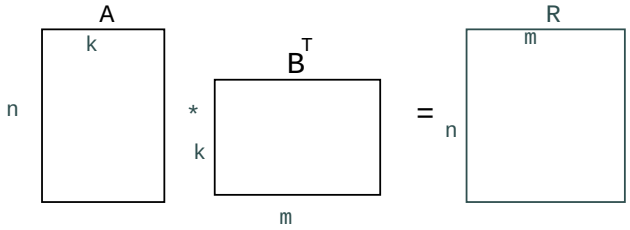
$$\forall v \in H^1_\gamma(\Omega) \quad \text{where } H^1_\gamma(\Omega) := \{u \in H^1(\Omega) : u = 0 \text{ on } \gamma\}$$

Define the discrete system : $Ax = c$.

$$A_{ij} := a(b_i, b_j) := \int_\Omega \alpha(x,y)(\nabla b_i, \nabla b_j)dx; \int_\Omega fb_j dx + \int_{\partial\Omega\setminus\Gamma} gb_j dx := c_j.$$

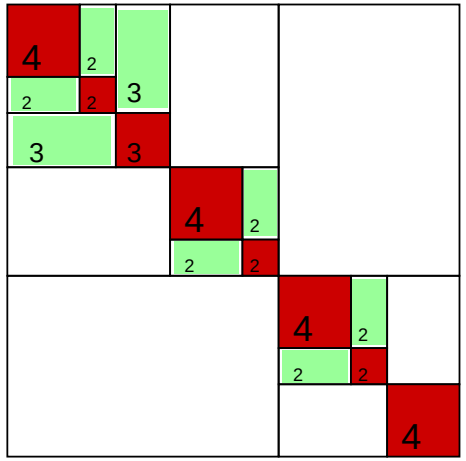
Rank-k matrices

1. $R \in \mathbb{R}^{n\times m}$, $A \in \mathbb{R}^{n\times k}$, $B \in \mathbb{R}^{m\times k}$, $k \ll \min(n,m)$. The storage $R = AB^T$ is $k(n+m)$ instead of $n \cdot m$ for R represented in full matrix format.



$\mathcal{H}$-**matrices** (Hackbusch '99)

2. Grid $\rightarrow$ cluster tree (T_I) $\rightarrow$ blockcluster tree $(T_{I\times J})$ + admissibility condition $\rightarrow$ admissible partitioning $\rightarrow$ $\mathcal{H}$-matrix $\rightarrow$ $\mathcal{H}$-matrix arithmetics .

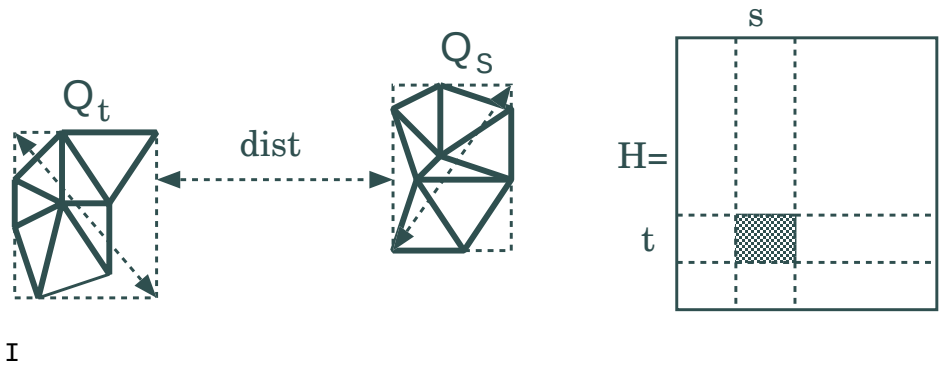


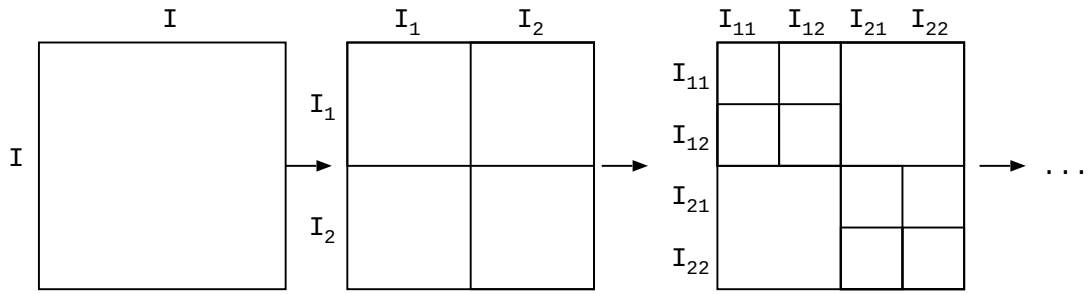
3. Let $I := I(\Omega)$, $t, s \in T_I$, $(t \times s) \in T_{I \times I}$.

Admissibility : $\max\{diam(t), diam(s)\} \leq \eta \cdot dist(t, s)$.

if(adm=true) then $M|_{t \times s}$ is a rank-k matrix block

if(adm=false) then divide $M|_{t \times s}$ further or define as a dense matrix block, if small enough.





Definition 0.1 $\mathcal{H}(T_{I\times J},k) := \{M \in \mathbb{R}^{I\times J} \mid rank(M\,|_{t\times s}) \leq k$ *for all admissible leaves* $t\times s$ *of* $T_{I\times J}\}$.

Operation	Sequential Compl.	Parallel Complexity (R.Kriemann 2005)
$building(M)$	$N = \mathcal{O}(n \log n)$	$\frac{N}{q}$
$storage(M)$	$N = \mathcal{O}(kn \log n)$	N
Mx	$N = \mathcal{O}(kn \log n)$	$\frac{N}{q}$
$M' \oplus M''$	$N = \mathcal{O}(k^2 n \log n)$	$\frac{N}{q}$
$M' \odot M''$	$N = \mathcal{O}(k^2 n \log^2 n)$	$\frac{N}{q}$
M^{-1}	$N = \mathcal{O}(k^2 n \log^2 n)$	$\frac{N}{q} + \mathcal{O}(n)$
$\mathcal{H}$-LU	$N = \mathcal{O}(k^2 n \log^2 n)$	$\frac{N}{q} + \mathcal{O}(\frac{k^2 n \log^2 n}{n^{1/d}})$

$n := \max(|I|,|J|)$, $d = 1,2,3$ is the spatial dimension.

$\mathcal{H}$-LU Factorisation (M.Lintner, 2004)

$A \approx L_{\mathcal{H}} U_{\mathcal{H}}$ implies $A^{-1} \approx U_{\mathcal{H}}^{-1} L_{\mathcal{H}}^{-1}$.

Suppose that

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}.$$

M.Bebendorf, 05 :

1. Compute L_{11} and U_{11} as $\mathcal{H}$-LU decomposition of A_{11}.
2. Compute U_{12} from $L_{11} U_{12} = A_{12}$ (use a recursive block forward substitution).
3. Compute L_{21} from $L_{21} U_{11} = A_{21}$ (use a recursive block backward substitution).
4. Compute L_{22} and U_{22} as $\mathcal{H}$-LU decomposition of $L_{22} U_{22} = A_{22} \ominus L_{21} \odot U_{12}$.

All steps are executed in the class of $\mathcal{H}$-matrices.

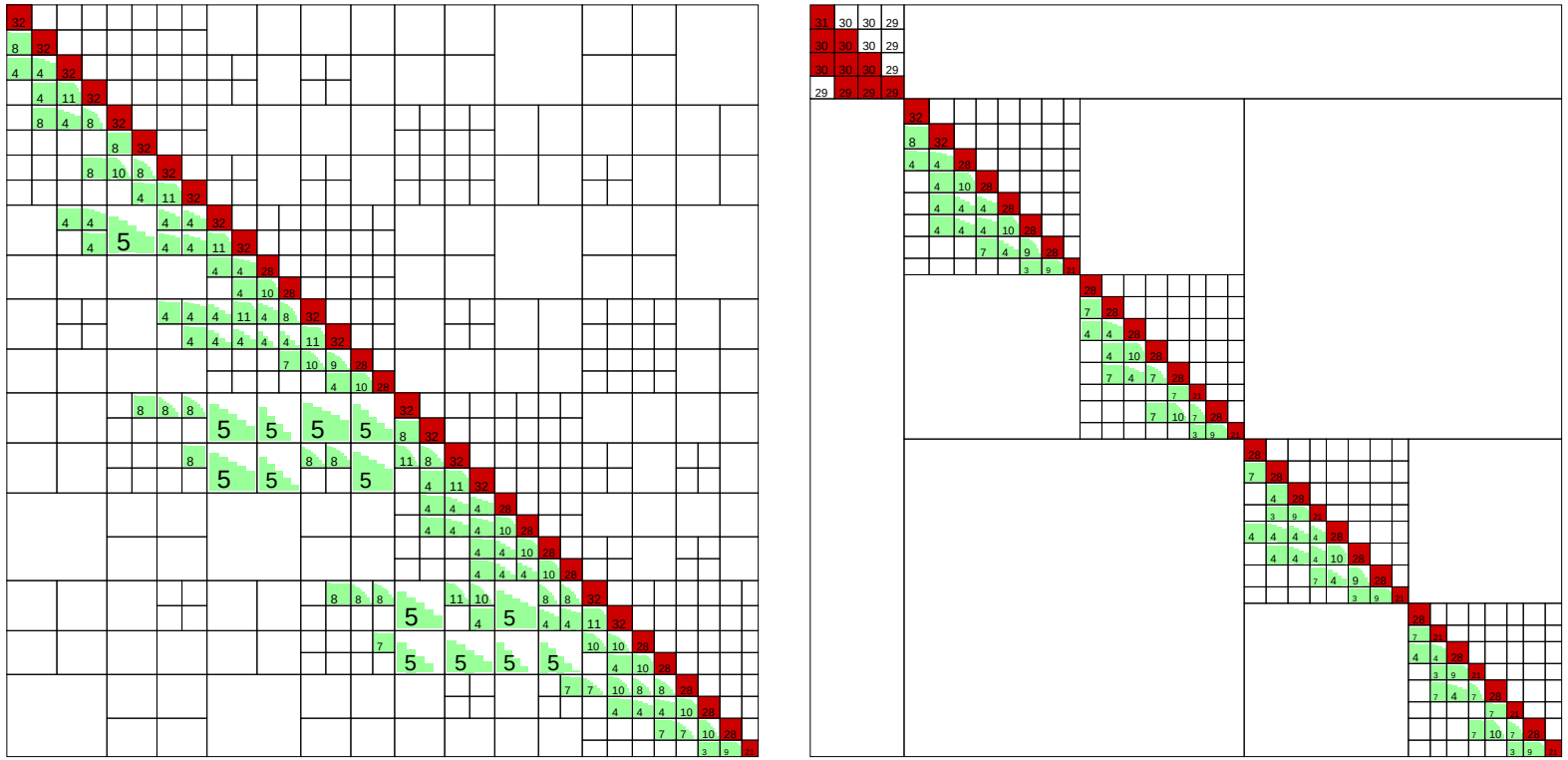
Spectral equivalence

Let $A = \begin{pmatrix} A_{11} & \varepsilon A_{12} \\ \varepsilon A_{21} & \varepsilon A_{22} \end{pmatrix}$, $W := \begin{pmatrix} A_{11} & 0 \\ 0 & \varepsilon A_{22} \end{pmatrix}$ be given, Ω_l be the lipid layer, $\Omega_c := \Omega \setminus \Omega_l$, u_1 the solution in Ω_l and u_2 the solution in Ω_c.

Proposition 0.1 *Let the component u_2 be discretely harmonic in the subdomain $\Omega_c \subset \Omega$ then*
$\exists c_1 > 0 : c_1(A_{11}u_1, u_1) \geq (A_{22}u_2, u_2)$ *with c_1 independent of h.*

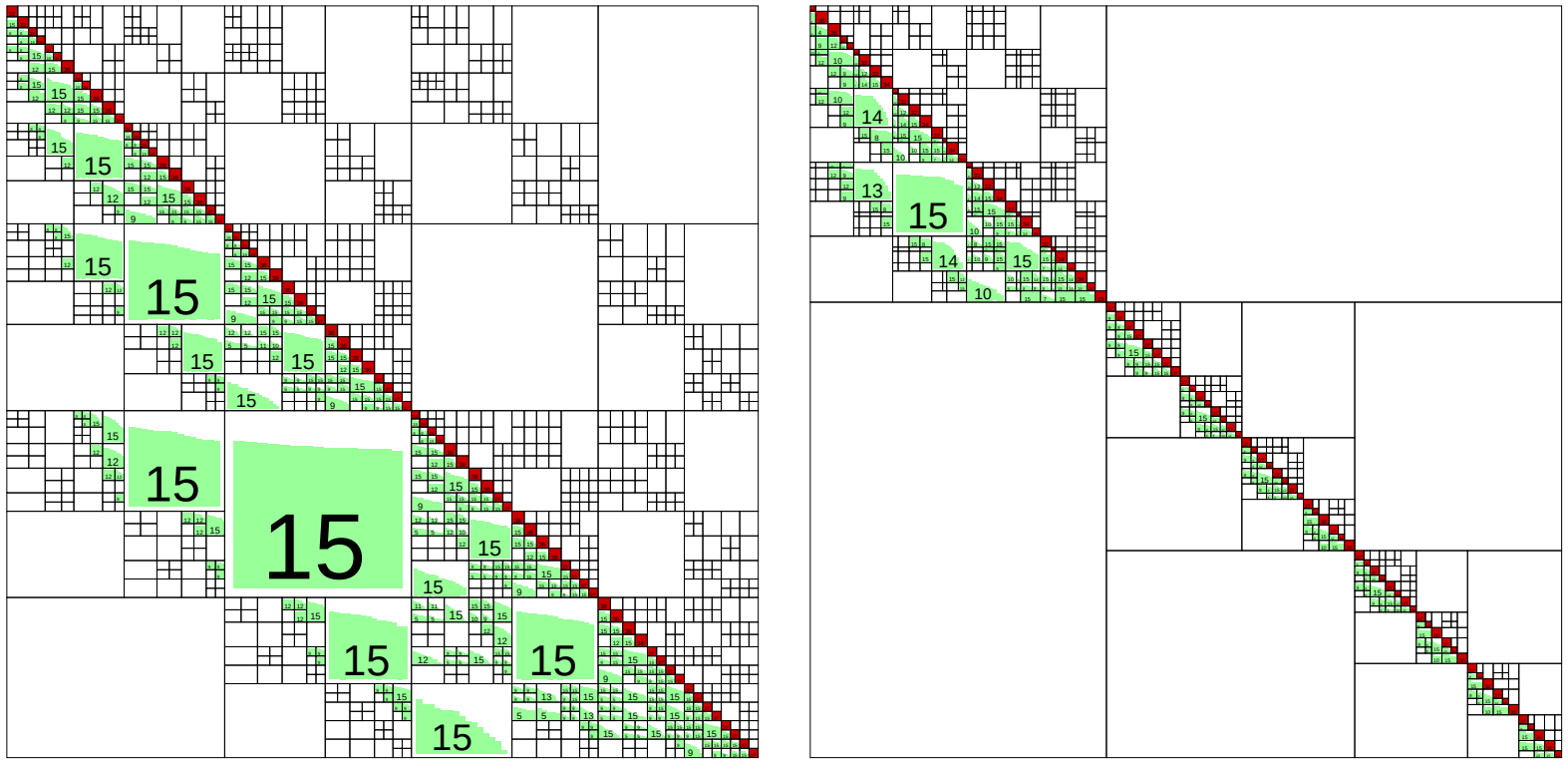
Lemma 0.1 *Let Prop. 0.1 holds, then the matrices A and W are spectrally equivalent $cW \leq A \leq 2W$ with $c = \frac{1-\varepsilon}{1+c_1\varepsilon}$.*

$\mathcal{H}$-Cholesky Preconditioner and New Preconditioner in 2D



(**left**) before resorting and (**right**) after resorting $I(\Omega) := I(\Omega_l) \cup I(\Omega_c)$ and after omitting the coupling. The numbers indicate the local rank.

$\mathcal{H}$-Cholesky Preconditioner and New Preconditioner in 3D

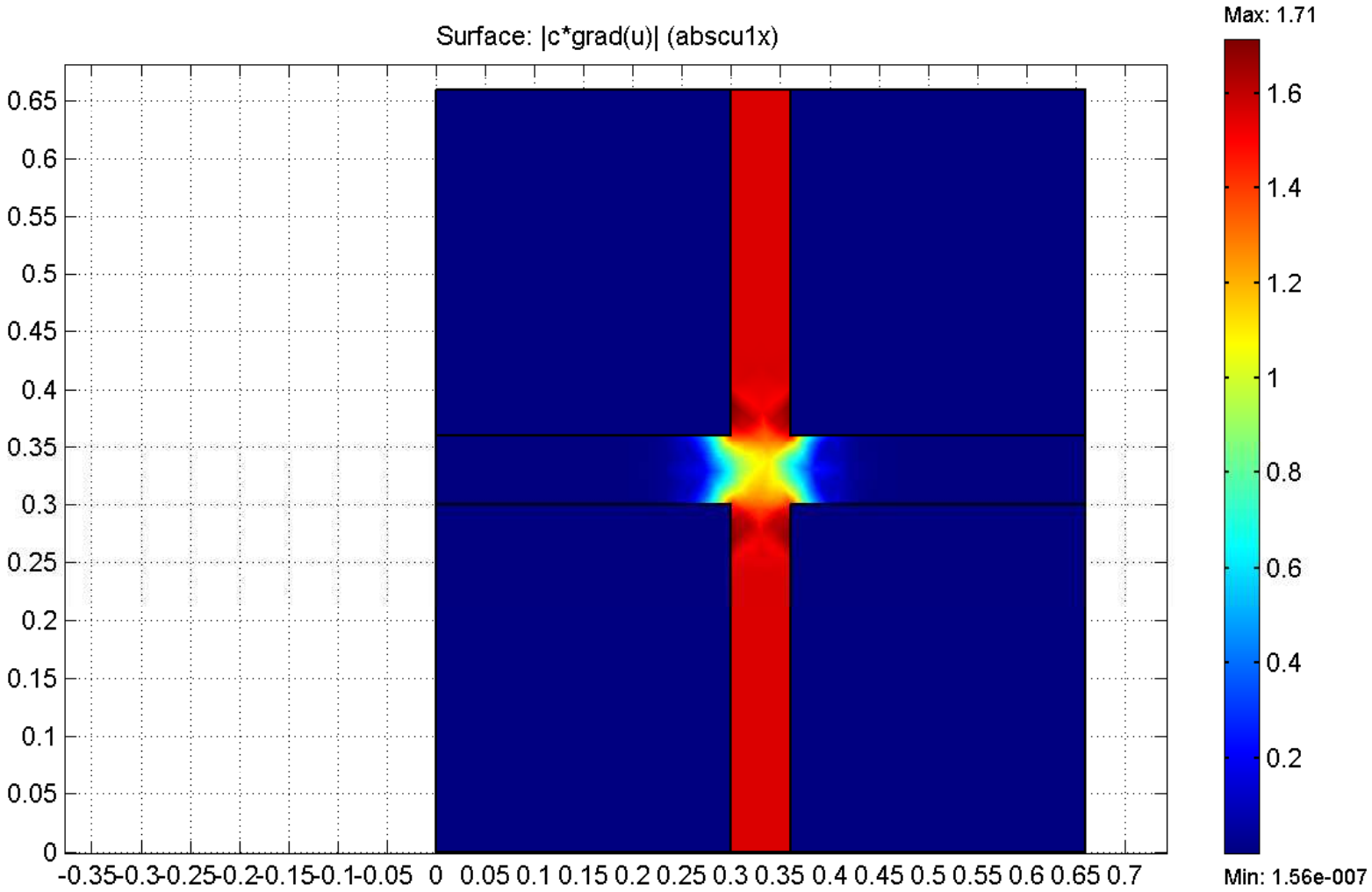


(**left**) before resorting and (**right**) after resorting $I(\Omega) := I(\Omega_l) \cup I(\Omega_c)$ and after omitting the coupling.

Lemma 0.2 *Let A be the standard stiffness matrix, n the number of all dofs, n_I the number of dofs in the lipid layer, p the number of processors, $n_0 := \frac{n-n_I}{p-1}$, W_1 and W_2 the Cholesky factorizations of A and* $\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}$ *respectively, where $A_{11} \in \mathbb{R}^{n_I \times n_I}$, $A_{22} \in \mathbb{R}^{(n-n_I)\times(n-n_I)}$. The sequential and parallel computational costs of W_1 and W_2 are as in the following Table.*

Preconditioner	*Complexity*	*Parallel Complexity*
W_1	$\mathcal{O}(n \log^2 n)$	$\mathcal{O}(n \log^2 n)$
W_2	$\mathcal{O}(n_I \log^2 n_I)$ $+\mathcal{O}((n-n_I)\log^2(n-n_I))$	$\max\{\mathcal{O}(n_I \log^2 n_I),$ $\mathcal{O}(n_0 \log^2 n_0)\}$

Penetration of drugs in 2D (computed in MATLAB)



Blue color means low penetration and red color high penetration.

Preconditioned CG-method

$$x^{m+1} = x^m - W^{-1}(Ax^m - c),$$

where $W = LL^T$ and $W^{-1/2}AW^{-1/2} = L^{-T}AL^{-1}$ is symmetric and positive definite.

u = solve_cg(A, $prec$, rhs, ...) ;

$\kappa(A) \leq \max(\frac{\alpha(\triangle_i)}{\alpha(\triangle_j)})h^{-d}$ - is the condition number of A, $d = 1, 2, 3$ and $\triangle_i$, $\triangle_j$ are finite elements.

PCG stops as soon as $\|Ax^m - c\|_2 \leq \varepsilon$.

Numerical results in 3D

(Laptop, 1.3Ghz, 512 Mb)

Tab. 1 – Comparison of times for W_1 and W_2 in 3D. 40^3 dofs, $\|Ax - b\|_2 = 10^{-8}$, $\alpha(x) = 10^{-5}$.

k	$t_p^{(1)} + t_{it}^{(1)}$	$t_p^{(2)} + t_{it}^{(2)}$	$t_l + t_c$
1	24+10.6	8.7 + 10	2.8 + 0.9
2	70+11.3	21.6+ 13.3	4.7 + 2.1
4	208+12.5	68 + 13.5	13.5 + 6.9
6	484+82	123 + 26	29.6 + 11.4

$t_p^{(1,2)}$, $t_{it}^{(1,2)}$ contain the respective times for computing the preconditioners W_1 and W_2 and for performing the pcg iterations.

t_l and t_c show the computational times in the lipid layer and in one cell, respectively.

For all ranks k the time for W_2 (red number) is much smaller than the time for W_1 (blue number) !

Tab. 2 – Comparison of W_1 and W_2 in 3D. 40^3 dofs, $\|Ax-b\| = 10^{-8}$, $\alpha(x) = 10^{-5}$.

k	$S^{(1)}$, $S^{(2)}$	iter$^{(1)}$,$^{(2)}$
1	2e+2, 1e+2	69, 99
2	3.8e+2, 1.8e+2	46, 91
4	7.5e+2, 3.5e+2	17, 60
6	1.1e+3, 5.1e+2	11, 74

The new preconditioner W_2 requires less memory ($S^{(1)} > S^{(2)}$) !

Tab. 3 – Dependence of the number of iterations and the computational time on the coefficient $\alpha(x)$. 40^3 dofs, $\|Ax-b\| = 10^{-8}$, rank k=1 for $\mathcal{H}$-matrices.

α	iter$^{(1)}$,$^{(2)}$	$t^{(1)}$, $t^{(2)}$
1	86, 89	70, 33
10^{-1}	77, 100	67, 35
10^{-2}	79, 113	63, 37
10^{-4}	79, 113	65, 37
10^{-6}	82, 116	67, 37
10^{-8}	85, 120	67, 38

For all α the time for W_2 (red number) is almost two times smaller than the time for W_1 (blue number).

Conclusion

The rank $k = 1$ in $\mathcal{H}$-arithmetic with a larger number of iterations leads to faster performance than a large rank k with a small number of iterations.

(+) The new preconditioner W_2 is well parallelisable ,

(+) W_2 has sequential complexity

$\mathcal{O}(n_I \log^2 n_I) + \mathcal{O}((n - n_I) \log^2 (n - n_I))\}$,

(+) W_2 has parallel complexity

$\max\{\mathcal{O}(n_I \log^2 n_I), \mathcal{O}(n_D \log^2 n_D)\}$, $n_D := \frac{n - n_I}{p-1}$,

(+) W_2 requires less memory than W_1,

[0] www.hlib.org

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[4] Sabine Le Borne, Ronald Kriemann, Lars Grasedyck, *Parallel Black Box Domain Decomposition Based $\mathcal{H}$-LU Preconditioning*, Preprint 115, 2005, Max-Planck-Institut MIS, Leipzig.

[5] A. Litvinenko, *Application of Hierarchical Matrices for Solving Multiscale Problems. PhD Dissertation, Leipzig University, submitted, April 2006.*