

The Relation Between Optimized Schwarz Methods for Scalar and Systems of Partial Differential Equations

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Outline of the talk

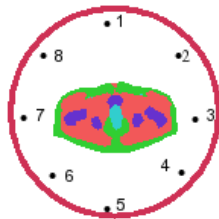
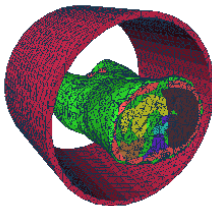
- 1 Introduction
 - Motivation
 - References
- 2 One domain problem
 - Mathematical formulation
 - Relation to a scalar equation
- 3 Domain decomposition algorithm
 - Classical Schwarz algorithm
 - Optimized Schwarz methods
 - General interface conditions
- 4 Numerical results
- 5 Conclusions and future work

Motivation

Local hyperthermia using electromagnetic waves

Treatment of a cancerous tumour by rising locally the temperature of the tumour.

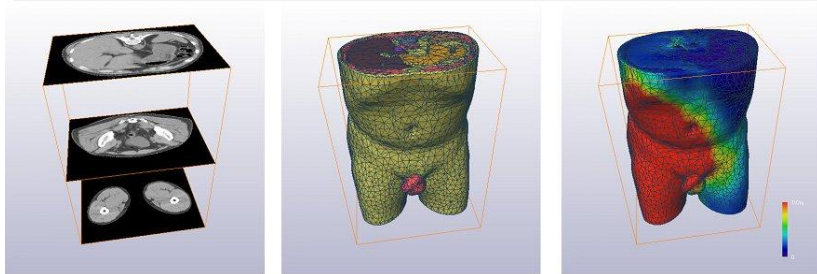
Tool : use an electromagnetic field radio-frequencies or micro-waves.



Motivation

Therapeutical planning

- 1 Segmentation of scanners images
- 2 Mesh of the body
- 3 Electromagnetic and thermic computations + optimization of the parameters.



Electromagnetic computation

- Mathematical model:

$$\begin{cases} (i\omega\epsilon + \sigma)\mathbf{E} - \text{curl } \mathbf{H} = -\mathbf{J}_{\text{imp}}, \\ i\omega\mu\mathbf{H} + \text{curl } \mathbf{E} = 0. \end{cases}$$

- Other features:
 - Unbounded domain.
 - Antennas : courant source terms inside the domain.
 - Linear isotropic material for a given frequency.
 - Unstructured mesh and heterogeneous media.

Optimized Schwarz: from scalar problems to systems

- Schwarz algorithms that are convergent without overlap: Lions '90.
- Approximate radiation conditions for Helmholtz: Despres, '91.
- The use of non-local operators first invoked in Hagstrom, '88.
- Approximations of non-local interface conditions for advection-diffusion equation Charton '91, Nataf '95, optimized transmission conditions Japhet '00.
- Helmholtz equations: Chevalier '98, Gander, Magoules, Nataf '01.
- Optimized conditions for symmetric, positive definite problems Gander '06, time-dependent problems Gander, Halpern, Nataf '03.
- Maxwell's equations (curl-curl) Alonso, Gerardo-Giorda '06.
- Derivation of optimized conditions for Cauchy-Riemann equations using the equivalence with a scalar problem V.D., Gander '06.

Systematic approach: from scalar problems to systems using Smith factorization for Euler V.D., Nataf '05 and Stokes V.D., Nataf, Rapin '06

Mathematical model

Scattering problem - total field

$$\begin{cases} (i\omega G_0 + G'_0)\mathbf{W} + G_x\partial_x\mathbf{W} + G_y\partial_y\mathbf{W} + G_z\partial_z\mathbf{W} = 0, & \text{in } \Omega, \\ (M_{\Gamma_m} - G_n)\mathbf{W} = 0 & \text{on } \Gamma_m, \\ (M_{\Gamma_a} - G_n)(\mathbf{W} - \mathbf{W}_{\text{inc}}) = 0 & \text{on } \Gamma_a. \end{cases}$$

- Unknown electromagnetic vector field \mathbf{W} : $\mathbf{W} = (\mathbf{E}, \mathbf{H})^T$.
- Properties of different media :

$$G_0 = \begin{pmatrix} \epsilon I_3 & 0_{3 \times 3} \\ 0_{3 \times 3} & \mu I_3 \end{pmatrix} \text{ and } G'_0 = \begin{pmatrix} \sigma I_3 & 0_{3 \times 3} \\ 0_{3 \times 3} & 0_{3 \times 3} \end{pmatrix}.$$

- Vector product with \mathbf{e}_l , l in $\{x, y, z\}$:

$$G_l = \begin{pmatrix} 0_{3 \times 3} & N_{\mathbf{e}_l} \\ N_{\mathbf{e}_l}^t & 0_{3 \times 3} \end{pmatrix} \text{ with } N_{\mathbf{n}} = \begin{pmatrix} 0 & \mathbf{n}_z & -\mathbf{n}_y \\ -\mathbf{n}_z & 0 & \mathbf{n}_x \\ \mathbf{n}_y & -\mathbf{n}_x & 0 \end{pmatrix}$$

Mathematical model

- Taking into account the boundary conditions :

$$M_{\Gamma_m} = \begin{pmatrix} 0_{3 \times 3} & N_{\mathbf{n}} \\ -N_{\mathbf{n}}^t & 0_{3 \times 3} \end{pmatrix} \text{ and } M_{\Gamma_a} = |G_{\mathbf{n}}|.$$

- Characteristic variables in direction \mathbf{n} : $\mathbf{w} = T_{\mathbf{n}}^{-1} \mathbf{W}$ (where $G_{\mathbf{n}} = G_x n_x + G_y n_y + G_z n_z = T_{\mathbf{n}} \Lambda_{\mathbf{n}} T_{\mathbf{n}}^{-1}$) used to impose a simple approximation of absorbing boundary conditions at $\partial\Omega$ where \mathbf{n} is the outward normal.

Characteristic variables associated with the direction $\tilde{\mathbf{n}} = (1, 0, 0)$

$$\begin{aligned} w_1 &= -\frac{1}{2}(E_2 - H_3), \quad w_2 = \frac{1}{2}(E_3 + H_2), \quad w_3 = H_1, \\ w_4 &= E_1, \quad w_5 = \frac{1}{2}(E_2 + H_3), \quad w_6 = -\frac{1}{2}(E_3 - H_2) \\ \mathbf{w}_- &= (w_1, w_2)^T, \quad \mathbf{w}_0 = (w_3, w_4)^T, \quad \mathbf{w}_+ = (w_5, w_6)^T. \end{aligned}$$

Relation to a scalar equation

Consider a simplified Maxwell system on the domain $\Omega = [0, 1] \times \mathbb{R}^2$:

- No conductivity: $\sigma = 0$.
- Homogeneous media (ϵ, μ constants) and normalization of the variables: equivalent system with $\epsilon = \mu = 1$.
- No source of current: $\mathbf{J} = 0$.

Maxwell system written in characteristic variables:

$$\begin{aligned}
 (i\omega - \partial_x)w_1 + \frac{1}{2}\partial_z w_3 - \frac{1}{2}\partial_y w_4 &= 0 \\
 (i\omega - \partial_x)w_2 + \frac{1}{2}\partial_y w_3 + \frac{1}{2}\partial_z w_4 &= 0 \\
 i\omega w_3 + \partial_z w_1 + \partial_y w_2 - \partial_z w_5 - \partial_y w_6 &= 0 \\
 i\omega w_4 - \partial_y w_1 + \partial_z w_2 - \partial_y w_5 + \partial_z w_6 &= 0 \\
 (i\omega + \partial_x)w_5 - \frac{1}{2}\partial_z w_3 - \frac{1}{2}\partial_y w_4 &= 0 \\
 (i\omega + \partial_x)w_6 - \frac{1}{2}\partial_y w_3 + \frac{1}{2}\partial_z w_4 &= 0
 \end{aligned}$$

with the characteristic boundary conditions + radiation condition \Rightarrow well-posed problem.

$$\mathbf{w}_+(0, y, z) = \mathbf{r}(y, z), \quad \mathbf{w}_-(1, y, z) = \mathbf{s}(y, z), \quad (y, z) \in \mathbb{R}^2,$$

Equivalence result

Let \mathbf{w} be the characteristic variables. Any component \tilde{w}_j , $j = 1, \dots, 6$, of the characteristic variables of the Maxwell system satisfies, in the interior of $\Omega = [0, 1] \times \mathbb{R}^2$, the Helmholtz equation,

$$-(\omega^2 + \Delta)w_j = 0, \quad j = 1, 2, \dots, 6,$$

together with the boundary conditions

$$\begin{aligned} (\partial_x - i\omega)\tilde{w}_j(0, y, z) &= \tilde{r}_j(y, z), \\ \tilde{w}_j(1, y, z) &= \tilde{s}_j(1, y, z), (y, z) \in \mathbb{R}^2. \end{aligned}$$

Equivalence between Schwarz algorithms

Classical Schwarz algorithm for Maxwell

Decomposition into domains: $\Omega_1 = [0, \alpha] \times \mathbb{R}^2$, $\Omega_2 = [\beta, 1] \times \mathbb{R}^2$

$$i\omega \mathbf{w}^{1,n} + \sum_{l=x,y,z} G_l \partial_l \mathbf{w}^{1,n} = 0, \Omega_1 \quad i\omega \mathbf{w}^{2,n} + \sum_{l=x,y,z} \mathbf{G}_l \partial_l \mathbf{w}^{2,n} = 0, \Omega_2,$$

$$\mathbf{w}_+^{1,n} = \mathbf{r}, \partial\Omega_1 \cap \Omega,$$

$$\mathbf{w}_-^{2,n} = \mathbf{s}, \partial\Omega_2 \cap \Omega,$$

$$\mathbf{w}_-^{1,n} = \mathbf{w}_-^{2,n-1}, \partial\Omega_1 \cap \Omega_2,$$

$$\mathbf{w}_+^{2,n} = \mathbf{w}_+^{1,n-1}, \partial\Omega_2 \cap \Omega_1,$$

Schwarz algorithm for Helmholtz

$$-(\omega^2 + \Delta) \tilde{w}_j^{1,n} = 0, \Omega_1,$$

$$-(\omega^2 + \Delta) \tilde{w}_j^{2,n} = \tilde{0}, \Omega_2,$$

$$(\partial_x - i\omega) \tilde{w}_j^{1,n} = \tilde{r}_j, \partial\Omega_1 \cap \Omega,$$

$$\tilde{w}_j^{2,n} = \tilde{s}_1, \partial\Omega_2 \cap \Omega,$$

$$\tilde{w}_j^{1,n} = \tilde{w}_j^{2,n-1}, \partial\Omega_1 \cap \Omega_2,$$

$$(\partial_x - i\omega) \tilde{w}_j^{2,n} = (\partial_x - i\omega) \tilde{w}_j^{1,n-1}, \partial\Omega_2 \cap \Omega_1.$$

Convergence rate of the algorithm

Proposition Let $\Omega = \mathbb{R}^3$, and consider the Maxwell system in Ω with the radiation condition

$$\lim_{r \rightarrow \infty} r(\mathbf{n} \times \mathbf{E} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H})) = 0,$$

where $r = |\mathbf{x}|$, $\mathbf{n} = \mathbf{x}/|\mathbf{x}|$. Let Ω be decomposed into $\Omega_1 := (-\infty, L) \times \mathbb{R}^2$ and $\Omega_2 := (0, +\infty) \times \mathbb{R}^2$, ($L \geq 0$). For any given initial guess $\mathbf{w}^{1,0} \in (L^2(\Omega_1))^6$, $\mathbf{w}^{2,0} \in (L^2(\Omega_2))^6$, the Schwarz algorithm applied to system converges for all Fourier modes such that $k_y^2 + k_z^2 \neq \omega^2$. The convergence factor is

$$R_{th} = \begin{cases} \left| \frac{\sqrt{\omega^2 - (k_y^2 + k_z^2)} - \omega}{\sqrt{\omega^2 - (k_y^2 + k_z^2)} + \omega} \right|, & \text{for } k_y^2 + k_z^2 < \omega^2, \\ e^{-\sqrt{k_y^2 + k_z^2 - \omega^2} L}, & \text{for } k_y^2 + k_z^2 > \omega^2. \end{cases}$$

Absorbing boundary conditions for Maxwell's equations

The exact **absorbing boundary conditions** for the time harmonic Maxwell equations on the domain $\Omega = (0, 1) \times \mathbb{R}^2$:

$$(\mathbf{w}_+ + \mathcal{S}_1 \mathbf{w}_-)(0, y, z) = 0, \quad (\mathbf{w}_- + \mathcal{S}_2 \mathbf{w}_+)(1, y, z) = 0, \quad (y, z) \in \mathbb{R}^2,$$

where the operators \mathcal{S}_l , $l = 1, 2$, are general, pseudodifferential operators acting in the y and z directions.

Absorbing boundary conditions for Maxwell

Lemma If the operators \mathcal{S}_l , $l = 1, 2$ have the Fourier symbol

$$\mathcal{F}(\mathcal{S}_l) = \frac{1}{(\sqrt{|k|^2 - \omega^2} + i\omega)^2} \begin{bmatrix} k_z^2 - k_y^2 & -2k_y k_z \\ -2k_y k_z & k_y^2 - k_z^2 \end{bmatrix}, \quad j = 1, 2,$$

then the solution of the Maxwell equations in Ω coincides with the restriction on Ω of the solution of the Maxwell system on \mathbb{R}^3 .

Absorbing boundary conditions for Helmholtz's equation

Absorbing boundary conditions for the Helmholtz equation in $\Omega = (0, 1) \times \mathbb{R}^2$

$$(\partial_x - \tilde{\mathcal{S}}_1)\mathbf{u}(0, y, z) = 0, \quad (\partial_x + \tilde{\mathcal{S}}_2)\mathbf{u}(1, y, z) = 0, \quad (y, z) \in \mathbb{R}^2,$$

where $\tilde{\mathcal{S}}_j$ ($j = 1, 2$) are general, pseudodifferential operators acting in the y and z directions.

Absorbing boundary conditions for Helmholtz

Lemma If the operators $\tilde{\mathcal{S}}_l$ ($l = 1, 2$) have the Fourier symbol

$$\tilde{\sigma}_l = \mathcal{F}(\tilde{\mathcal{S}}_l) = \sqrt{|k|^2 - \omega^2}$$

then the solution of Helmholtz equation in Ω coincides with the restriction on Ω of the solution of the Helmholtz equation on \mathbb{R}^3 .

More general interface conditions

$$\Omega_1 : [(\mathbf{w}_- + \mathcal{S}_1 \mathbf{w}_+)(L, y, z)]^{1,n} = [(\mathbf{w}_- + \mathcal{S}_1 \mathbf{w}_+)(L, y, z)]^{2,n-1}, \quad (y, z) \in \mathbb{R}^2,$$

$$\Omega_2 : [(\mathbf{w}_+ + \mathcal{S}_2 \mathbf{w}_-)(0, y, z)]^{2,n} = [(\mathbf{w}_+ + \mathcal{S}_2 \mathbf{w}_-)(0, y, z)]^{1,n-1}, \quad (y, z) \in \mathbb{R}^2.$$

BUT the operators $\mathcal{S}_l, l = 1, 2$, which lead to this optimal performance, are non-local operators \rightarrow the necessity of approximating operators in the transmission conditions.

General form of the interface conditions

The operators \mathcal{S}_1 and \mathcal{S}_2 have the Fourier symbol

$$\sigma_l := \mathcal{F}(\mathcal{S}_l) = \gamma_l \begin{bmatrix} k_z^2 - k_y^2 & -2k_y k_z \\ -2k_y k_z & k_y^2 - k_z^2 \end{bmatrix}, \quad \gamma_l \in \mathbb{C}(k_y, k_z) \quad (l = 1, 2),$$

Equivalence between optimized methods

Different choices of transmission conditions in the optimized Schwarz algorithm

Maxwell equations	Helmholtz
Case 1: Dirichlet/Dirichlet	Desprès conditions
Case 2: Optimized 1 param	Optimized/Desprès
Case 3: Optimized 2 param	Optimized/Optimized
Exact absorbing	Exact absorbing

Asymptotical behavior of the OSM

Five variants of the optimized Schwarz method applied to Maxwell's equations, when the mesh parameter h is small, and the maximum numerical frequency is estimated by $k_{\max} = \frac{C}{h}$, and where $C_\omega = \min(k_+^2 - \omega^2, \omega^2 - k_-^2)$, $\bar{C}_\omega = k_+^2 - \omega^2$.

Convergence rate after optimization

without overlap, $L = 0$		
Case	ρ	parameters
1	1	none
2	$1 - \frac{\sqrt{2}C_\omega^{\frac{1}{4}}}{\sqrt{C}} \sqrt{h}$	$p = \frac{\sqrt{C}C_\omega^{\frac{1}{4}}}{\sqrt{2}\sqrt{h}}$
3	$1 - \frac{\sqrt{2}(\bar{C}_\omega)^{\frac{1}{4}}}{\sqrt{C}} \sqrt{h}$	$p = \frac{\sqrt{C}(\bar{C}_\omega)^{\frac{1}{4}}}{\sqrt{2}\sqrt{h}}$
4	$1 - \frac{C_\omega^{\frac{1}{8}}}{C^{\frac{1}{4}}} h^{\frac{1}{4}}$	$p_1 = \frac{C_\omega^{\frac{3}{8}} \cdot C^{\frac{1}{4}}}{2 \cdot h^{\frac{1}{4}}}, p_2 = \frac{C_\omega^{\frac{1}{8}} \cdot C^{\frac{3}{4}}}{h^{\frac{3}{4}}}$
5	$1 - \frac{(\bar{C}_\omega)^{\frac{1}{8}}}{C^{\frac{1}{4}}} h^{\frac{1}{4}}$	$p_1 = \frac{(\bar{C}_\omega)^{\frac{3}{8}} \cdot C^{\frac{1}{4}}}{2 \cdot h^{\frac{1}{4}}}, p_2 = \frac{(\bar{C}_\omega)^{\frac{1}{8}} \cdot C^{\frac{3}{4}}}{h^{\frac{3}{4}}}$

Comparison of the different methods

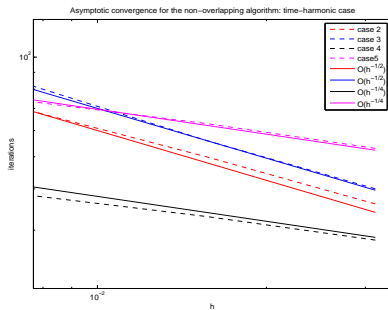
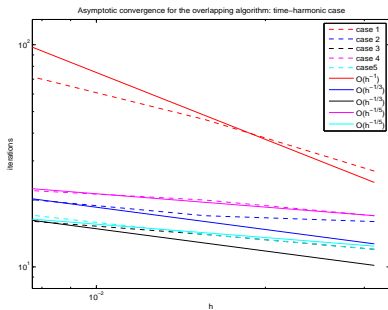
- Two-dimensional case: transverse electric waves
- unit square decomposed into two subdomains $\Omega_1 = (0, \beta) \times (0, 1)$ and $\Omega_2 = (\alpha, 1) \times (0, 1)$, where $0 < \alpha \leq \beta < 1$
- tolerance fixed at $\varepsilon = 10^{-6}$

Non-overlapping and overlapping optimized methods

	with overlap, $L = h$				without overlap, $L = 0$			
h	1/16	1/32	1/64	1/128	1/16	1/32	1/64	1/128
Case 1	18	27	46	71	-	-	-	-
Case 2	16	16	17	20	28	36	50	68
Case 3	10	12	14	16	31	40	56	81
Case 4	17	17	20	22	26	28	33	38
Case 5	10	12	14	17	41	53	63	73

Comparison of the different methods

Theoretical and numerical asymptotics for overlapping and non-overlapping optimized methods

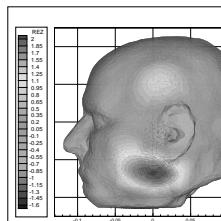
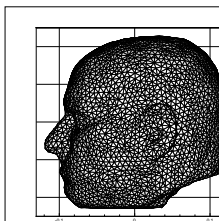


Preliminary three-dimensional results: a bioelectromagnetism example

Propagation of a plane wave in realistic geometrical models of head tissues: collaboration with S. Lanteri (INRIA Sophia-Antipolis)

Table: Characteristics of the tetrahedral meshes.

Mesh	# tetrahedra	L_{\min} (m)	L_{\max} (m)	L_{avg} (m)
M1	361,848	0.00185	0.04537	0.01165
M2	1,853,832	0.00158	0.02476	0.00693



Conclusions

- derivation of all possible optimized conditions for first order Maxwell system and optimization whenever no equivalence with scalar algorithm was found.
- validation on a simple 2d geometry and implementation in three-dimensions.

Ongoing work

- The use of optimized interface conditions with high order discretization methods (DG methods) in collaboration with R. Perrussel (Lab. Ampère, Lyon) and S. Lanteri (INRIA).
- Promising results concerning the robustness of optimized parameters with respect to the polynomial order (2d numerical simulations).

Future works

- Optimization of the parameters in the general case by taking into account the conductivity and application to realistic three-dimensional bioelectromagnetism simulations.