

Hybrid iterative-direct domain decomposition based solvers for the time-harmonic Maxwell equations

1st workshop of the joint INRIA-UIUC laboratory for Petascale Computing

Victorita Dolean¹, Mohamed El Bouajaji², Stéphane Lanteri² and
Ronan Perrussel³

¹J.A. Dieudonné Mathematics Laboratory (UMR 6621)
University of Nice/Sophia Antipolis, France

²NACHOS project-team, INRIA Sophia Antipolis - Méditerranée research center, France

³Ampère Laboratory (UMR 5005), Ecole Centrale de Lyon, France

June 10-12 2009, Hôtel Concorde Montparnasse, Paris

Opening: NACHOS project-team

Scientific objectives

- Design, analysis and validation of numerical methods and high performance resolution algorithms for the computer simulation of evolution problems in **complex domains** and **heterogeneous media**
- Research directions
 - High-order finite element discretization methods on simplicial meshes
 - Hybrid explicit/implicit time integration strategies
 - Domain decomposition resolution algorithms
 - High performance computing related aspects

Computational electromagnetics

- **System of Maxwell equations**
- Interaction of EM fields with biological tissues
- Interaction of charged particles with EM fields (Vlasov/Maxwell equations)

Computational geoseismics

- **System of elastodynamic equations**
- Propagation of seismic waves in heterogeneous geological media
- Numerical modeling of planar and non-planar faults (earthquake dynamics)

Opening: context and goal

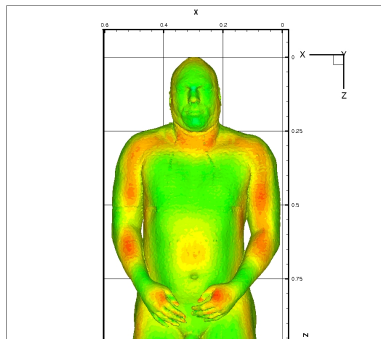
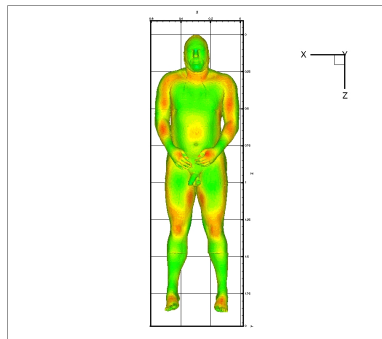
- Modeling issues
 - Electromagnetic wave propagation in heterogeneous media
 - Time-harmonic regime, high frequency (100 MHz to 3 GHz)
 - Irregularly shaped domains, complex geometrical features
- Target applications
 - Human exposure to electromagnetic fields
 - Medical applications (in-body miniaturized sensor/antenna design for wireless monitoring systems)
- Numerical ingredients
 - Unstructured meshes (triangles in 2D, tetrahedra in 3D)
 - High order Discontinuous Galerkin DG discretization methods
- Goal of this study
 - Design of domain decomposition based hybrid iterative-direct solvers for algebraic systems resulting from DG discretization
 - Part of this work is undertaken in the context of the PhyLeaS associate team

Opening: context and goal

- Modeling issues
 - Electromagnetic wave propagation in heterogeneous media
 - Time-harmonic regime, high frequency (100 MHz to 3 GHz)
 - Irregularly shaped domains, complex geometrical features
- Target applications
 - Human exposure to electromagnetic fields
 - Medical applications (in-body miniaturized sensor/antenna design for wireless monitoring systems)
- Numerical ingredients
 - Unstructured meshes (triangles in 2D, tetrahedra in 3D)
 - High order Discontinuous Galerkin DG discretization methods
- Goal of this study
 - Design of domain decomposition based hybrid iterative-direct solvers for algebraic systems resulting from DG discretization
 - Part of this work is undertaken in the context of the PhyLeaS associate team

Opening: example application

- Human exposure to electromagnetic fields
 - Multi-parametric studies, uncertainty quantification (source position, morphology, electromagnetic parameters)



- Plane wave exposure ($F=2.14$ GHz)
- Tetrahedral mesh: 899,872 vertices and 5,335,521 elements
- Discretization by a DG- \mathbb{P}_2 method: 320,131,260 d.o.f

Opening: related works

- Full set of Maxwell equations
- High order finite element discretization
- Domain decomposition solver
 - J.J.W. van der Vegt, M.A. Botchev *at al.*, University of Twente
 - High order edge element, *hp*-adaptivity, sparse direct solver
 - P. Solin, *h*-FEM group, University of Nevada
 - High order edge element, *hp*-adaptivity, sparse direct solver
 - J. Zou *at al.*, The Chinese University of Hong Kong
 - Low order edge element, non-overlapping DD solver
 - J.-F. Lee *at al.*, Ohio State University
 - High order edge element, non-overlapping DD solver, non-matching grid
 - Schwarz algorithm with Robin interface conditions
 - A. Schädle, F. Schmidt *at al.*, ZIB
 - Schwarz algorithm with transparent interface conditions approximated by a PML method
 - High order edge element (mixed triangular/quadrangular mesh)
 - Scattering by periodic structures

Opening: related works

- J. Jin *at al.*, UIUC, Department of Electrical and Computer Engineering
 - Full set of Maxwell equations
 - Time-harmonic and time-domain formulations
 - High order edge element discretization
 - Domain decomposition solver
- Mini-symposium at the 19th International Conference on Domain Decomposition Methods (DD19), August 17-22, 2009, Zhangjiajie of China
 - Domain decomposition methods for electromagnetic wave propagation problems
 - J. Jin
 - J.-F. Lee, Ohio State University
ElectroScience Laboratory, ECE Department
 - J. Zou, The Chinese University of Hong Kong
Department of Mathematics
 - Wei Hong, Southeast University, Nanjing
State Key Laboratory of Millimeter Waves
 - M. Gander, University of Geneva, Mathematics Section

Opening: related works

- J. Jin *et al.*, UIUC, Department of Electrical and Computer Engineering
 - Full set of Maxwell equations
 - Time-harmonic and time-domain formulations
 - High order edge element discretization
 - Domain decomposition solver
- Mini-symposium at the 19th International Conference on Domain Decomposition Methods (DD19), August 17-22, 2009, Zhangjiajie of China
[Domain decomposition methods for electromagnetic wave propagation problems](#)
 - J. Jin
 - J.-F. Lee, Ohio State University
ElectroScience Laboratory, ECE Department
 - J. Zou, The Chinese University of Hong Kong
Department of Mathematics
 - Wei Hong, Southeast University, Nanjing
State Key Laboratory of Millimeter Waves
 - M. Gander, University of Geneva, Mathematics Section

- 1 The time-harmonic Maxwell equations
- 2 Discontinuous Galerkin discretization methods
 - Basic properties
 - Formulation
 - Matricial system
 - Numerical results for the 2D time-harmonic Maxwell equations
- 3 Domain decomposition solver
 - Formulation in the continuous case
 - Formulation in the discrete case
 - 3D application
- 4 Closure

The time-harmonic Maxwell equations

$$\begin{cases} \varepsilon i\omega \mathbf{E} - \text{rot}(\mathbf{H}) = 0, \\ \mu i\omega \mathbf{H} + \text{rot}(\mathbf{E}) = 0 \end{cases}$$

- $\mathbf{E} = \mathbf{E}(\mathbf{x})$: electric field
- $\mathbf{H} = \mathbf{H}(\mathbf{x})$: magnetic field
- $\varepsilon = \varepsilon(\mathbf{x})$: electric permittivity
- $\mu = \mu(\mathbf{x})$: magnetic permeability
- $\sigma = \sigma(\mathbf{x})$: electric conductivity
- Vacuum impedance: $z_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}}$
- Boundary conditions
 - PEC boundary (Γ^m): $\mathbf{n} \times \mathbf{E} = 0$
 - Absorbing boundary (Γ^a): $\mathbf{n} \times \mathbf{E} + \mathbf{z}\mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^\infty + \mathbf{z}\mathbf{n} \times (\mathbf{n} \times \mathbf{H}^\infty)$

The time-harmonic Maxwell equations

Pseudo-conservative system form

$$Q\mathbf{W}_t + \nabla \cdot \mathbf{F}(\mathbf{W}) = \mathbf{J}$$

$$F_x(\mathbf{W}) = \begin{bmatrix} 0_{3 \times 3} & N_x \\ -N_x & 0_{3 \times 3} \end{bmatrix} \mathbf{W} = {}^t(0, H_z, -H_y, 0, -E_z, E_y)$$

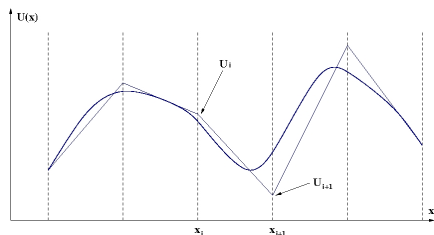
$$F_y(\mathbf{W}) = \begin{bmatrix} 0_{3 \times 3} & N_y \\ -N_y & 0_{3 \times 3} \end{bmatrix} \mathbf{W} = {}^t(-H_z, 0, H_x, E_z, 0, -E_x)$$

$$F_z(\mathbf{W}) = \begin{bmatrix} 0_{3 \times 3} & N_z \\ -N_z & 0_{3 \times 3} \end{bmatrix} \mathbf{W} = {}^t(H_y, -H_x, 0, -E_y, E_x, 0)$$

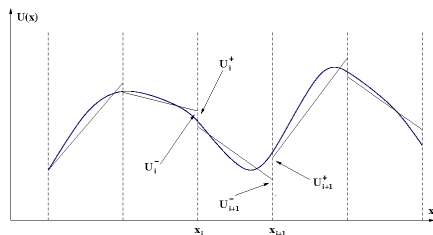
$$N_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad N_y = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad N_z = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Discontinuous Galerkin discretization methods

Basic properties



FE, continuous P1 interpolation



DG, local P1 interpolation

- Can easily deal with discontinuous coefficients and solutions
- Can handle unstructured, non-conforming meshes
- High order accurate methods with compact stencils
- Naturally lead to discretization (h -) and interpolation order (p -) adaptivity
- Amenable to efficient parallelization
- **But lead to larger problems compared to continuous finite element methods**

Discontinuous Galerkin discretization methods

Basic properties

DG for electromagnetic wave propagation in heterogeneous media

- The basic support of the DG method is the **element** (triangle in 2D and tetrahedron in 3D)
- Heterogeneity is ideally treated at the element level
 - Mesh generation process is simplified
 - Discontinuities occur at material (i.e element) interfaces
- Wavelength varies with ϵ and μ
 - For a given mesh density, approximation order can be set on an element basis to fit to the local frequency resolution criteria

Discretization of irregularly shaped domains

- Unstructured meshes are preferred
- Local refinement is made easier by allowing non-conformity
- Non-conformity opens the route to the coupling of different discretization methods (e.g structured/unstructured)

Discontinuous Galerkin discretization methods

Formulation

- Triangulation: $\mathcal{T}_h = \bigcup_{i=1}^N \tau_i$
- Assume $\mathbf{J} = 0$ for simplicity of the presentation
- φ is a sufficiently regular test function
- $\mathbf{n}_{ij} = {}^t(n_{ij}^{x_1}, n_{ij}^{x_2}, n_{ij}^{x_3})$

$$\int_{\tau_i} \varphi (\mathbf{i}\omega \mathbf{Q}\mathbf{W} + \nabla \cdot \mathbf{F}(\mathbf{W})) \, d\mathbf{x} = 0$$

$$\Leftrightarrow \int_{\tau_i} \mathbf{i}\omega \mathbf{Q}\mathbf{W} \varphi \, d\mathbf{x} - \int_{\tau_i} \nabla \varphi \cdot \mathbf{F}(\mathbf{W}) \, d\mathbf{x} + \int_{\partial\tau_i} (\mathbf{F}(\mathbf{W}) \cdot \mathbf{n}) \varphi \, d\sigma = 0$$

- Local set of degrees of freedom for τ_i : $\mathbf{W}_{ij} \in \mathbf{R}^6$

- Local approximation: $\mathbf{W}_i(\mathbf{x}) \in \mathcal{P}_i = \mathbb{P}_m[\tau_i]$ and $\mathbf{W}_i(\mathbf{x}) = \sum_{j=1}^{d_i} \mathbf{W}_{ij} \varphi_{ij}(\mathbf{x})$

$$\Leftrightarrow \mathbf{i}\omega \mathbf{Q}_i \int_{\tau_i} \mathbf{W}_i \varphi \, d\mathbf{x} - \int_{\tau_i} \nabla \varphi \cdot \mathbf{F}(\mathbf{W})_i \, d\mathbf{x} + \sum_{j \in \mathcal{V}_i} \int_{a_{ij}} (\mathbf{F}(\mathbf{W}) \cdot \mathbf{n}_{ij}) \varphi \, d\sigma = 0$$

Discontinuous Galerkin discretization methods

Formulation

$$F(\mathbf{W})_i \equiv F(\mathbf{W})|_{\tau_i} \quad \text{and} \quad Q_i = \begin{bmatrix} \varepsilon_i I_{3 \times 3} & 0_{3 \times 3} \\ 0_{3 \times 3} & \mu_i I_{3 \times 3} \end{bmatrix}$$

- $\phi_i = (\varphi_{i1}, \varphi_{i2}, \dots, \varphi_{id_i})$
- $\mathcal{V}_i = \{j | \tau_i \cap \tau_j \neq \emptyset\}$ and $a_{ij} = \tau_i \cap \tau_j$
- Calculation of the boundary term on a_{ij} : **numerical flux**
 - Centered scheme : $F(\mathbf{W})|_{a_{ij}} \approx \frac{F(\mathbf{W})_i + F(\mathbf{W})_j}{2}$
 - Upwind scheme : $F(\mathbf{W})|_{a_{ij}} \approx F^+(\mathbf{W})_i + F^-(\mathbf{W})_j$
- Integration by parts + algebraic manipulations

$$\begin{aligned} \sum_{j \in \mathcal{V}_i} \int_{a_{ij}} (F(\mathbf{W}) \cdot \mathbf{n}_{ij}) \varphi d\sigma &= \frac{1}{2} \int_{\tau_i} ((\nabla \cdot F(\mathbf{W}))_i) \varphi + \nabla \varphi \cdot F(\mathbf{W})_i dx \\ &+ \frac{1}{2} \sum_{j \in \mathcal{V}_i} \int_{a_{ij}} (F(\mathbf{W})_j \cdot \mathbf{n}_{ij}) \varphi d\sigma \end{aligned}$$

Discontinuous Galerkin discretization methods

Formulation

Weak formulation

$$\begin{aligned} i\omega Q_i \int_{\tau_i} \mathbf{W}_i \varphi dx &+ \frac{1}{2} \int_{\tau_i} \left(\left(\sum_{k=1}^3 \partial_{x_k} \Psi^{x_k} \mathbf{W}_i \right) \varphi - \sum_{k=1}^3 \partial_{x_k} \varphi \Psi^{x_k} \mathbf{W}_i \right) dx \\ &+ \frac{1}{2} \sum_{j \in \mathcal{V}_i} \int_{a_{ij}} M_{ij} \mathbf{W}_j \varphi d\sigma = 0 \end{aligned}$$

$$\left\{ \begin{array}{l} \Psi^{x_k} = \begin{bmatrix} \mathbf{0}_{3 \times 3} & N_{x_k} \\ -N_{x_k} & \mathbf{0}_{3 \times 3} \end{bmatrix} \\ M_n = \sum_{k=1}^3 n^{x_k} \Psi^{x_k} = \begin{bmatrix} \mathbf{0}_{3 \times 3} & N_n \\ -N_n & \mathbf{0}_{3 \times 3} \end{bmatrix} \quad \text{and} \quad M_{ij} = M_{n_{ij}} \\ N_n = \sum_{k=1}^3 n^{x_k} N_{x_k} \\ N_{ij} = N_{n_{ij}} \end{array} \right.$$

Discontinuous Galerkin discretization methods

Matricial system

Local algebraic system of equations

$$\begin{aligned} 2i\omega \mathcal{Y}_i \mathbf{W}_i &+ \sum_{k=1}^3 \mathcal{Y}_i^{x_k} \mathbf{W}_i + \sum_{a_{ij} \in \mathcal{F}_d^i} \mathcal{Y}_{ij} \mathbf{W}_j \\ &+ \sum_{a_{ij} \in \mathcal{F}_m^i} \mathcal{Y}_{im} \mathbf{W}_i + \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{ia} \mathbf{W}_i = - \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{i\infty} \mathbf{W}_i^\infty \end{aligned}$$

- $\mathbf{W}_i = {}^t(\mathbf{W}_{i1}, \mathbf{W}_{i2}, \dots, \mathbf{W}_{id_i})$, \mathbf{W}_i is a $6d_i \times 1$ vector
- $\mathcal{F}^i = \mathcal{F}_d^i \cup \mathcal{F}_a^i \cup \mathcal{F}_m^i$: set of faces of τ_i

Global algebraic system of equations: $\mathbf{A}\mathbf{W} = \mathbf{b}$

$$\begin{cases} A_{ij} &= 2i\omega \mathcal{Y}_i + \sum_{k=1}^3 \mathcal{Y}_i^{x_k} + \sum_{a_{ij} \in \mathcal{F}_m^i} \mathcal{Y}_{im} + \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{ia} \\ A_{ij} &= \mathcal{Y}_{ij}, \text{ for } j \in \mathcal{F}_d^i, \quad \mathbf{b}_i = \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{i\infty} \mathbf{W}_i^\infty \end{cases}$$

- A_{ij} and A_{ji} are $6d_i \times 6d_j$ matrices

Discontinuous Galerkin discretization methods

Matricial system

Local algebraic system of equations

$$\begin{aligned} 2i\omega \mathcal{Y}_i \mathbf{W}_i &+ \sum_{k=1}^3 \mathcal{Y}_i^{x_k} \mathbf{W}_i + \sum_{a_{ij} \in \mathcal{F}_d^i} \mathcal{Y}_{ij} \mathbf{W}_j \\ &+ \sum_{a_{ij} \in \mathcal{F}_m^i} \mathcal{Y}_{im} \mathbf{W}_i + \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{ia} \mathbf{W}_i = - \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{i\infty} \mathbf{W}_i^\infty \end{aligned}$$

- $\mathbf{W}_i = {}^t(\mathbf{W}_{i1}, \mathbf{W}_{i2}, \dots, \mathbf{W}_{id_i})$, \mathbf{W}_i is a $6d_i \times 1$ vector
- $\mathcal{F}^i = \mathcal{F}_d^i \cup \mathcal{F}_a^i \cup \mathcal{F}_m^i$: set of faces of τ_i

Global algebraic system of equations: $\mathbf{A}\mathbf{W} = \mathbf{b}$

$$\begin{cases} A_{ii} &= 2i\omega \mathcal{Y}_i + \sum_{k=1}^3 \mathcal{Y}_i^{x_k} + \sum_{a_{ij} \in \mathcal{F}_m^i} \mathcal{Y}_{im} + \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{ia} \\ A_{ij} &= \mathcal{Y}_{ij}, \text{ for } j \in \mathcal{F}_d^i, \quad \mathbf{b}_i = \sum_{a_{ij} \in \mathcal{F}_a^i} \mathcal{Y}_{i\infty} \mathbf{W}_i^\infty \end{cases}$$

- A_{ii} and A_{ij} are $6d_i \times 6d_i$ matrices

Discontinuous Galerkin discretization methods

Numerical results for the 2D time-harmonic Maxwell equations

$$\left\{ \begin{array}{l} \mu i \omega H_x + \frac{\partial E_z}{\partial y} = 0 \\ \mu i \omega H_y - \frac{\partial E_z}{\partial x} = 0 \\ \varepsilon i \omega E_z - \frac{\partial H_y}{\partial x} + \frac{\partial H_x}{\partial y} = 0 \end{array} \right.$$

- DGTH- \mathbb{P}_p method based on Lagrange (nodal) interpolation
 - Triangular mesh
 - Sparse block matrix, $3n_p \times 3n_p$ (with $n_p = ((p+1)(p+2))/2$)
 - MUMPS multifrontal sparse matrix solver
(P.R. Amestoy, I.S. Duff and J.-Y. L'Excellent, CMAME, Vol. 184, 2000)

Discontinuous Galerkin discretization methods

Numerical results for the 2D time-harmonic Maxwell equations

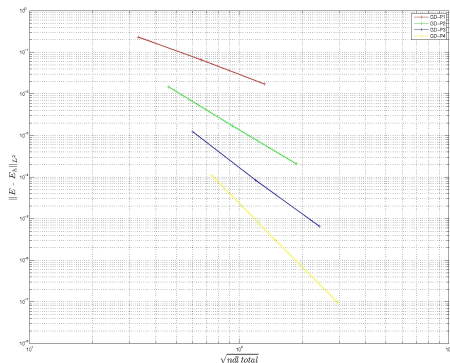
- Plane wave in vacuum, $F=600$ MHz
- Non-uniform triangular mesh
 - h_m and h_M : minimal and maximal edge length
 - CPU: factorization + solution time (Intel Xeon/2.33 GHz)

| # triangles | n_z | h_m/h_M | Method | CPU | RAM (LU/total) |
|-------------|------------|-------------|--------------------|-----------|----------------|
| 366 | 35,466 | 0.021/0.130 | DG- \mathbb{P}_1 | < 1.0 sec | 1 MB/ 6 MB |
| - | 108,120 | - | DG- \mathbb{P}_2 | < 1.0 sec | 3 MB/ 16 MB |
| - | 295,152 | - | DG- \mathbb{P}_3 | < 1.0 sec | 6 MB/ 33 MB |
| - | 644,922 | - | DG- \mathbb{P}_4 | < 2.0 sec | 12 MB/ 60 MB |
| 1,464 | 142,440 | 0.011/0.066 | DG- \mathbb{P}_1 | < 1.0 sec | 5 MB/ 26 MB |
| - | 433,200 | - | DG- \mathbb{P}_2 | < 1.0 sec | 15 MB/ 69 MB |
| - | 1,182,336 | - | DG- \mathbb{P}_3 | 2.1 sec | 32 MB/ 149 MB |
| - | 2,582,712 | - | DG- \mathbb{P}_4 | 4.0 sec | 57 MB/ 266 MB |
| 5,856 | 570,912 | 0.005/0.033 | DG- \mathbb{P}_1 | 1.8 sec | 28 MB/ 125 MB |
| - | 1,734,240 | - | DG- \mathbb{P}_2 | 4.7 sec | 76 MB/ 326 MB |
| - | 4,732,800 | - | DG- \mathbb{P}_3 | 10.0 sec | 156 MB/ 682 MB |
| - | 10,336,896 | - | DG- \mathbb{P}_4 | 20.6 sec | 274 MB/1217 MB |

Discontinuous Galerkin discretization methods

Numerical results for the 2D time-harmonic Maxwell equations

- Numerical convergence: **non-uniform** triangular mesh

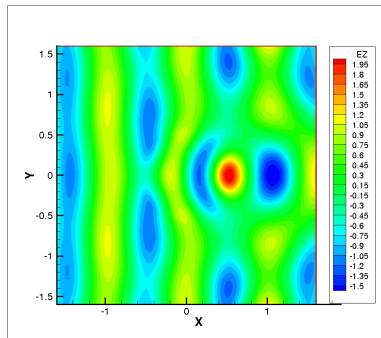
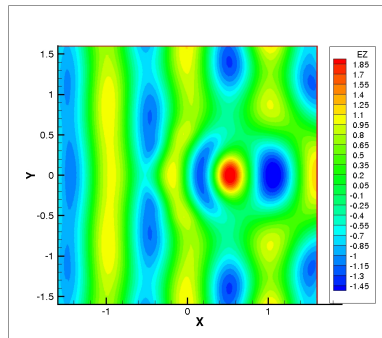


| | P1 | P2 | P3 | P4 |
|-------|-----|-----|-----|-----|
| E_z | 1.9 | 3.0 | 3.8 | 5.1 |
| H | 1.2 | 2.2 | 2.9 | 4.0 |

Discontinuous Galerkin discretization methods

Numerical results for the 2D time-harmonic Maxwell equations

- Scattering of a plane wave by a dielectric cylinder, $F=300$ MHz



Contour lines of E_z

Left: exact solution - Right: DG- \mathbb{P}_2 method

Discontinuous Galerkin discretization methods

Numerical results for the 2D time-harmonic Maxwell equations

- Scattering of a plane wave by a dielectric cylinder, $F=300$ MHz
 - # vertices = 4,108 and # elements = 8,054
 - h_m and h_M : minimal and maximal edge length
 - CPU: factorization + solution time (Intel Xeon/2.33 GHz)

| n_z | h_m/h_M | Method | CPU | RAM (LU/total) |
|-----------|-----------------|--------------------|----------|----------------|
| 791,522 | 0.00071/0.14020 | DG- \mathbb{P}_1 | 3.0 sec | 50 MB/ 179 MB |
| 2,402,104 | - | DG- \mathbb{P}_2 | 13.4 sec | 149 MB/ 463 MB |
| 6,543,232 | - | DG- \mathbb{P}_3 | 99.6 sec | 366 MB/ 964 MB |

Domain decomposition solver

Formulation in the continuous case

Time harmonic Maxwell system

$$\mathcal{L}\mathbf{W} = i\omega G_0\mathbf{W} + G_x\partial_x\mathbf{W} + G_y\partial_y\mathbf{W} + G_z\partial_z\mathbf{W} = 0$$

- Flux matrices

$$G_l = \begin{bmatrix} 0_{3 \times 3} & N_l \\ -N_l & 0_{3 \times 3} \end{bmatrix} \quad \text{for } l = x, y, z \quad \text{and with } {}^t N_l = -N_l$$

- Property : for any $\mathbf{n} = {}^t(n_x, n_y, n_z)$ with $\|\mathbf{n}\| = 1$,

$$C(\mathbf{n}) = G_0^{-1}(n_x G_x + n_y G_y + n_z G_z) \quad \text{is diagonalizable}$$

$$C(\mathbf{n}) = T(\mathbf{n})\Lambda(\mathbf{n})T^{-1}(\mathbf{n})$$

$$\text{Eigenvalues : } \lambda_{1,2} = -c, \quad \lambda_{3,4} = 0, \quad \lambda_{5,6} = c \quad \text{with } c = \frac{1}{\sqrt{\varepsilon\mu}}$$

Domain decomposition solver

Formulation in the continuous case

Schwarz algorithm

- $\Omega = \bigcup_{j=1}^{N_s} \Omega_j$, $\mathbf{W}^j = \mathbf{W}|_{\Omega_j}$
- $\Gamma = \Gamma_a$ (for the presentation)
- Overlapping subdomains

$$\begin{cases} \mathcal{L}\mathbf{W}^{j,p+1} & = 0 \text{ in } \Omega_j \\ \mathcal{B}_{\mathbf{n}_{jl}}\mathbf{W}^{j,p+1} & = \mathcal{B}_{\mathbf{n}_{jl}}\mathbf{W}^{l,p} \text{ on } \Gamma_{jl} = \partial\Omega_j \cap \bar{\Omega}_l \\ \mathcal{G}_{\mathbf{n}}^-\mathbf{W}^{j,p+1} & = \mathcal{G}_{\mathbf{n}}^-\mathbf{W}_{\text{inc}} \text{ on } \Omega_j \cap \Gamma_a \end{cases}$$

Classical (natural) interface conditions

$$\mathcal{B}_{\mathbf{n}} \equiv \mathcal{G}_{\mathbf{n}}^-$$

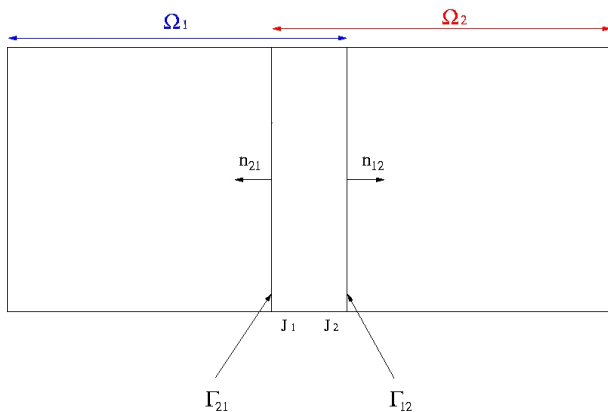
$$\mathcal{G}_{\mathbf{n}}^-\mathbf{W} \iff \mathbf{n} \times \mathbf{E} + \mathbf{z}\mathbf{n} \times (\mathbf{n} \times \mathbf{H}) \quad (\text{impedance condition})$$

Domain decomposition solver

Convergence analysis (2D case) in the non-conductive case

- Two subdomain case and $\Omega = \mathbb{R}^2$

$$\Omega_1 =]-\infty, b[\times \mathbb{R} \quad \text{and} \quad \Omega_2 =]a, +\infty[\times \mathbb{R} \quad \text{with} \quad a \leq b$$



Domain decomposition solver

Convergence analysis (2D case) in the non-conductive case

- V. Dolean, M.J. Gander and L. Gerardo-Giorda, SISC, to appear (2009)
- Fourier analysis

$$\widehat{\mathcal{E}}^{j,p}(x, k) = \mathcal{F}_y(\mathcal{E}^{j,p}) = \int_{\mathbb{R}} e^{-iky} \mathcal{E}^{j,p}(x, y) dy$$

with $\mathcal{E}^{j,p} = \mathbf{U}^{j,p} - \mathbf{U}_{|\Omega_j}^{\text{ex}}$ where $\mathbf{U} = T^{-1}\mathbf{W}$ (characteristic variables)

Convergence rate

$$\rho(k, \delta) = \left| \left(\frac{\sqrt{k^2 - \omega^2} - i\omega}{\sqrt{k^2 - \omega^2} + i\omega} \right) e^{-\delta\sqrt{k^2 - \omega^2}} \right|$$

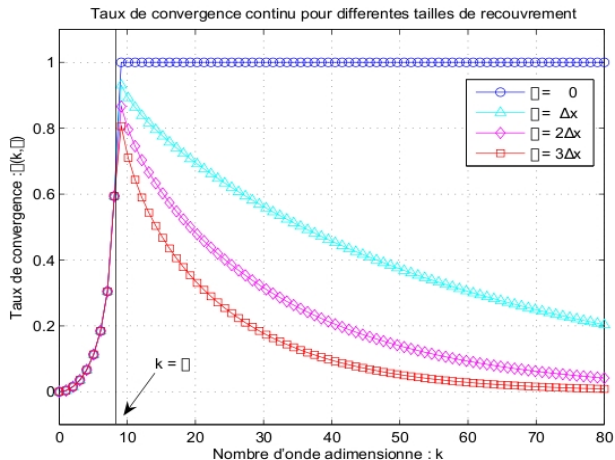
with $\delta = b - a$

$$\rho(k, \delta) = \begin{cases} \left| \frac{\sqrt{\omega^2 - k^2} - \omega}{\sqrt{\omega^2 - k^2} + \omega} \right| & \text{si } |k| < \omega \text{ (propagative modes)} \\ e^{-\delta\sqrt{k^2 - \omega^2}} & \text{si } |k| \geq \omega \text{ (evanescent modes)} \end{cases}$$

Domain decomposition solver

Convergence analysis (2D case) in the non-conductive case

Convergence rate as a function of the frequency parameter



Domain decomposition resolution algorithms

Schwarz algorithm: algebraic formulation

- Global system (two-subdomain case)

$$\begin{pmatrix} A_1 & 0 & R_1 & 0 \\ 0 & A_2 & 0 & R_2 \\ 0 & -B_2 & \text{Id} & 0 \\ -B_1 & 0 & 0 & \text{Id} \end{pmatrix} \begin{pmatrix} \mathbf{W}_h^1 \\ \mathbf{W}_h^2 \\ \lambda_h^1 \\ \lambda_h^2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_h^1 \\ \mathbf{f}_h^2 \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}$$

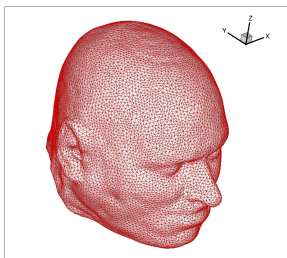
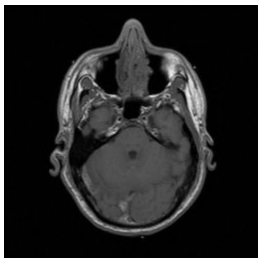
- Interface system: $\mathcal{T}_h \lambda_h = \mathbf{g}_h$

$$\mathcal{T}_h = \begin{pmatrix} \text{Id} & B_2 A_2^{-1} R_2 \\ B_1 A_1^{-1} R_1 & \text{Id} \end{pmatrix} \quad \text{and} \quad \mathbf{g}_h = \begin{pmatrix} B_2 A_2^{-1} F^2 \\ B_1 A_1^{-1} F^1 \end{pmatrix}$$

- Schwarz iteration $\Leftrightarrow \lambda_h^{p+1} = (\text{Id} - \mathcal{T}_h) \lambda_h^p + \mathbf{d}_h$
- Accelerated iteration \Rightarrow Krylov method

Domain decomposition resolution algorithms

3D application



Geometric models

- Built from segmented medical images
- Extraction of surfacic (triangular) meshes of the tissue interfaces using specific tools
 - Marching cubes + adaptive isotropic surface remeshing
 - Delaunay refinement
- Generation of tetrahedral meshes using a Delaunay/Voronoi tool

Domain decomposition resolution algorithms

3D application

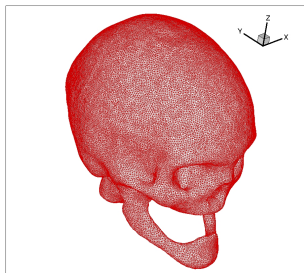
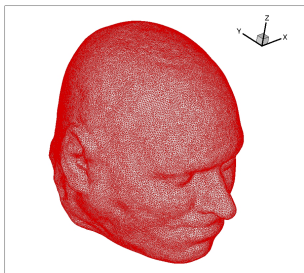
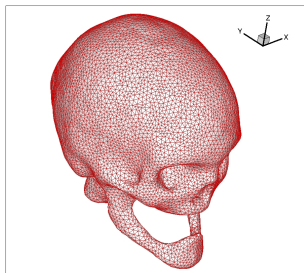
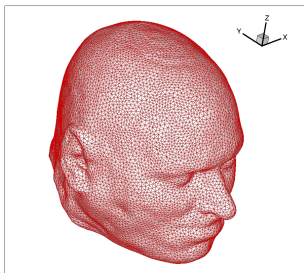
- Plane wave exposure: $F=1.8$ GHz
- Characteristics of the tetrahedral meshes

| Mesh | # vertices | # tetrahedra | L_{\min} (mm) | L_{\max} (mm) | L_{avg} (mm) |
|------|------------|--------------|-----------------|-----------------|-----------------------|
| M1 | 188,101 | 1,118,952 | 9.04 | 23.86 | 9.09 |
| M2 | 309,599 | 1,853,832 | 1.15 | 24.76 | 6.93 |

- Solution methods
 - Interface system
 - BiCGstab(ℓ) (G.L.G. Sleijpen and D.R. Fokkema, ETNA, Vol.1, 1993)
 - No preconditioner, $\ell = 6$
 - Local systems
 - Sparse direct solvers: MUMPS or PasTiX
 - Mixed arithmetic strategy: LU in 32 bit + iterative refinement
- Hardware platform
 - Bull Novascale 3045 system of the CEA/CCRT center (Centre de Calcul Recherche et Technologie)
 - Intel Itanium 2/1.6 GHz, InfiniBand

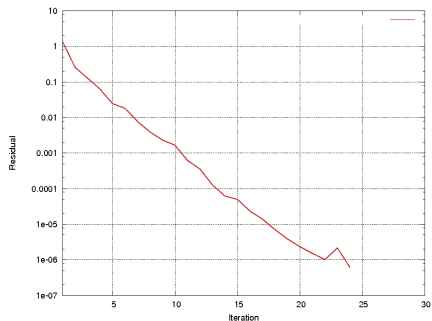
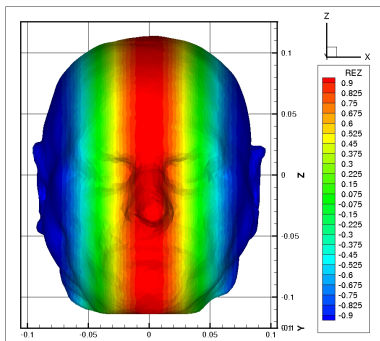
Domain decomposition resolution algorithms

3D application



Domain decomposition resolution algorithms

3D application: homogeneous propagation media

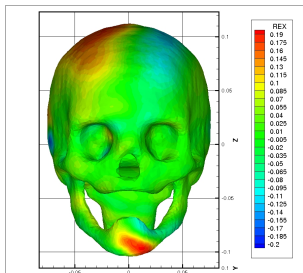
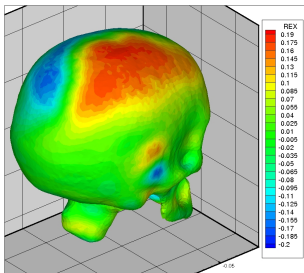
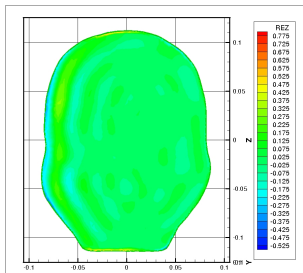
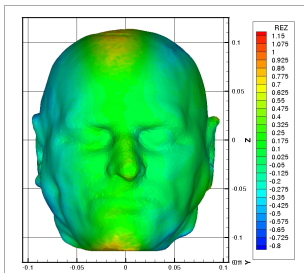


| Mesh | Method | # d.o.f | N_s | # it | CPU (min/max) | Elapsed time |
|------|----------------------|------------|-------|------|-------------------|--------------|
| M1 | DGTH- \mathbb{P}_1 | 26,854,848 | 160 | 24 | 1204 sec/1209 sec | 1210 sec |

| | | |
|---------------|----------------------|---------------------|
| LU (min/max) | CPU factor (min/max) | Elapsed time factor |
| 2.1 GB/3.1 GB | 493 sec/494 sec | 495 sec |

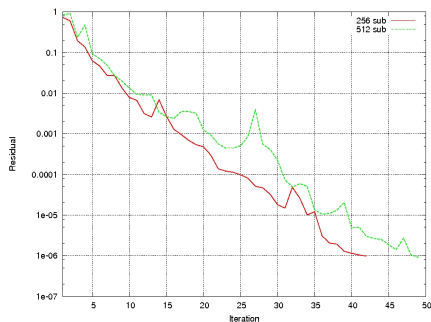
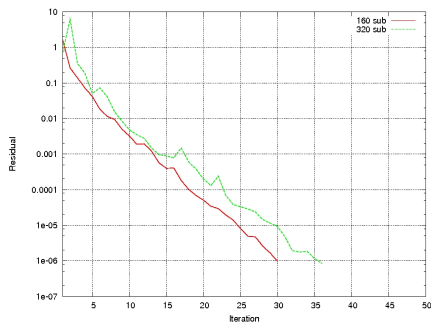
Domain decomposition resolution algorithms

3D application: heterogeneous propagation media



Domain decomposition resolution algorithms

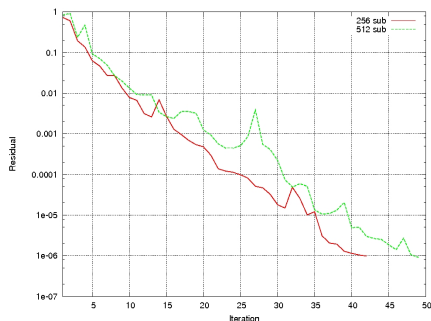
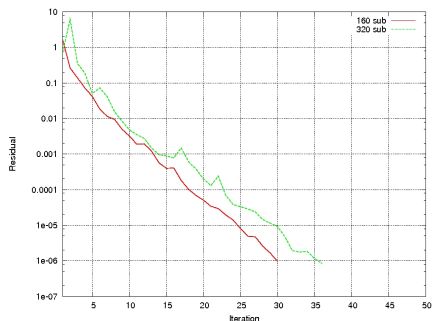
3D application: heterogeneous propagation media



| Mesh | Method | # d.o.f | N_s | # it | CPU (min/max) | Elapsed time |
|------|----------------------|------------|-------|------|-------------------|---------------|
| M1 | DGTH- \mathbb{P}_1 | 26,854,848 | 160 | 30 | 1311 sec/1313 sec | 1314 sec |
| - | - | - | 320 | 36 | 525 sec/ 527 sec | 528 sec (2.5) |
| M2 | DGTH- \mathbb{P}_1 | 44,491,968 | 256 | 42 | 1816 sec/1823 sec | 1824 sec |
| - | - | - | 512 | 49 | 782 sec/ 784 sec | 785 sec (2.3) |

Domain decomposition resolution algorithms

3D application: heterogeneous propagation media



| Mesh | N_s | LU (min/max) | CPU factor (min/max) | Elapsed time factor |
|------|-------|---------------|----------------------|---------------------|
| M1 | 160 | 2.1 GB/3.1 GB | 490 sec/495 sec | 496 sec |
| - | 320 | 0.8 GB/1.2 GB | 130 sec/131 sec | 132 sec (3.8) |
| M2 | 256 | 2.2 GB/3.2 GB | 525 sec/527 sec | 528 sec |
| - | 512 | 0.8 GB/1.3 GB | 138 sec/140 sec | 142 sec (3.7) |

DGTH method

- Non-conforming (both in h and p) DGTH method
- hp -adaptivity

Solution methods

- Schwarz algorithms based on optimized interface conditions (in collaboration with M. Gander, University of Geneva)
- Subdomain solver
 - Block ILU preconditioned iterative solver
 - Hierarchical solution strategies

High performance computing

- Hierarchical SPMD model (multiple parallelism levels)
- DG method on hybrid CPU/GPU systems

Thank you for your attention!