Three-level parallelization for Finite Element Code with Hybrid Meshes

Adrian Amor-Martin(1) Daniel Garcia-Donoro(2), Luis E. Garcia-Castillo(1)
September 5, 2018
URSI 2018, Granada

(1) Radiofrequency, Microwaves, Electromagnetics and Antennas Group.
University Carlos III of Madrid.
[aamor,luise]@tsc.uc3m.es

(2) Xidian University, Xi’an, China.
daniel@xidian.edu.cn
Introduction
Intro: HOFEM

- User-friendly.
- Based on GiD.

\[ \nabla \times \left( f_r^{-1} \times \vec{V} \right) - i \omega \mu_0 \vec{V} = -j k_0 \vec{H}_0 + \nabla \times f_r^{-1} \vec{Q} \]

LHS\( g_i \) = \( RH\vec{S} \)

\[ \vec{E} = \sum_{i} g_i \vec{N}_i \]
Intro: design by blocks

<table>
<thead>
<tr>
<th>MODULES</th>
<th>TESTS - MMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOMAIN</td>
<td>FAMILY</td>
</tr>
<tr>
<td>Systematic</td>
<td>MUMPS</td>
</tr>
<tr>
<td>Hierarchical</td>
<td>PARDISO</td>
</tr>
</tbody>
</table>

HOFEM
HIGHER ORDER
FINITE ELEMENT METHOD

13.0.0
Intro: where do we go?

- Efficient use of HPC in electromagnetics.
- Memory limits (use of MUMPS).
- Domain Decomposition Method.
  - Memory.
  - Flexibility.
Intro: DDM
Intro: DDM

- Nonoverlapping, nonconformal and nonmatching.
- Hybrid meshes.
- Geometry aware optimization.
- $hp$ adaptivity in 3D.
Formulation
Formulation: classic FEM

\[ \nabla \times \frac{1}{\mu_r} (\nabla \times \mathbf{E}) - k_0^2 \varepsilon_r \mathbf{E} = \mathbf{0} \]

\[ \hat{n} \times \mathbf{E} = 0, \text{on } \Gamma_D \]

\[ \hat{n} \times \frac{1}{\mu_{ri}} (\nabla \times \mathbf{E}) = 0, \text{on } \Gamma_N \]

\[ \hat{n} \times \frac{1}{\mu_{ri}} (\nabla \times \mathbf{E}) + jk_0 \hat{n} \times \hat{n} \times \mathbf{E} = \Psi, \text{on } \Gamma_C \]
Find $\mathbf{E} \in \mathbf{W}$ such that

$$c_1(\mathbf{F}, \mathbf{E}) - k_0^2 c_2(\mathbf{F}, \mathbf{E}) + \gamma c_3(\mathbf{F}, \mathbf{E}) = l(\mathbf{F}), \quad \forall \mathbf{F} \in \mathbf{W}$$

$$c_1(\mathbf{F}, \mathbf{E}) = \int_{\Omega} (\nabla \times \mathbf{F}) \cdot \left( \frac{1}{\mu_r} \nabla \times \mathbf{E} \right) \, d\Omega$$

$$c_2(\mathbf{F}, \mathbf{E}) = \int_{\Omega} \mathbf{F} \cdot \varepsilon_r \mathbf{E} \, d\Omega$$

$$c_3(\mathbf{F}, \mathbf{E}) = \int_{\Gamma_c} (\mathbf{n} \times \mathbf{F}' \mathbf{)} \cdot (\mathbf{n} \times \mathbf{E}) \, d\Gamma_c$$

$$l(\mathbf{F}) = \int_{\Omega} (\mathbf{F} \cdot \mathbf{O}) \, d\Omega - \int_{\Gamma_c} (\mathbf{F} \cdot \mathbf{\Psi}) \, d\Gamma_c$$

$$\mathbf{W} := \{ \mathbf{A} \in \mathbf{H}(\text{curl}, \Omega), \, \mathbf{n} \times \mathbf{A} = 0 \, \text{on} \, \Gamma_D \}$$
\documentclass{article}

\begin{document}

\textbf{Formulation: FEM with DDM}

\[ \nabla \times \frac{1}{\mu_{ri}} (\nabla \times E_i) - k_0^2 \varepsilon_{ri} E_i = 0 \]

\[ \hat{n}_i \times E_i = 0, \text{ on } \Gamma_{i,D} \]

\[ \hat{n}_i \times \frac{1}{\mu_{ri}} (\nabla \times E_i) = 0, \text{ on } \Gamma_{i,N} \]

\[ \hat{n}_i \times \frac{1}{\mu_{ri}} (\nabla \times E_i) + jk_0 \hat{n}_i \times \hat{n}_i \times E_i = \Psi_i, \text{ on } \Gamma_{i,C} \]

\[ \hat{n}_i \times E_i \times \hat{n}_i = \hat{n}_j \times E_j \times \hat{n}_j, \text{ on } \Gamma_{ij} \]

\[ \hat{n}_i \times \frac{1}{\mu_{ri}} (\nabla \times E_i) = -\hat{n}_j \times \frac{1}{\mu_{rj}} (\nabla \times E_j), \text{ on } \Gamma_{ij} \]

\end{document}
Formulation: cement variables and TC

\[ e_i = \hat{n}_i \times E_i \times \hat{n}_i \]

\[ j_i = \frac{1}{k_0} \hat{n}_i \times \frac{1}{\mu_{ri}} (\nabla \times E_i) \]

\[ \rho_i = \frac{1}{k_0} \nabla_\tau \cdot j_i \]

\[ (\alpha I + \beta_i S_{TE})(e_i) + (I + \gamma_i S_{TM})(j_i) = \]

\[ (\alpha I + \beta_j S_{TE})(e_j) - (I + \gamma_j S_{TM})(j_j) \]

\[ S_{TE} = \nabla_\tau \times \nabla_\tau \times \]

\[ S_{TM} = \nabla_\tau \nabla_\tau . \]
Find $\mathbf{E}_i \in \mathbf{W}_i, \mathbf{j}_i \in \mathbf{X}_i, \rho_i \in Y_i$ such that

$$c_1(\mathbf{F}_i, \mathbf{E}_i) - k_0^2 c_2(\mathbf{F}_i, \mathbf{E}_i) + jk_0 c_{\tau,1}(\mathbf{n}_i \times \mathbf{F}_i, \mathbf{n}_i \times \mathbf{E}_i) = l(\mathbf{F}_i), \forall \mathbf{F}_i \in \mathbf{W}_i$$

$$\alpha c_{\tau,1}(\mathbf{l}_i, \mathbf{e}_i) + k_0 c_{\tau,1}(\mathbf{l}_i, \mathbf{j}_i) + k_0^2 c_{\tau,1}(\mathbf{l}_i, \nabla_{\tau} \rho_i) + \beta_i k_0 c_{\tau,1}(\nabla_{\tau} \times \mathbf{l}_i, \nabla_{\tau} \times \mathbf{e}_i) = \alpha c_{\tau,1}(\mathbf{l}_i, \mathbf{e}_j) - k_0 c_{\tau,1}(\mathbf{l}_i, \mathbf{j}_j) - k_0^2 c_{\tau,1}(\mathbf{l}_i, \nabla_{\tau} \rho_j) + \beta_j k_0 c_{\tau,1}(\nabla_{\tau} \times \mathbf{l}_i, \nabla_{\tau} \times \mathbf{e}_j), \forall \mathbf{l}_i \in \mathbf{X}_i$$

$$c_{\tau,1}(\nabla_{\tau} \phi_i, \mathbf{j}_i) + k_0 c_{\tau,2}(\phi_i, \rho_i) = 0, \forall \phi_i \in Y_i$$

$\mathbf{F}_i \in \mathbf{W}_i := H_0(\text{curl}; \Omega_i), \mathbf{l}_i \in \mathbf{X}_i := H_0(\text{curl}_\tau; \Gamma_{ij}), \phi_i \in Y_i := H_0^{-1/2}(\Gamma_{ij})$
Formulation: variational formulation with DDM (\(\& ii\))

\[
c_1(F_i, E_i) = \int_{\Omega_i} (\nabla \times F_i) \cdot \frac{1}{\mu r_i} (\nabla \times E_i) \, d\Omega_i
\]

\[
c_2(F_i, E_i) = \int_{\Omega_i} F_i \cdot \varepsilon r_i E_i \, d\Omega_i
\]

\[
c_{\tau, 1}(l_i, e_j) = \int_{\Gamma_{ij}} (l_i \cdot e_j) \, d\Gamma_{ij}
\]

\[
c_{\tau, 2}(\phi_i, \rho_j) = \int_{\Gamma_{ij}} (\phi_i \rho_j) \, d\Gamma_{ij}
\]

\[
l(F_i) = \int_{\Omega_i} (F_i \cdot O_i) \, d\Omega_i - \int_{\Gamma_{i,C}} (F_i \cdot \Psi_i) \, \Gamma_{i,C}
\]
Implementation
Implementation: parallelization

- Algorithm: DDM.
- Process: MPI.
- Thread: OpenMP.
Implementation: workflow (i)

MPI Division

P₀ P₁ P₂ P₃

... Read input data

P₀ P₁ P₂ P₃

... Create dom. and surf. mesh

P₀ P₁ P₂ P₃

... Destroy global mesh

P₀ P₁ P₂ P₃
Implementation: workflow (ii)

Fill surf. mesh

... Numbering DOFs

Evaluate shared points

Fill surf. mesh

Numbering DOFs
Implementation: workflow (iii)

Build solver structures

Calculate and fill dom. LHS

Factorize dom. matrices
Implementation: workflow (iv)

1. Generate surf. matrices
2. Fill surf. problem
3. Solve surf. problem

Diagram:

- P0, P1, P2, P3
- Pn-1, Pn
Implementation: workflow (& v)

Create mesh object

Generate postprocess

Recover full solution

END
Numerical results
Results: setup

- Pre and postprocessing: GiD.
- Direct solver: MUMPS.
- Iterative solver: GCR through PETSC.
  - Residual: $10^{-6}$.
- SOTC-TE.
Results: long waveguide

- WR-90 empty waveguide.
- Working frequency $f = 10$ GHz.
- Length of $10\lambda_g$.
- 3 simulations:
  - Without DDM: 750688 unknowns.
  - With nonconformal DDM: tetrahedra, prisms and hexahedra: 512622 unknowns, 10 dom.
Results: long waveguide
Results: long waveguide
<table>
<thead>
<tr>
<th>Case of study</th>
<th>Time (s)</th>
<th>Peak memory (Mb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No DDM (MPI 1, OpenMP 8)</td>
<td>397.49</td>
<td>6867</td>
</tr>
<tr>
<td>No DDM (MPI 10, OpenMP 4)</td>
<td>58.475</td>
<td>2187</td>
</tr>
<tr>
<td>DDM (MPI 10, OpenMP 1)</td>
<td>228.48</td>
<td>1550</td>
</tr>
<tr>
<td>DDM (MPI 10, OpenMP 2)</td>
<td>184.02</td>
<td>1550</td>
</tr>
<tr>
<td>DDM (MPI 10, OpenMP 4)</td>
<td>163.18</td>
<td>1550</td>
</tr>
</tbody>
</table>
Results: very long waveguide

- WR-90 empty waveguide.
- Working frequency $f = 10\, \text{GHz}$.
- Length of $100\lambda_g$.
- 2 simulations:
  - Without DDM: 5042688 unknowns.
  - With conformal DDM, METIS: 26500 unknowns per dom., 200 dom.
## Results: performance of simulation

<table>
<thead>
<tr>
<th>Case of study</th>
<th>Time (s)</th>
<th>Peak memory (Mb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No DDM (MPI 12, OpenMP 4)</td>
<td>416.561</td>
<td>23060</td>
</tr>
<tr>
<td>DDM, 30 dom. (MPI 12, OpenMP 4)</td>
<td>1457.60</td>
<td>13467</td>
</tr>
<tr>
<td>DDM, 40 dom. (MPI 12, OpenMP 4)</td>
<td>1311.66</td>
<td>13244</td>
</tr>
<tr>
<td>DDM, 40 dom, direct (MPI 12, OpenMP 4)</td>
<td>1454.78</td>
<td>13399</td>
</tr>
<tr>
<td>DDM, 50 dom. (MPI 12, OpenMP 4)</td>
<td>1108.97</td>
<td>13329</td>
</tr>
<tr>
<td>DDM, 100 dom. (MPI 12, OpenMP 4)</td>
<td>1259.97</td>
<td>14217</td>
</tr>
<tr>
<td>DDM, 200 dom. (MPI 12, OpenMP 4)</td>
<td>2341.79</td>
<td>16076</td>
</tr>
</tbody>
</table>
Results: X-band waveguide filter

- WR-75 waveguide.
- X-band.
- 4 rectangular cavities:
  - Embedded resonator of $\varepsilon_r = 30$.
  - Support of $\varepsilon_r = 9$.
- 236690 unknowns for DDM, 412428 without DDM.

Results: X-band waveguide filter
Results: X-band waveguide filter
Results: X-band waveguide filter
Results: X-band waveguide filter
Results: X-band waveguide filter

Filter with four dielectric resonators

<table>
<thead>
<tr>
<th>$S_{11,DDM}$</th>
<th>$S_{21,DDM}$</th>
<th>$S_{11}$</th>
<th>$S_{21}$</th>
<th>$S_{21}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Frequency (GHz)

S-parameters (dB)
Results: X-band waveguide filter
Results: SWA

- Resonant SWA with length $4.5\lambda_g$.
- 7 elliptical slots.
- 9 subdomains.
- Working frequency: $f = 3.4045$ GHz.
- 611440 unknowns without DDM, 657256 with DDM.
- Systematic family of basis functions.
- Surface problem:
  - 141 iterations.
  - 61088 unknowns.

Results: SWA
Results: SWA
Results: SWA
Results: SWA
Results: SWA

Plane YZ

Plane XZ

No DDM

DDM
Results: 2D circular horn array

• 4x4 circular horns.
• Working frequency $f = 10 \text{ GHz}$
• Uniform excitation through WR-90 waveguides.
• 2261472 unknowns without DDM, 2368032 unknowns with DDM.
• Unstructured tetrahedra.
• Surface problem:
  • 73 iterations.
  • 185856 unknowns.
Results: 2D circular horn array
Results: 2D circular horn array
Results: 2D circular horn array
Results: 2D circular horn array
Results: 2D circular horn array

Plane YZ

- No DDM
- DDM

Plane XZ

- No DDM
- DDM
Results: RCS for F117

- Stealth design.
- Unstructured tetrahedra mesh.
- RCS for $f = 50$ MHz.
- Domains obtained through ParMETIS.
- Without DDM, 1011464 unknowns; with DDM, 1063208 unknowns.
- Surface problem (5 domains):
  - 360 iterations.
  - 68790 unknowns.
Results: RCS for F117
Results: RCS for F117
Results: RCS for F117
Results: RCS for F117

Plane XZ

Plane YZ
Bonus track: h adaptivity

- Singularity through l-shape domain
Bonus track: h adaptivity
Bonus track: h adaptivity
Bonus track: h adaptivity

- Representation of the singularity with ROT
- Uniform
- Maximum
- SER

- Representation of the singularity without ROT
- Uniform
- Maximum
- SER
Bonus track: h adaptivity for SWA
Bonus track: h adaptivity for SWA
Bonus track: h adaptivity for SWA
Bonus track: h adaptivity for SWA
Bonus track: h adaptivity for SWA
Bonus track: h adaptivity for SWA
Bonus track: h adaptivity for SWA
Hidden gem: hp adaptivity

- 134578 unknowns for h adaptivity.
- 67512 unknowns for hp adaptivity.
Hidden gem: hp adaptivity
Hidden gem: hp adaptivity
Conclusions
Conclusions

• Introduction of DDM as third level.
• Geometry aware optimization with hybrid meshes.
• Best use of memory for large scale problems.
• Controlled loss of accuracy.
• Flexibility.
Thanks for your attention!
Adrian Amor-Martin
aamor@ing.uc3m.es