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Towards an HPC tool for simulation of 3D CSEM surveys: and edge-based approach

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Computer Applications in Science & Engineering Department

My country

Universidad Veracruzana

Scholarship CONACyT

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BSC

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Marenostrum

92nd at Top500 (November 2015)
77th at Top500 (June 2015)

1,1 Petaflops as peak performance   155.5 TiB of main memory   3,056 nodes

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CASE department

Optimized applications for science and engineering:

- Biomechanics (Alya Red): coupled electrical/mechanical/fluid in very large grids (10^8 elements)
- Geophysics (BSIT): pioneers in acoustic RTM, elastic FWI with real data, electromagnetic methods
- Coupled Multiphysics (ALYA): Coupling fluids, solids, electromagnetics, particles, chemistry on grids with 10^9 elements. Several CFD modelization: free surface, compressible/incompressible, subsonic/supersonic, RANS/LES/DNS, ...

My research thesis

Main target:

- Implement an edge-based FE code on HPC platforms to simulate CSEM in geophysics.

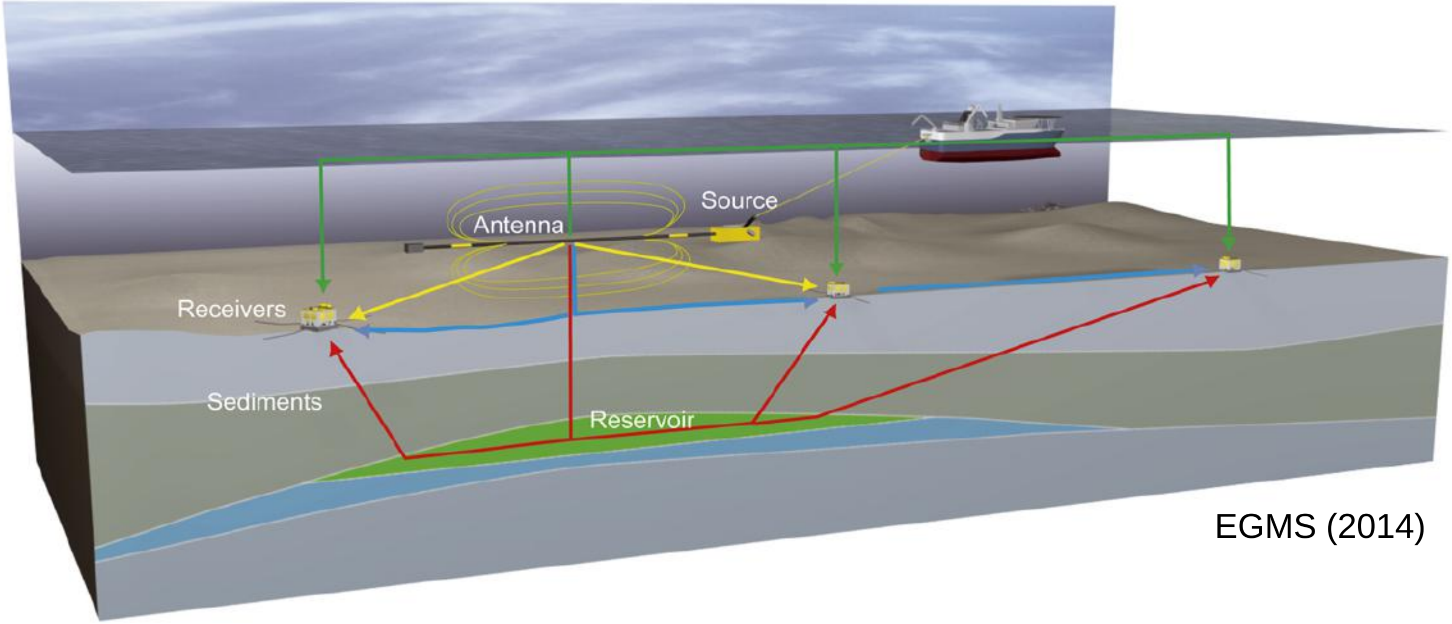
Team at BSC has experience with FD, FE but not with Edge Elements (Nédélec elements, curl-conforming elements).

My first job:

- Review the state of the art
- Understand the concept of Edge elements
- Understand the physical meaning
- Identify data structures needed

Controlled-source Electromagnetic Method (CSEM)

- CSEM uses a dipole to transmit a time-varying electromagnetic field into the earth.
- The field is modified by the presence of subsurface resistive layers
- Used as a complementary tool to seismic surveys and well data analysis



EGMS (2014)

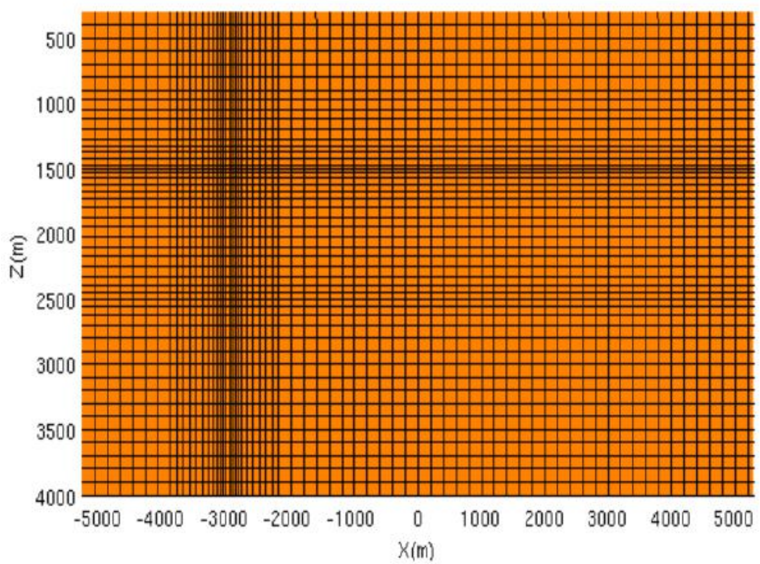
Controlled-source Electromagnetic Method (CSEM)

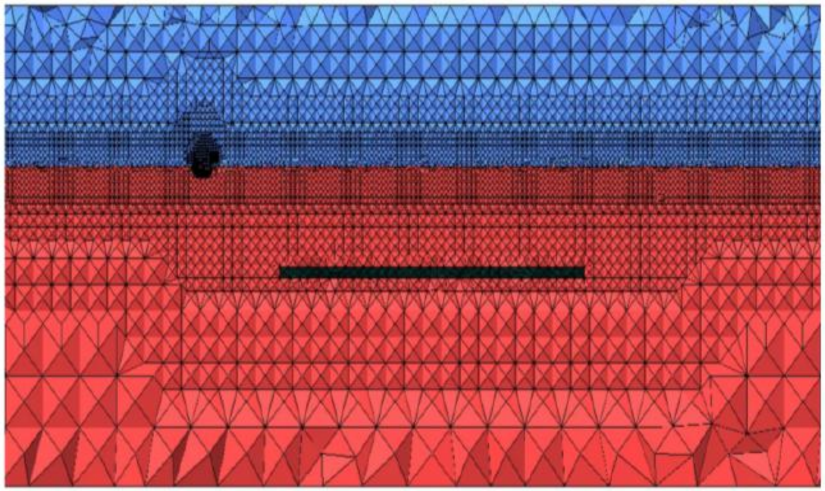
Finite difference (FD)

- Structured meshes
- Difficult to adapt to complex geometries
- Very fast approach

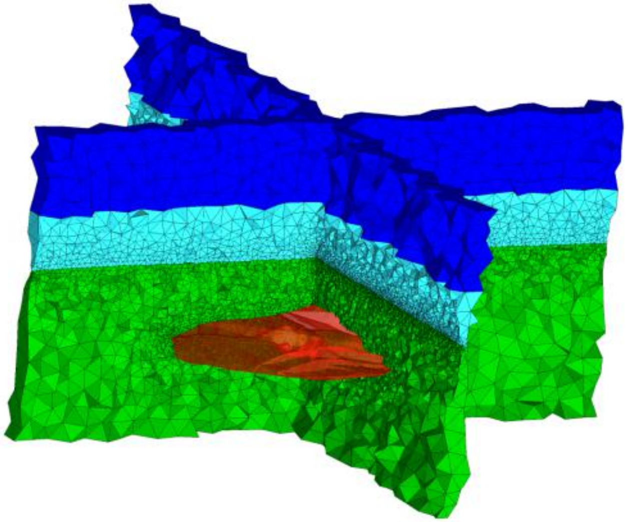
Finite Element (FE)

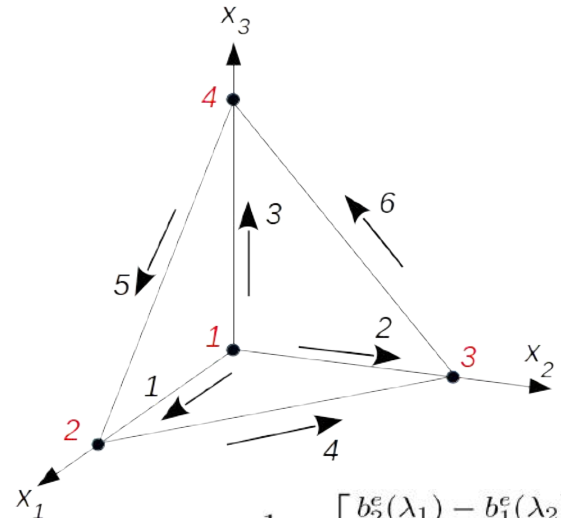
- Unstructured meshes
- Local refinement
- Nodal approach produces spurious solutions





Edge finite element method: basis functions





$$W_{12}\ell_1^e = \frac{1}{(6V^e)^2}\begin{bmatrix} b_2^e(\lambda_1) - b_1^e(\lambda_2)\cdot\hat{i} \\ c_2^e(\lambda_1) - c_1^e(\lambda_2)\cdot\hat{j} \\ d_2^e(\lambda_1) - d_1^e(\lambda_2)\cdot\hat{k} \end{bmatrix}\ell_1$$

$$W_{13}\ell_2^e = \frac{1}{(6V^e)^2}\begin{bmatrix} b_3^e(\lambda_1) - b_1^e(\lambda_3)\cdot\hat{i} \\ c_3^e(\lambda_1) - c_1^e(\lambda_3)\cdot\hat{j} \\ d_3^e(\lambda_1) - d_1^e(\lambda_3)\cdot\hat{k} \end{bmatrix}\ell_2$$

$$W_{14}\ell_3^e = \frac{1}{(6V^e)^2}\begin{bmatrix} b_4^e(\lambda_1) - b_1^e(\lambda_4)\cdot\hat{i} \\ c_4^e(\lambda_1) - c_1^e(\lambda_4)\cdot\hat{j} \\ d_4^e(\lambda_1) - d_1^e(\lambda_4)\cdot\hat{k} \end{bmatrix}\ell_3$$

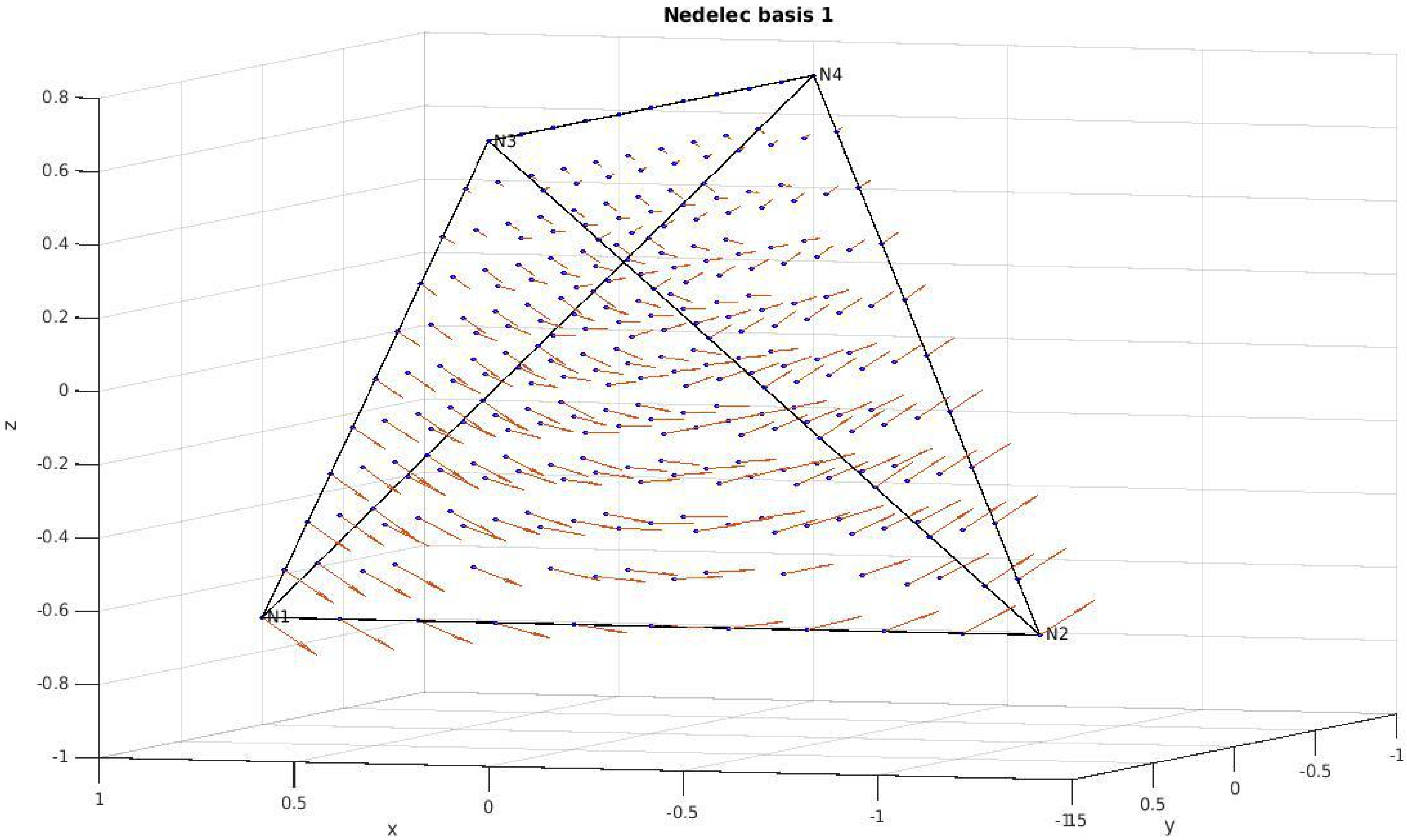
$$W_{23}\ell_4^e = \frac{1}{(6V^e)^2}\begin{bmatrix} b_3^e(\lambda_2) - b_2^e(\lambda_3)\cdot\hat{i} \\ c_3^e(\lambda_2) - c_2^e(\lambda_3)\cdot\hat{j} \\ d_3^e(\lambda_2) - d_2^e(\lambda_3)\cdot\hat{k} \end{bmatrix}\ell_4$$

$$W_{42}\ell_5^e = \frac{1}{(6V^e)^2}\begin{bmatrix} b_2^e(\lambda_4) - b_4^e(\lambda_2)\cdot\hat{i} \\ c_2^e(\lambda_4) - c_4^e(\lambda_2)\cdot\hat{j} \\ d_2^e(\lambda_4) - d_4^e(\lambda_2)\cdot\hat{k} \end{bmatrix}\ell_5$$

$$W_{34}\ell_6^e = \frac{1}{(6V^e)^2}\begin{bmatrix} b_4^e(\lambda_3) - b_3^e(\lambda_4)\cdot\hat{i} \\ c_4^e(\lambda_3) - c_3^e(\lambda_4)\cdot\hat{j} \\ d_4^e(\lambda_3) - d_3^e(\lambda_4)\cdot\hat{k} \end{bmatrix}\ell_6$$

- DOF are each edge in the mesh
- Linear vector basis functions (VBF)
- VBS are divergence free but not curl free (useful for the representation of the electric field)

Edge finite element method: basis functions



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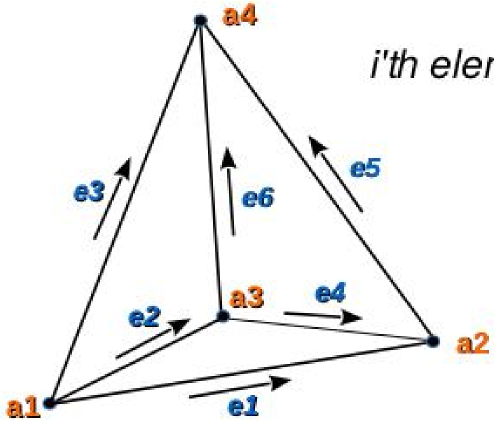
Edge finite element method: data structures



i'th element

Column ... a1 ... a2 ... a3 ... a4 ...

nodes = (... x ... x ... x ... x ... ; ... y ... y ... y ... y ... ; ... z ... z ... z ... z ...)

Column ... i ...

elements = (... a1 ... ; ... a2 ... ; ... a3 ... ; ... a4 ...)

Column ... e1 ... e2 ... e3 ... e4 ... e5 ... e6 ...

edges = (... a1 ... a1 ... a1 ... a3 ... a2 ... a3 ... ; ... a2 ... a3 ... a4 ... a2 ... a4 ... a4 ...)

Transformation stage in pre-processing

Column ... i ...

elements = (... e1 ... ; ... e2 ... ; ... e3 ... ; ... e4 ... ; ... e5 ... ; ... e6 ...)

Column ... i ...

signs = (... ±e1 ... ; ... ±e2 ... ; ... ±e3 ... ; ... ±e4 ... ; ... ±e5 ... ; ... ±e6 ...)

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Edge finite element method: data structures

Algorithm 1: Edge conductivity computation

Input: A finite set of conductivities values per element:
$\nu_\sigma = \{\nu_1, \nu_2, \ldots, \nu_t\}$.

Output: A finite set of conductivities values per edge:
$\varrho_\sigma = \{\varrho_1, \varrho_2, \ldots, \varrho_s\}$.

```
begin
    for i = 1 : s do        Loop over edges
        ϱ computation of edge i given by:
```

$$\varrho(i) = \frac{\sum \nu \in i}{\text{Number of } \nu \in i}$$

```
    end
end
```

Algorithm 1: Primary field computation

Input: A finite set of nodes expressed by their 3D coordinates:
$N(p_{i1}, p_{i2}, p_{i3}) \quad i = 1, 2, \ldots, r.$
A finite set of edges expressed by their two nodes $e(n_{i1}, n_{i2}) \quad i = 1, 2, \ldots, s$

Output: A finite set of projected primary electric fields in each edge:
$\epsilon = \{\epsilon_1, \epsilon_2, \ldots, \epsilon_m\}$

```
begin
    for i = 1 : s do        Loop over edges
        Mid-points computation of edge i given by:
```

$$h[x_i, y_i, z_i] = \begin{bmatrix} N(e(n_{i1},1)+N(e(n_{i2},1) \\ N(e(n_{i1},2)+N(e(n_{i2},2) \\ N(e(n_{i1},3)+N(e(n_{i2},3) \end{bmatrix} * 0.5$$

```
        Depending the source orientation, the primary field
        computation of edge i in his mid-point is given by:
```

$$E_{pi}(h) = \text{Equation 6, 7 or 8 of paper}$$

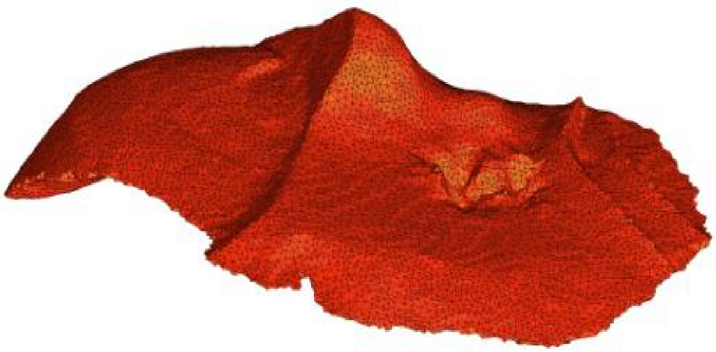
```
        Electric field projection ϵ_i, which is given by:
```

$$\epsilon_i(E_{pi}) = \text{Equation 10 of paper}$$

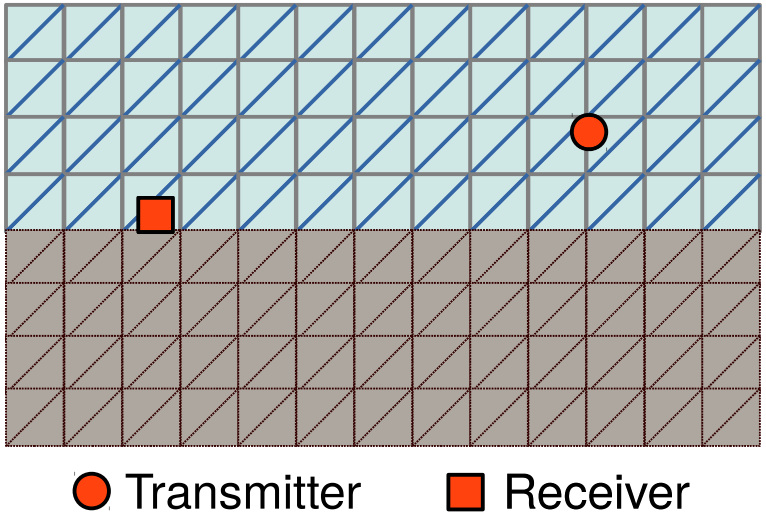
```
    end
end
```

Edge finite element method: PDE

- In our approach, the electric field is splitted into primary and secondary field
- Primary field is calculated analytically for a background layered-earth model
- Secondary field is discretized using Edge elements
- Maxwell's equations



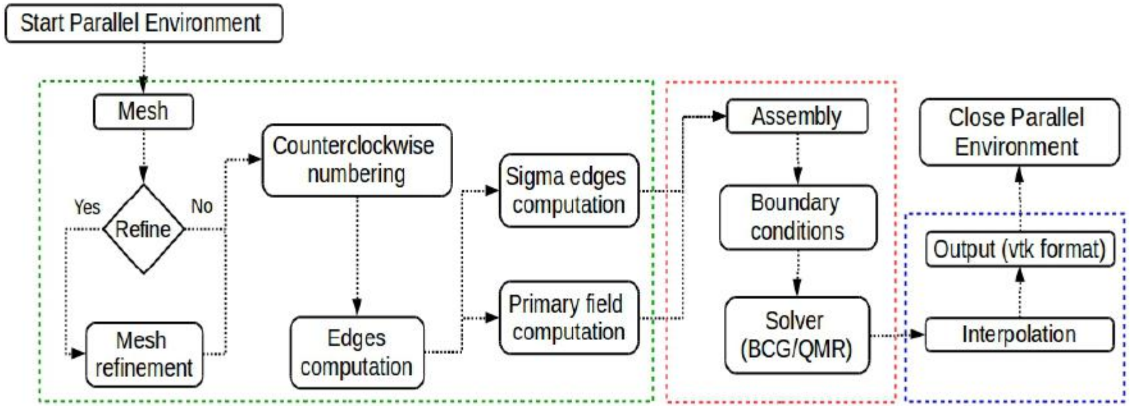
Repsol-BSC Research Center 2014



Slice of a CSEM mesh in X-Z plane

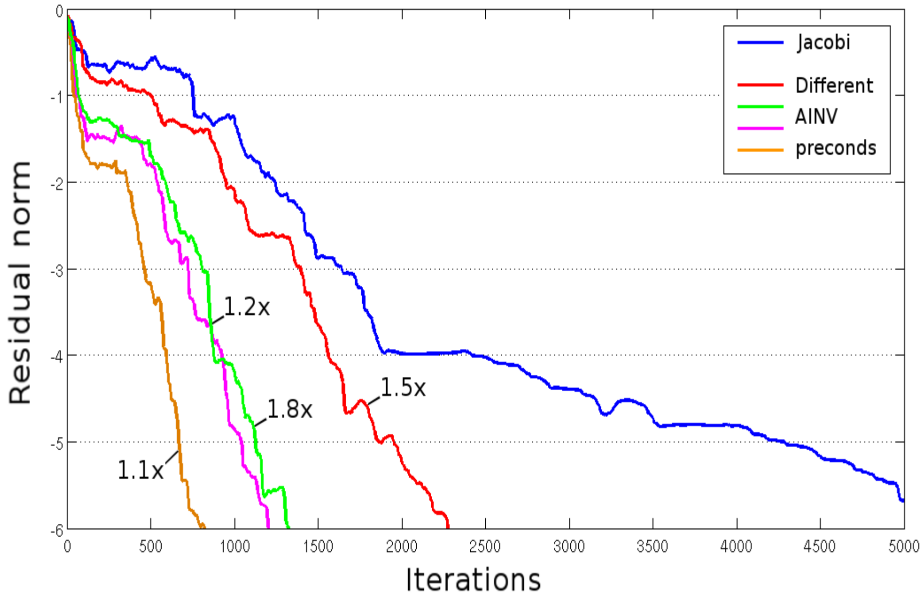
My research thesis

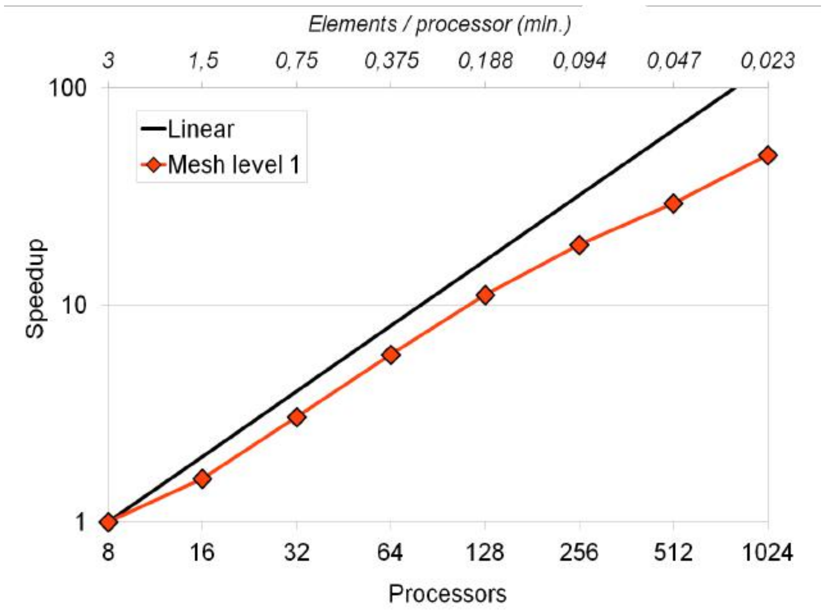
- Matlab prototype as proof of concept:
  - Modest parallel approach
  - Support for different mesh formats
  - Direct and iterative solvers
- Useful to study:
  - Convergence
  - Properties of elemental matrices
  - Errors (L1, L2, Linf)
  - Speed-up

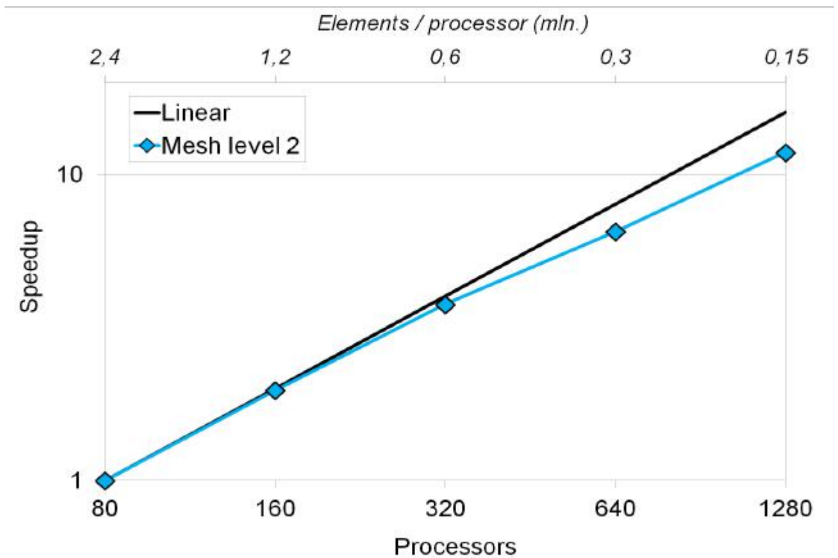


My research thesis

Convergence of the solvers and scalability







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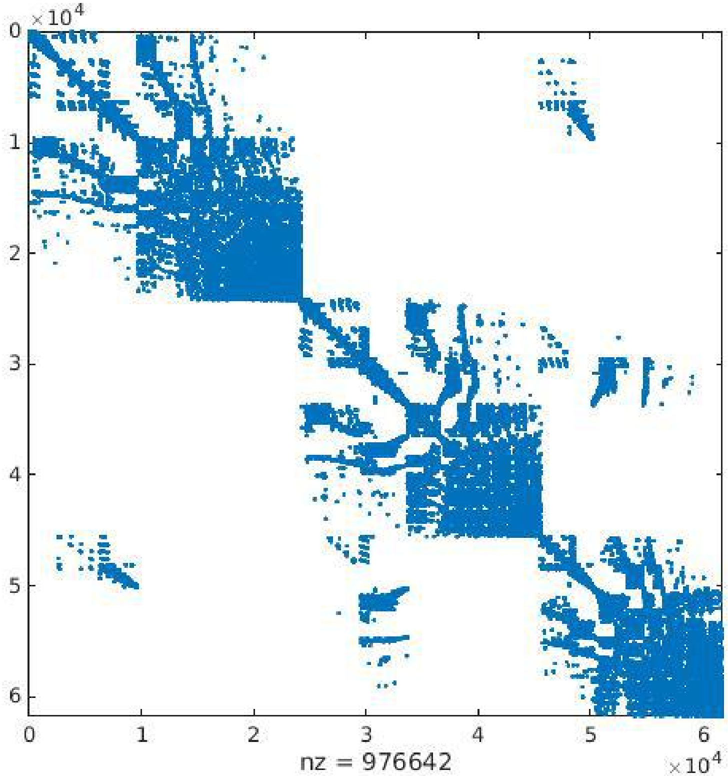
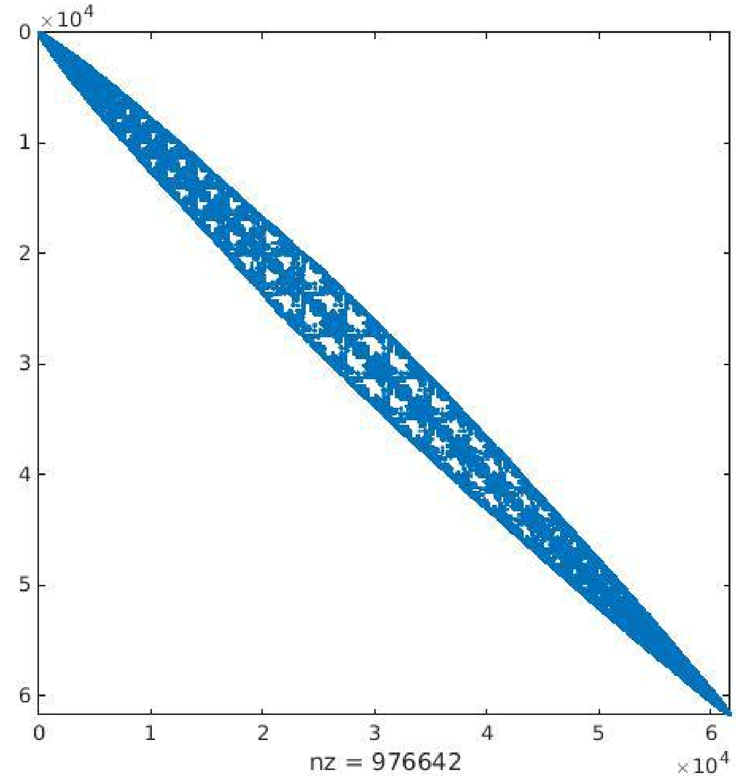
My reseach thesis

- Useful to study the matrices's properties in order to take advantages of the numerical method





- Improving locality

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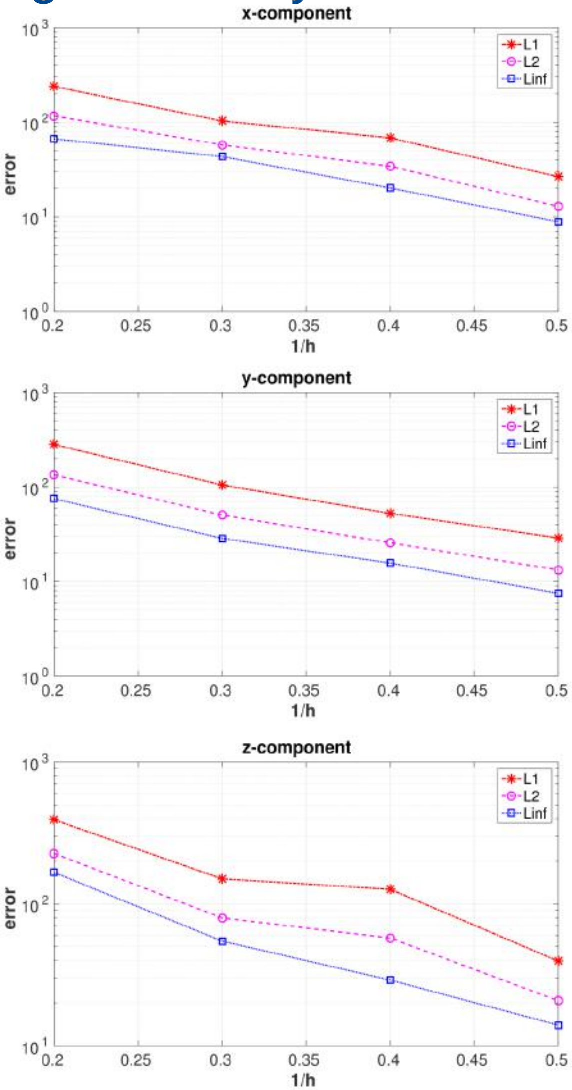
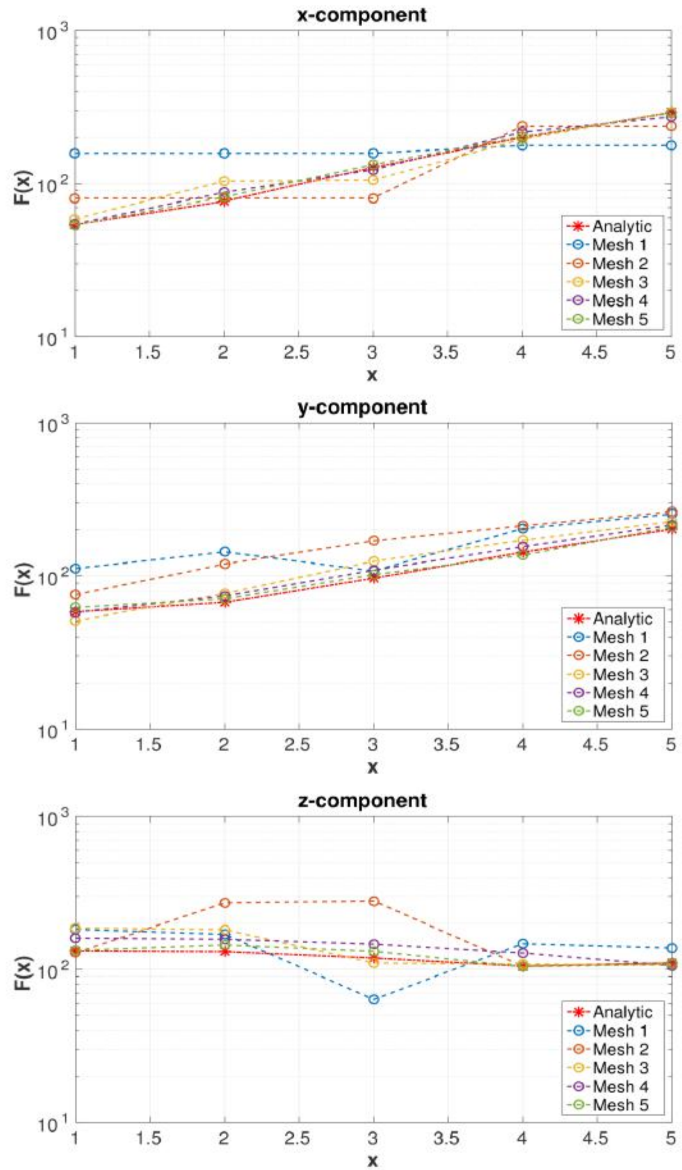
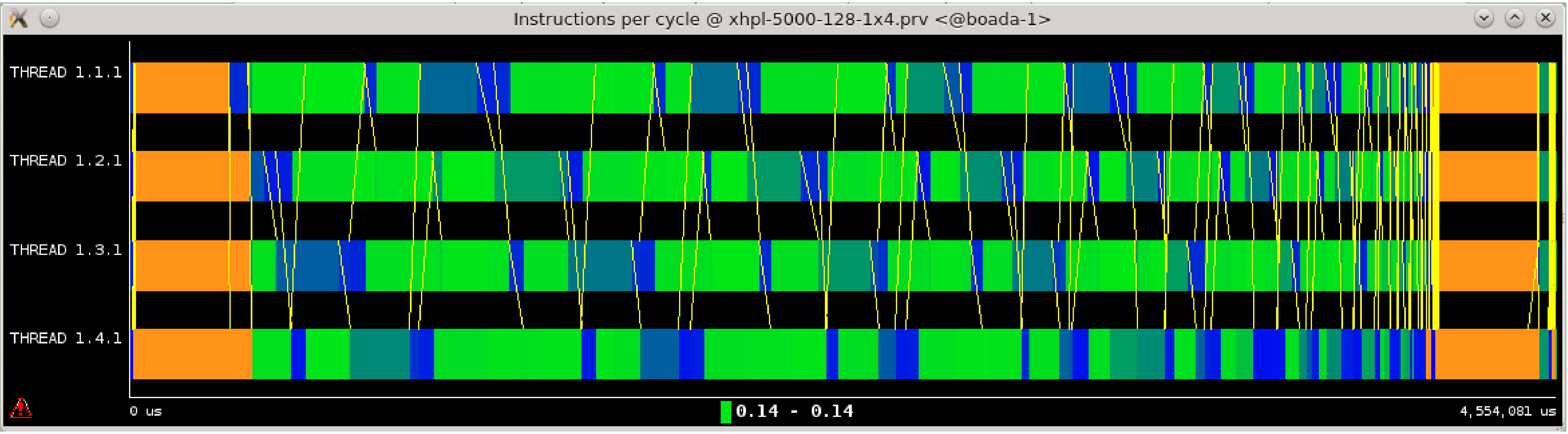
My reseach thesis

Convergence analysis

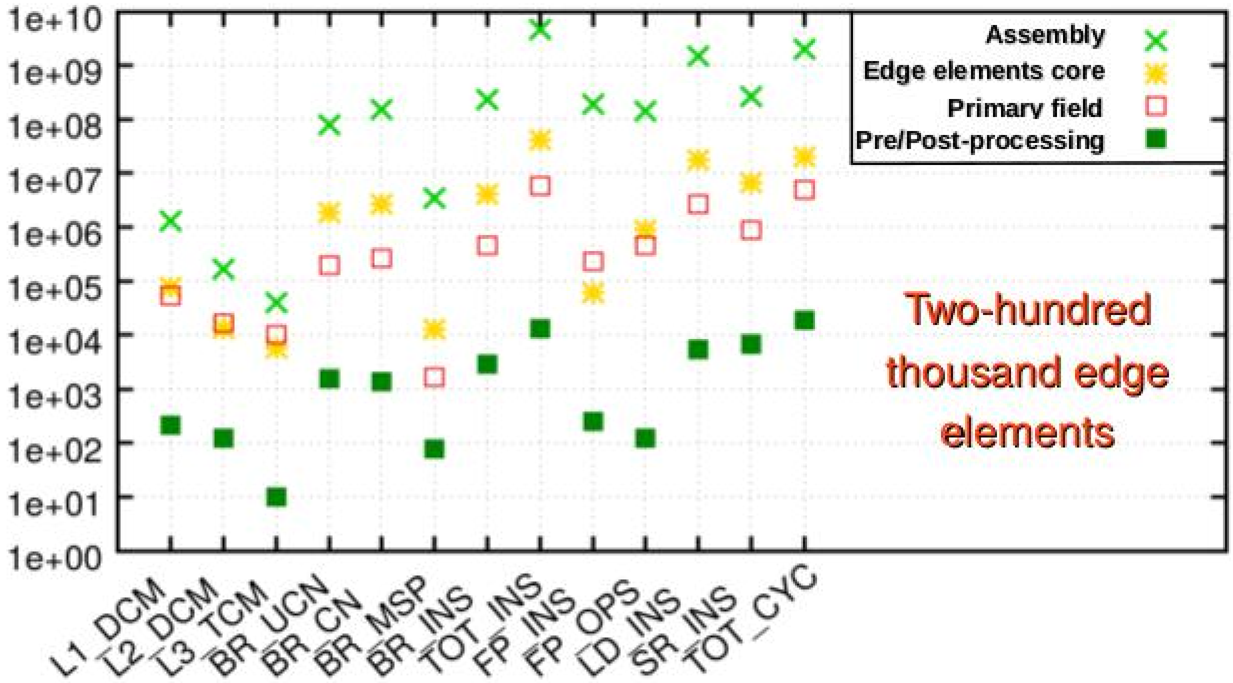




My research thesis



My research thesis



Performance Analysis

PAPI Counters

- Automatic generation of Hardware counters
- PARAVER: Performance analyzer developed at BSC

My research thesis

Journals & papers:

- Castillo, O., de la Puente, J., Modesto, D., Puzyrev, V., and Cela, J. M. (2015). Parallel edge-based tool for the simulation of 3D electromagnetic surveys in geophysics. Computación y Sistemas. National Polytechnic Institute. ISSN 1405-5546
- Castillo, O., de la Puente, J., Puzyrev, V., and Cela, J. M. (2015). Edge-based electric field formulation in 3D CSEM simulations: a parallel approach. In Proceedings of the 6th International Conference and Workshop on Computing and Communication. IEEE – 978-1-4799-6908-1. Vancouver, Canada.
- Castillo, O., de la Puente, J., Puzyrev, V., and Cela, J. M. (2015). Parallel and numerical issues of the edge finite element method for 3D controlled-source electromagnetic surveys. In Proceedings of the International Conference on Computing Systems and Telematics. IEEE– 978-1-4799-7639-3. Xalapa, Veracruz, México.
- Castillo, O., de la Puente, J., Puzyrev, V., and Cela, J. M. (2015). Assessment of edge-based finite element technique for geophysical electromagnetic problems: efficiency, accuracy and reliability. In Proceedings of the 1st Pan-American Congress on Computational Mechanics and XI Argentine Congress on Computational Mechanics, pages 984–995. ISBN 978-84-943928-2-5 CIMNE, Buenos Aires, Argentina.

Conferences:

- Castillo, O., de la Puente, J., Puzyrev, V., and Cela, J. M. (2015). HPC and edge elements for geophysical electromagnetic problems: an overview. In BSC Doctoral Symposium (2nd: 2015: Barcelona). Barcelona Supercomputing Center.
- Castillo, O., de la Puente, J., Puzyrev, V., and Cela, J. M. (2015). Edge-elements for geophysical electromagnetic problems: a new implementation challenge. In PRACEdays15. Partnership for Advanced Computing in Europe. Dublin, Ireland.
- Castillo, O. (2014). Soluciones HPC para el sector energético: Desafíos y oportunidades. In IV Simposio Becarios CONACyT en Europa. Casa Universitaria Franco-Mexicana - Consejo Nacional de Ciencia y Tecnología de México. Strasbourg, France.

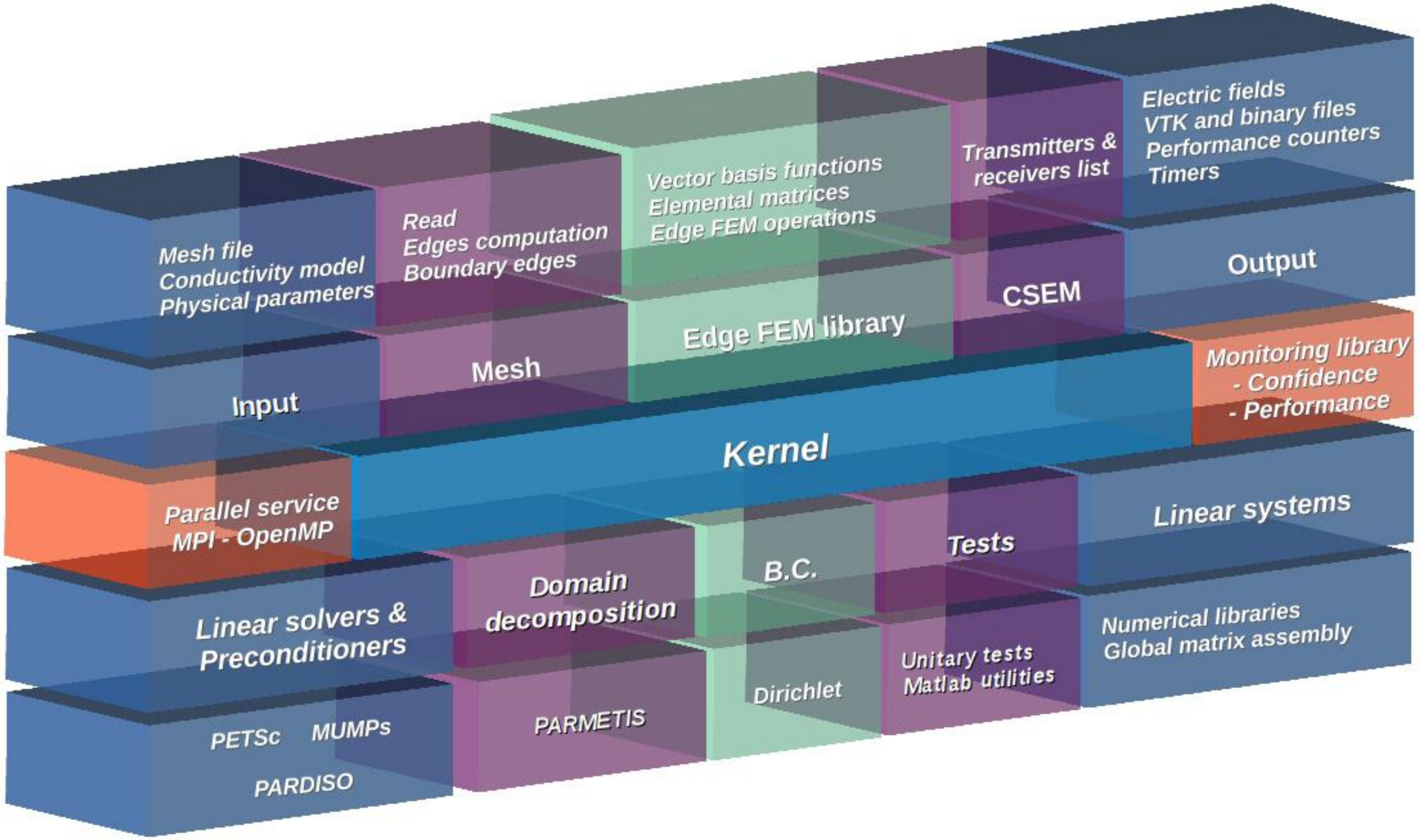
My stay at INRIA

- Investment of my time (during this month):
  - Finding a bug in RHS assembly
  - The proposal of the HPC software stack
  - Writing thesis
  - Two proposals for conferences (Deadline: november 30)

GROUP SUPPORTERS

This Project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 644202

HPC software stack: a proposal



Accuracy

reliability

efficiency

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My stay at INRIA

- I would like receive comments, opinions and new ideas about my prototype
  - Mathematical and physical formulation
  - Open to share the code

- I met the team and some of your research topics...

- Fruitful personal experience, so, I would like return next year...

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Thank you!

For further information please contact

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