

FINIS TERRAE COMPUTING CHALLENGES

CESGA-FINIS TERRAE COMPUTATIONAL SCIENCE CONFERENCE 2008

FINIS TERRAE

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❑ Finis Terrae computing challenges

✓ Selection

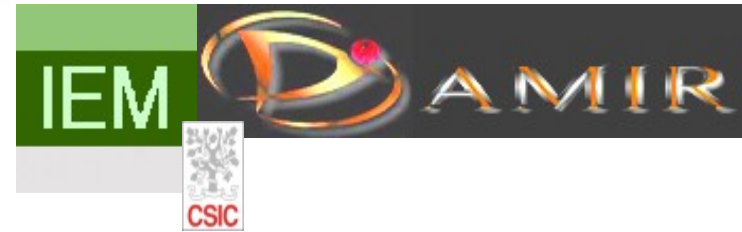
✓ Brief description

- **CHALLENGE 1: "PHASE SEPARATION"**
- **CHALLENGE 2: "POINT DISTRIBUTION ON BIDIMENSIONAL SPHERE"**
- **CHALLENGE 3: "ELECTROMAGNETIC COMPATIBILITY"**
- **CHALLENGE 4: "UNDERSTANDING THE MOST MASSIVE STARS OF THE UNIVERSE WITH GENETIC ALGORITHMS"**

✓ Conclusions

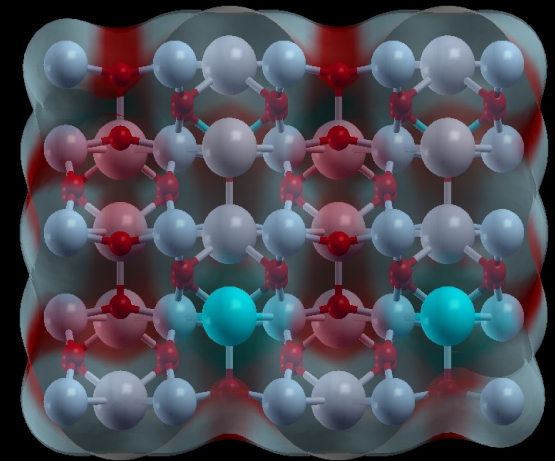
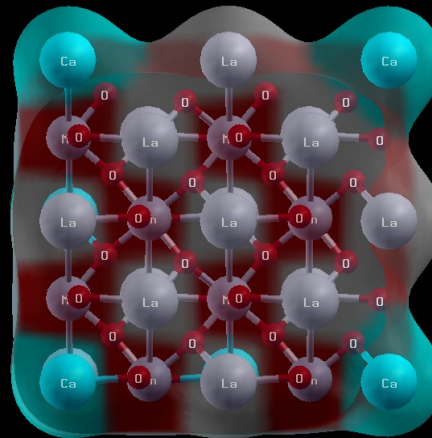
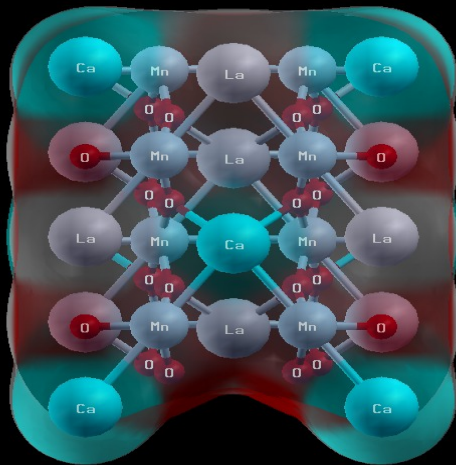
Challenges selection

- Different scientific fields / know-how
- Coming from different groups / Institutions / research projects
- Computationally highly demanding



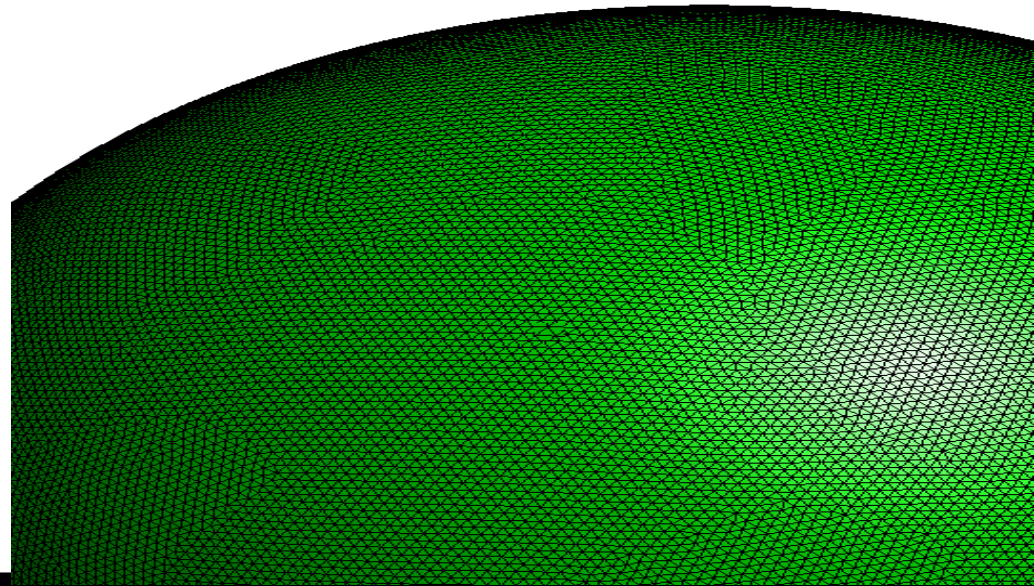
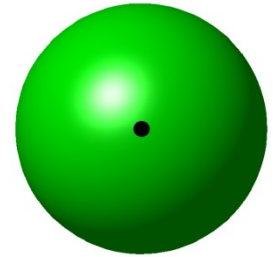
CHALLENGE 1: "PHASE SEPARATION"

- Solid State Physics: Materials Design
- Wien2k: electronic structure calculations of solids using density functional theory (DFT).
- Two levels parallelism:
 - Coarse grain: k points
 - Fine grain: Scalapack



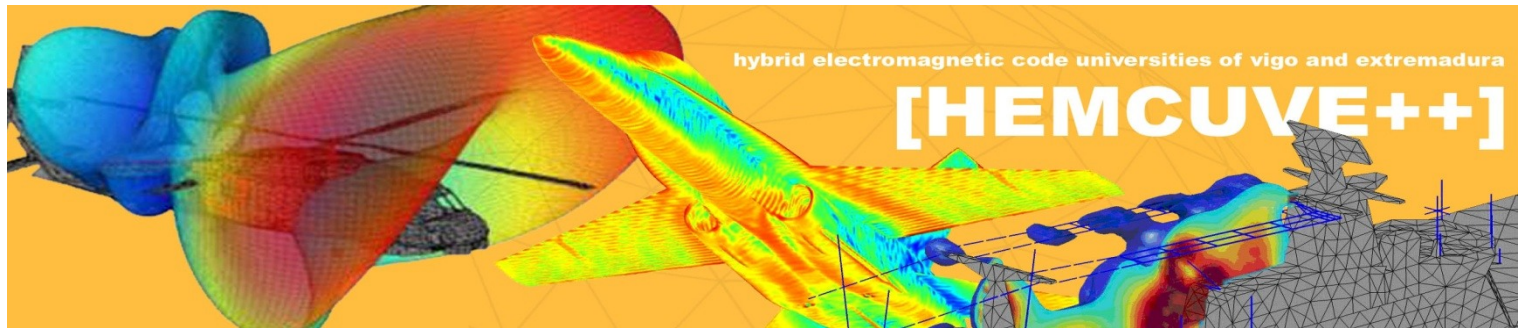
CHALLENGE 2: "POINT DISTRIBUTION ON BIDIMENSIONAL SPHERE"

- **I-MATH: Applied Maths (Potential Theory/Numerical Methods)**
- **Estimation of Fekete points**
- **Several parallelizations paradigms:**
 - **MPI**
 - **OpenMP**
 - **MPI/OpenMP**
 - **High Throughput**



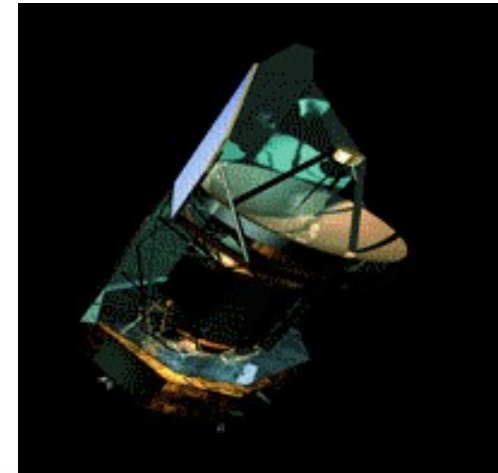
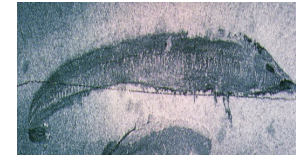
CHALLENGE 3: "ELECTROMAGNETIC COMPATIBILITY"

- Complex structures design
- HEmCUVE++: Electromagnetic calculations based on FAST MULTIPOLE methods
- Several parallelizations paradigms:
 - MPI
 - MPI/OpenMP
- Highly demanding on memory per process:
Balance between required CPU time and memory demand



CHALLENGE 4: "UNDERSTANDING THE MOST MASSIVE STARS OF THE UNIVERSE WITH GENETIC ALGORITHMS"

- Molecular and Infrared Astrophysics
- Genetic Algorithms: PIKAIA multimodal optimization problems / FASTWIND
- MPI master slave schema:
 - master task took care of the GA-related operations
 - slave tasks to perform the model calculations
- 7000 possible models



CONCLUSIONS

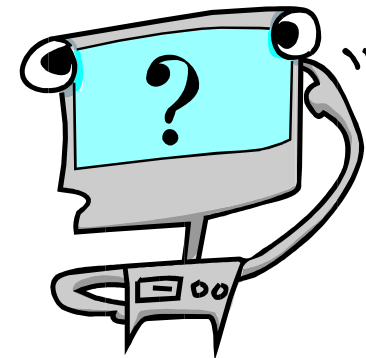
- ❑ **More computational challenges are running right now**
- ❑ **An infrastructure ready to use**
- ❑ **Decreasing time to solution on a wide spectrum of problems**

END



THANK YOU!

QUESTIONS



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