

CENTRO DE SUPERCOMPUTACIÓN DE GALICIA

Retos Computacionales en el Finis Terrae

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DESENVOLVEMENTO REXIONAL

FIDES TERRAE



EXPANDING
THE
FRONTIERS OF KNOWLEDGE

SANTIAGO DE COMPOSTELA, SPAIN,



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Spanish National Singular Scientific & Technological Infrastructure

More than: **16,000 GFLOPS**

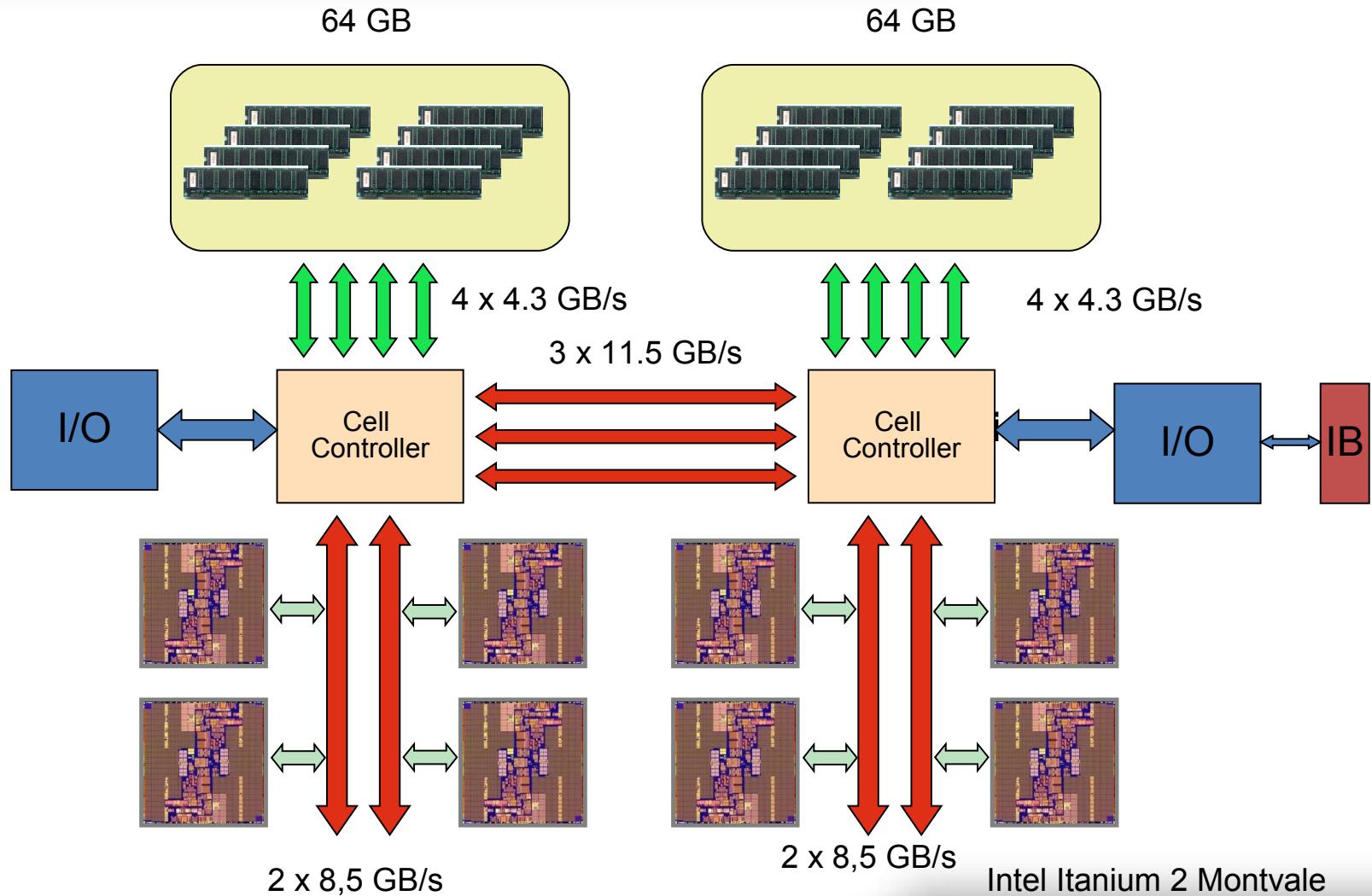
2,580 CPUs

19,640 GB Memory

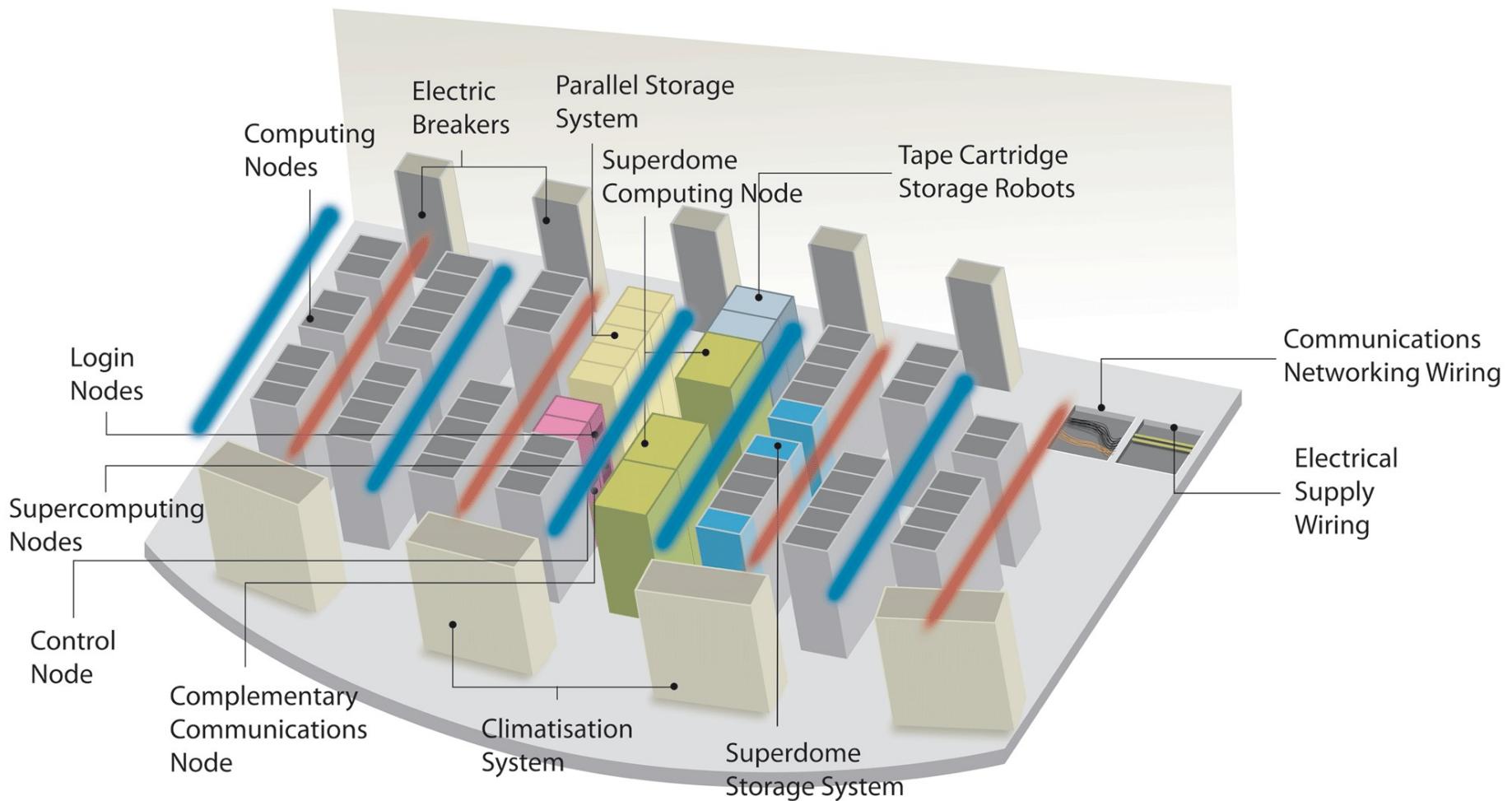
SuSE Linux Enterprise Server 10

SANTIAGO DE COMPOSTELA, SPAIN

RX 7640 Architecture



The Finis Terra Cluster



Technical Specs.

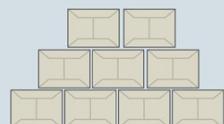
Surface Area: 140 m²

Weight:



35.000 Kg

Storage:



2.200.000 GB
on tape

390.000 GB
on disk

Memory:



19.670 GB

2.528 Processing Cores

142 nodes, each with 16 cores & 128 GB memory
1 node with 128 cores & 1.024 GB memory
1 node with 128 cores & 384 GB memory

Node Interconnect INFINIBAND
4x DDR at 20 Gbps

85 Km of interconnect cable
Open Software: Linux, Lustre, Globus...

CHALLENGES SELECTION

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

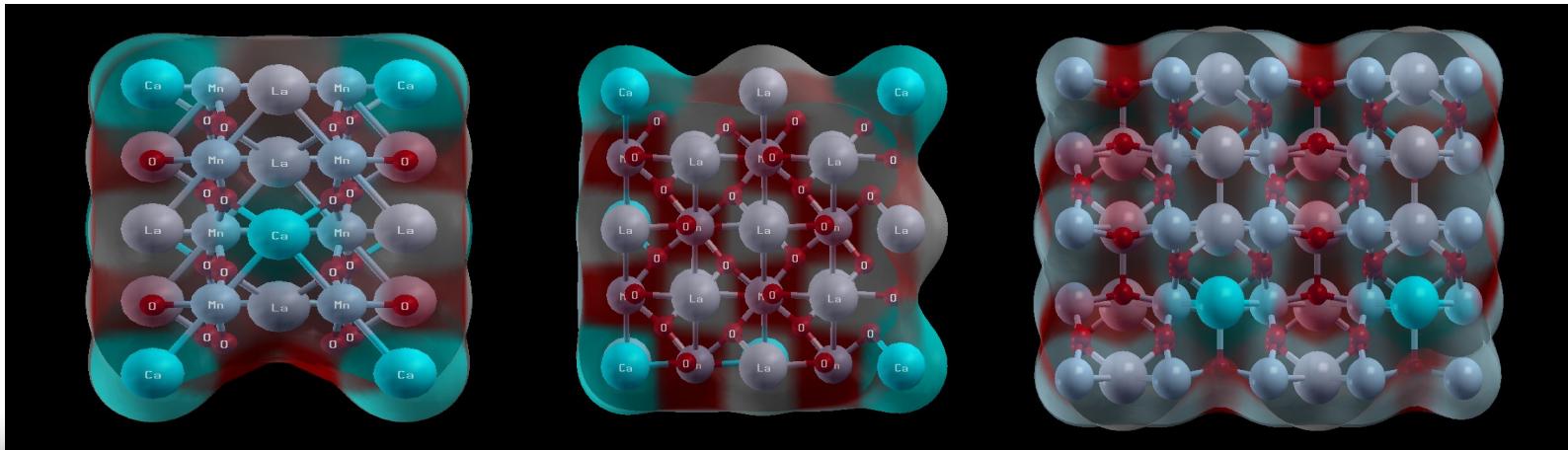


CHALLENGES

- Phase separation
- Massive stars
- Fekete Points
- HEmCUVE

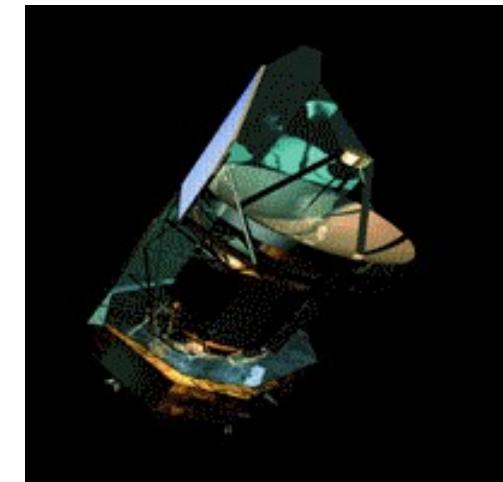
"PHASE SEPARATION"

- Condensed Matter Physics: Materials Design
- 3rd/4th physics most important problem of decade (AIP)
- Wien2k: electronic structure calculations of solids using density functional theory (DFT).
- Two levels parallelism:
 - Coarse grain: k points
 - Fine grain: ScaLapack
- 24 nodes: 384 cores, 100G memory, 300G disk -> 68.000h



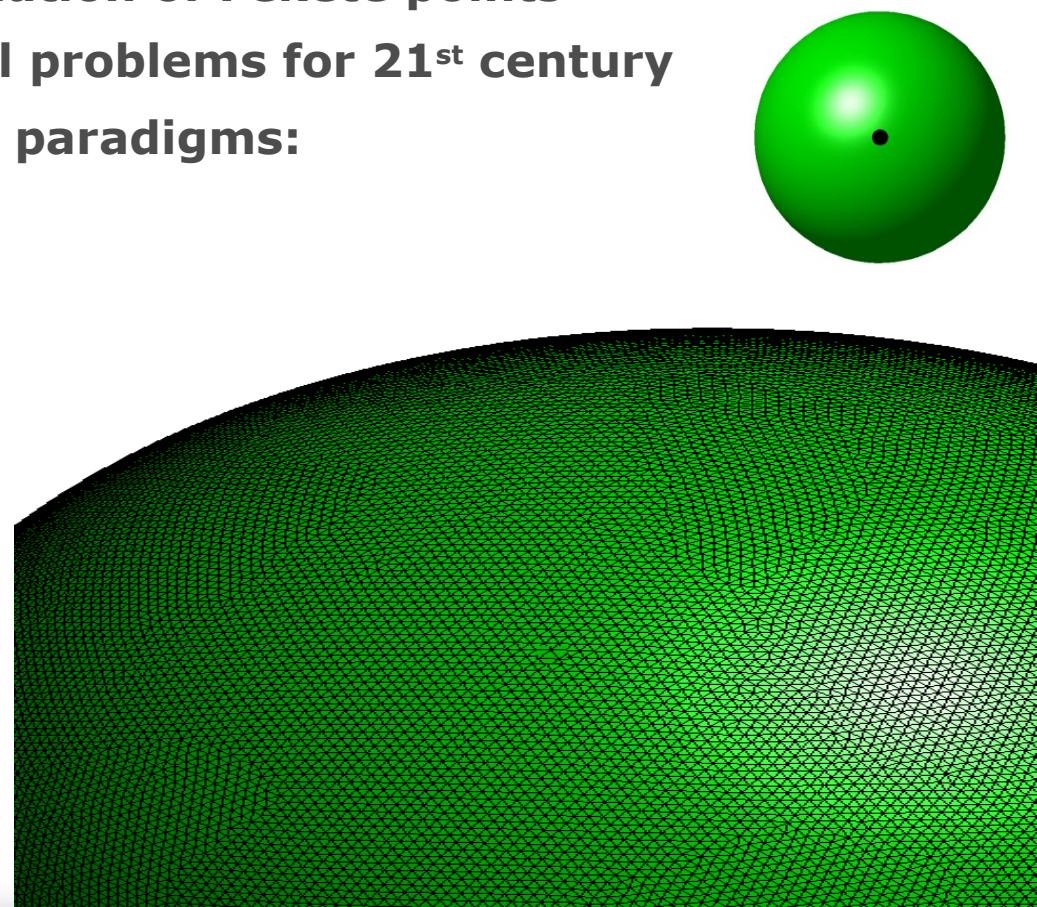
"GENETIC ALGORITHM FOR THE ASTROPHYSICS OF MASSIVE STARS"

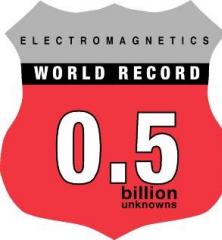
- Molecular and Infrared Astrophysics
- Genetic Algorithms: PIKAIA multimodal optimization problems / FASTWIND
- MPI master slave schema:
 - master task took care of the GA-related operations
 - slave tasks to perform the model calculations
- 20.000 – 40.000 models (15 min each)
- 80 cores



“FEKETE POINTS”

- I-MATH: Applied Maths (Potential theory/Numerical methods)
- Forces Method -> Estimation of Fekete points
- 7th Smale: Mathematical problems for 21st century
- Several parallelizations paradigms:
 - MPI
 - OpenMP
 - MPI/OpenMP
 - High Throughput
- 1024 cores
- 350.000 hours
- 50 million executions





"HEMCUVE"

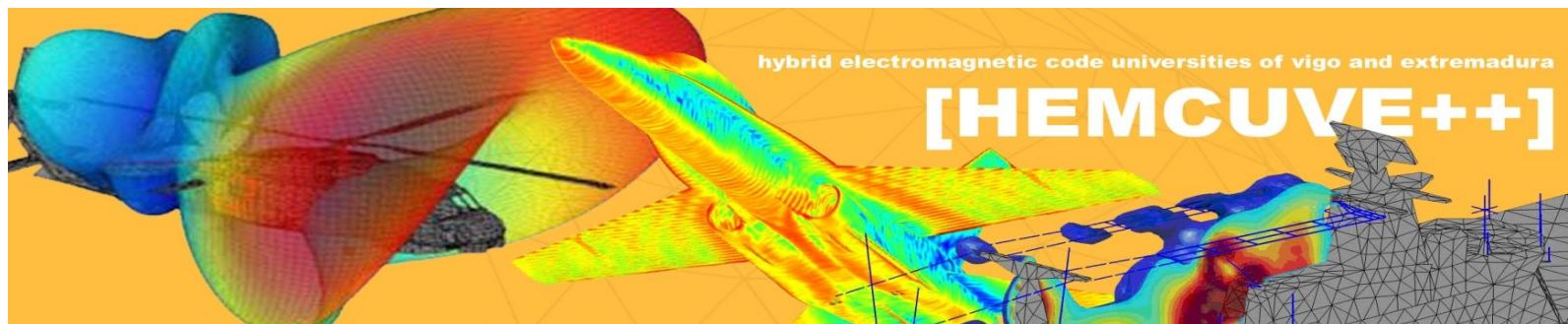


- Electromagnetic problems in large structures
- HEmCUVE++: Electromagnetic calculations based on FAST MULTIPOLE methods
- MPI/OpenMP
- Highly demanding on memory per process:
Balance between CPU time and memory
- 1024 cores, 6T of memory

presented at



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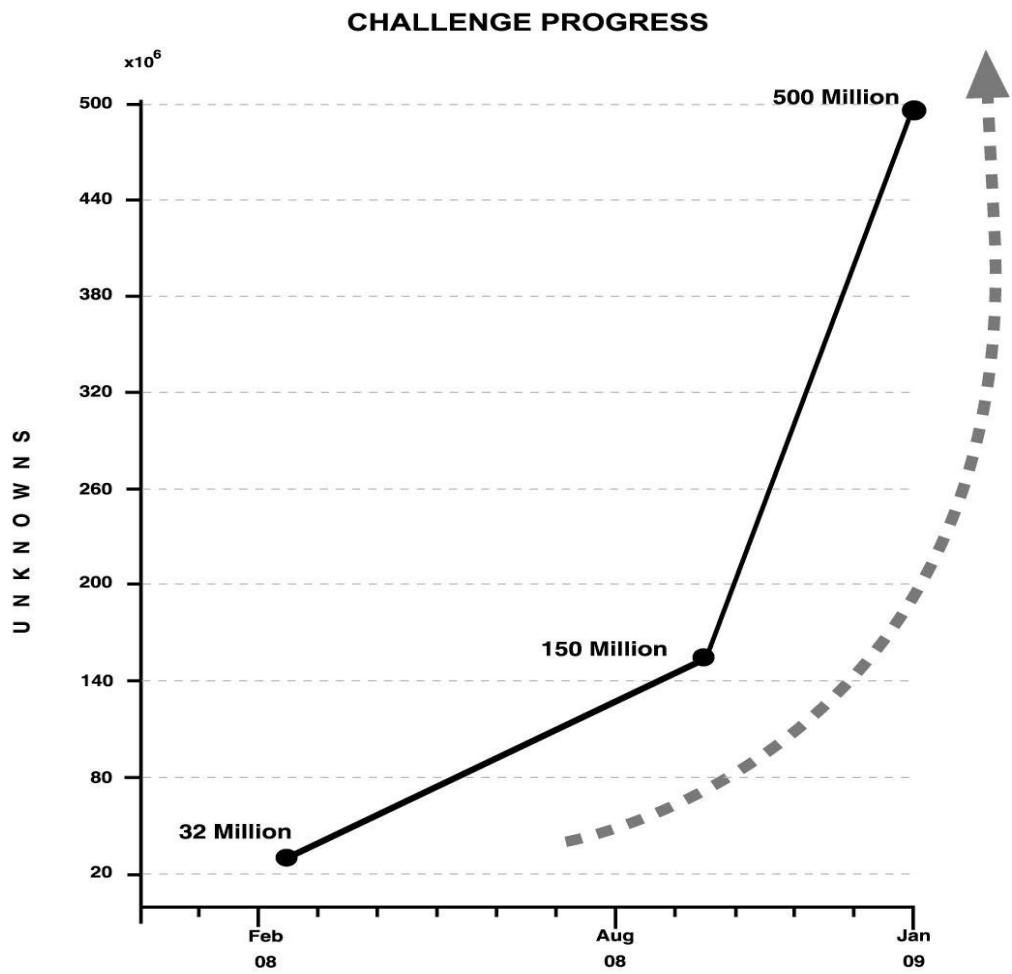


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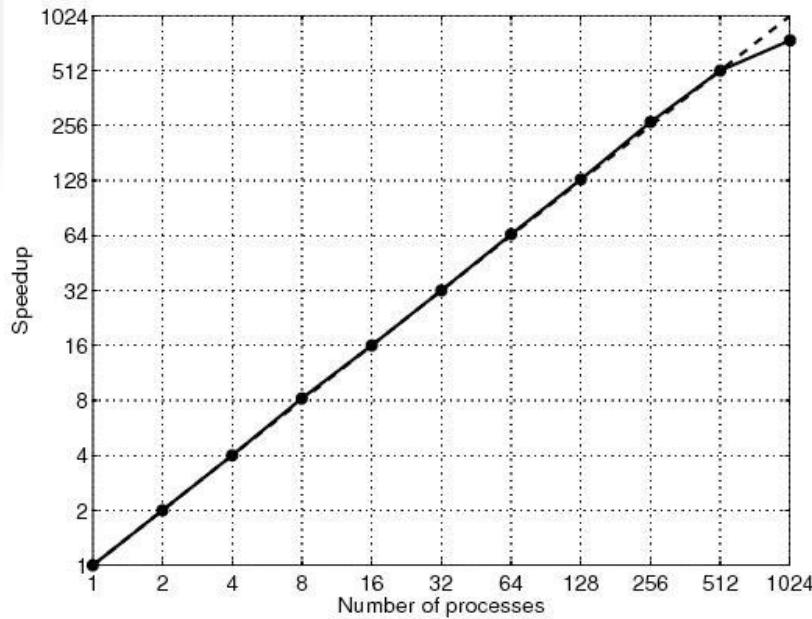


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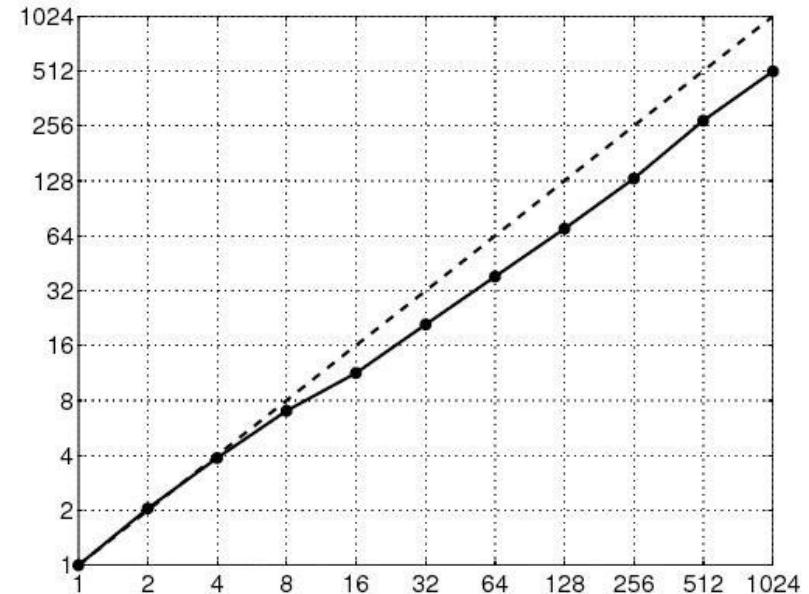
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Scalability



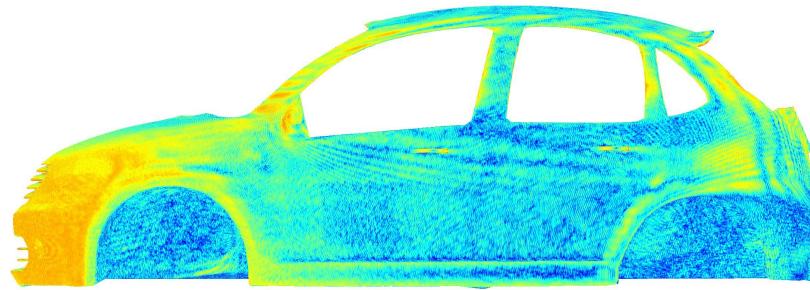
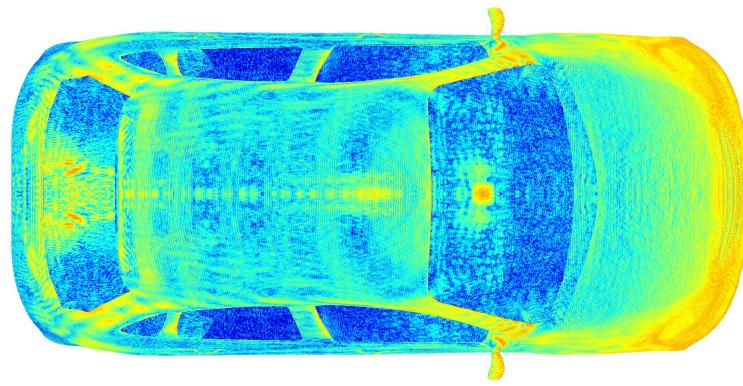
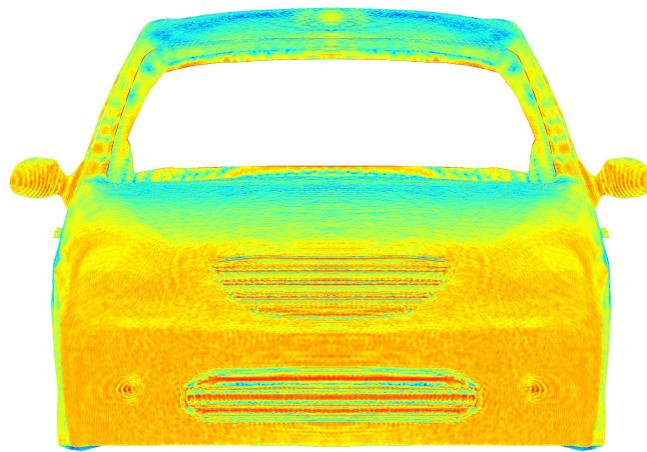
150M code



500M code

"HEMCUVE"

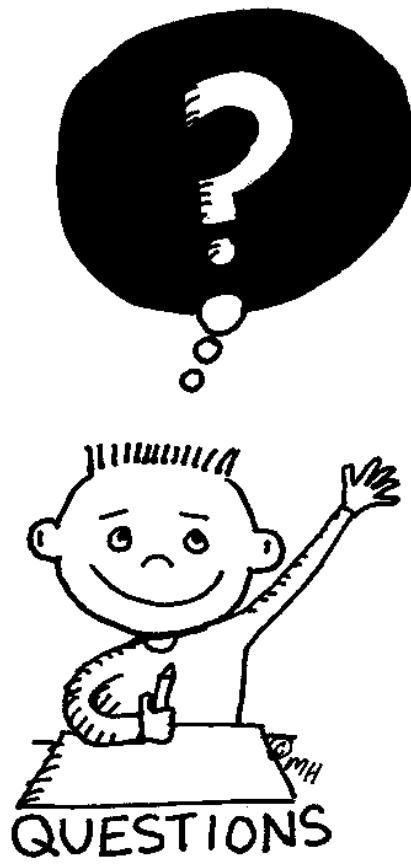
Citröen C3 at 24.125 GHz (radar frequency) 40M unknowns



In progress 79 GHz: 300M – 400M unknowns

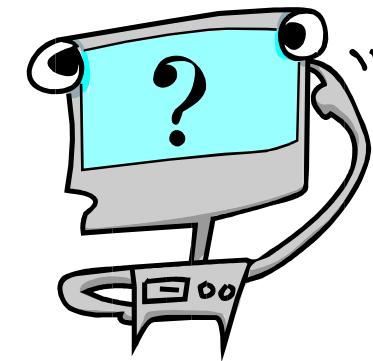
CONCLUSIONS

- Other Challenges are running just now
- New Challenges open call
- Finis Terrae fits this kind of applications
- Decreasing time to solution on a wide spectrum problems
- More than 10 scientific papers



THANK YOU!

QUESTIONS?



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