

**High-Performance Computing Infrastructure for
South East Europe's Research Communities**

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www.hp-see.eu



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High-Performance Computing Infrastructure
for South East Europe's Research Communities



- ❑ **Contract n°: RI-261499**
- ❑ **Project type: CP & CSA**
- ❑ **Call: INFRA-2010-1.2.3: VRCs**
- ❑ **Start date: 01/09/2010**
- ❑ **Duration: 24 + 9 months**
- ❑ **Total budget: 3 885 196 €**
- ❑ **Funding from the EC: 2 100 000 €**
- ❑ **Total funded effort, PMs: 539.5**
- ❑ **Web site: www.hp-see.eu**



HP-SEE Partnership



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Contractors (14)

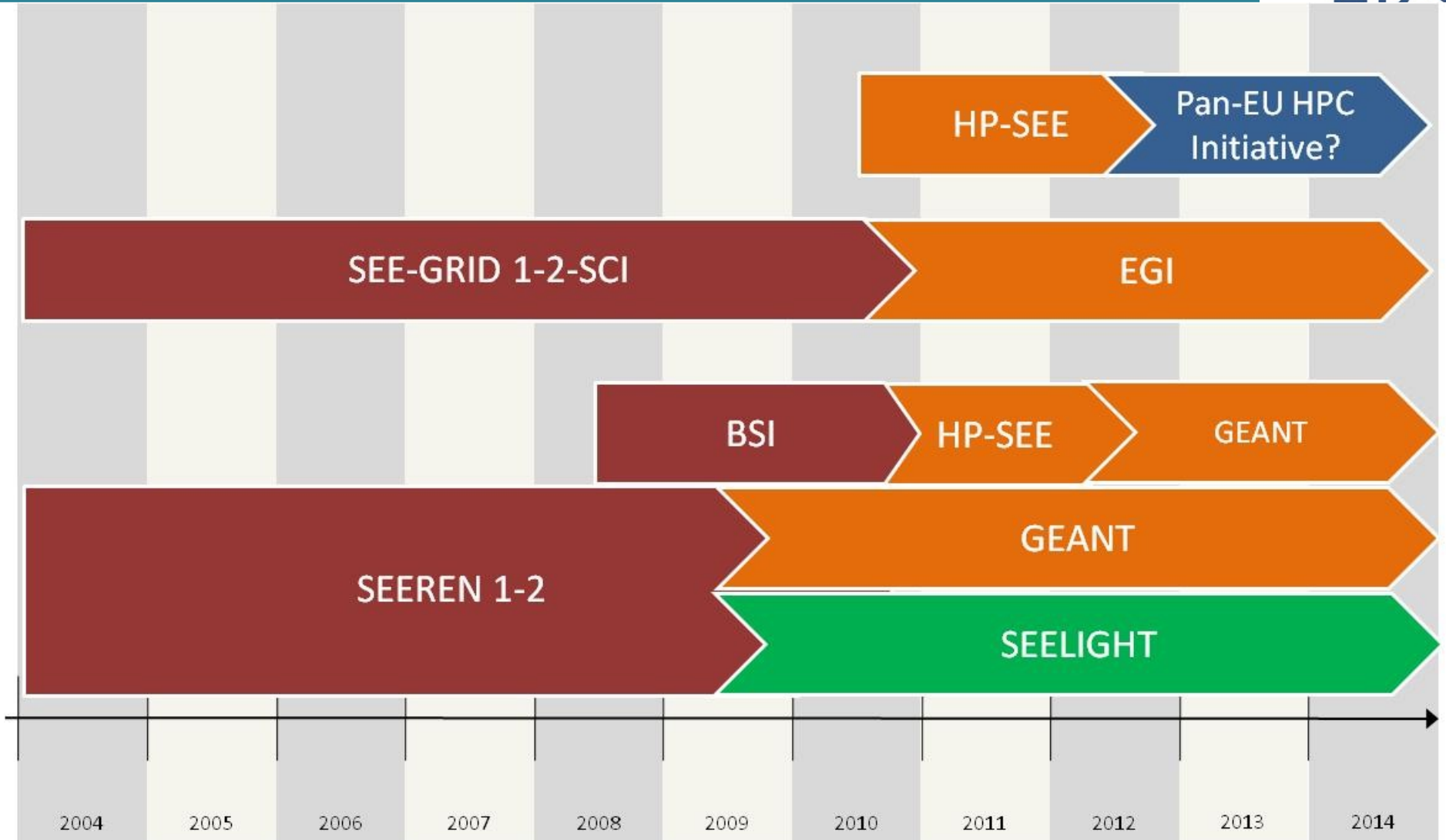
GRNET	Coordinating Contractor	Greece
IICT-BAS	Contractor	Bulgaria
IFIN-HH	Contractor	Romania
TÜBİTAK-ULAKBİM	Contractor	Turkey
NIIFI	Contractor	Hungary
IPB	Contractor	Serbia
UPT	Contractor	Albania
UOBL ETF	Contractor	Bosnia-Herzegovina
UKIM	Contractor	FYROM
UOM	Contractor	Montenegro
RENAM	Contractor	Moldova (Republic of)
IIAP NAS RA	Contractor	Armenia
GRENA	Contractor	Georgia
AZRENA	Contractor	Azerbaijan

**Third Party / JRU mechanism used
associate universities / research centres**

Context: the Timeline



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Building Infrastructure
for Research Communities



Context: the Model - Converged Communication & Service Infrastructure for South-East Europe



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Seismology,
Meteorology,
Environment

Comp physics,
Comp chem, Life science

User / Knowledge layer

SEE-GRID & EGI

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SEE-LIGHT & GEANT

HP-SEE Project Objectives



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- ❑ **Objective 1 – Empowering multi-disciplinary virtual research communities**
- ❑ **Objective 2 – Deploying integrated infrastructure for virtual research communities**
 - ❑ **Including a GEANT link to Southern Caucasus**
- ❑ **Objective 3 – Policy development and stimulating regional inclusion in pan-European HPC trends**
- ❑ **Objective 4 – Strengthening the regional and national human network**

Key results: HPC infrastructure



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Country	Center	Computing Cores	Teraflops
Bulgaria	BG Blue Gene/P	8192	27.85
	HPCG	576	3.23
FYR of Macedonia	FINKI SC	2016	9
	NIIIFI SC	144	0.5
Hungary	Pecs SC	1152	10
	Debrecen SC	3078	18
	Szeged	2112	14
	InfraGRID	400	2.5
Romania	IFIN_BIO	256	2.72
	IFIN_BC	368	3.9
	NCIT	562	3.4
	UVT Blue Gene/P	4096	13.9
	PARADOX	672	6.26
Serbia			
TOTAL		23624	115.26



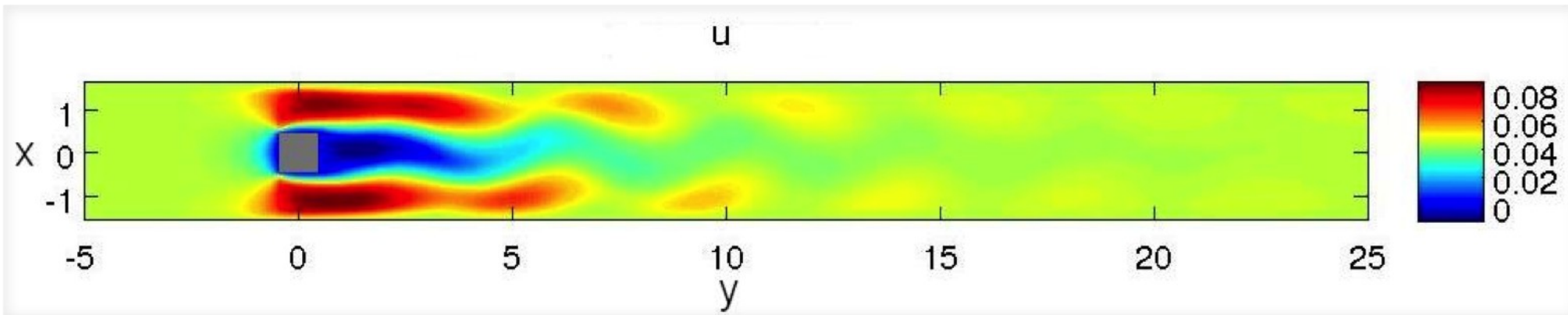
CP VRC – Selected Results



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- **Finite Volume Method for calculation of 2D gas-microflows using standard MPI**
- **Simulation of internal and external gas flows in or around micro mechanical devices**
-



Mach number 0.05, Knudsen number 0.001 (mean free path of molecules / square size)

CC VRC – Selected Results



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- Design of fullerene and metal-dithiolene-based materials for photonic applications
- Development of computational methods for the reasonably accurate determination of the linear and nonlinear optical properties of nano-systems.
- The investigation of a series of novel nano-systems with possible photonic applications.
- Achieved Scalability: 512 cores
-

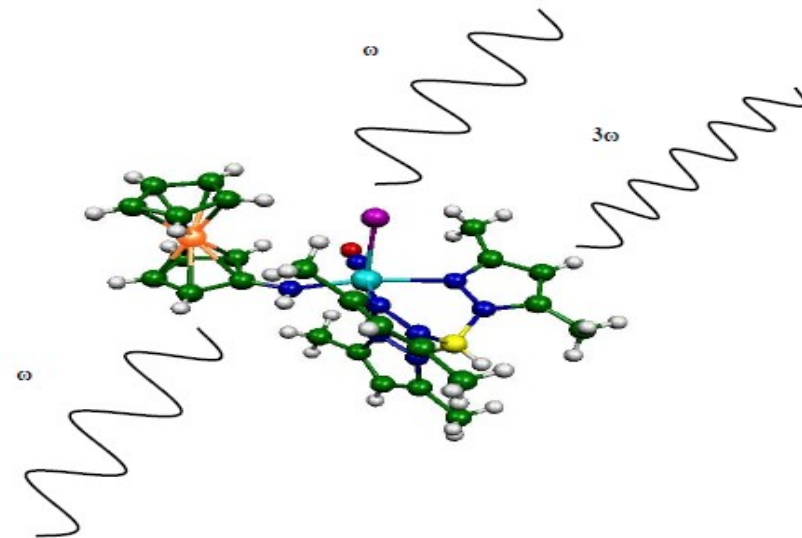


Figure. Third harmonic generation by a ferrocene derivative.

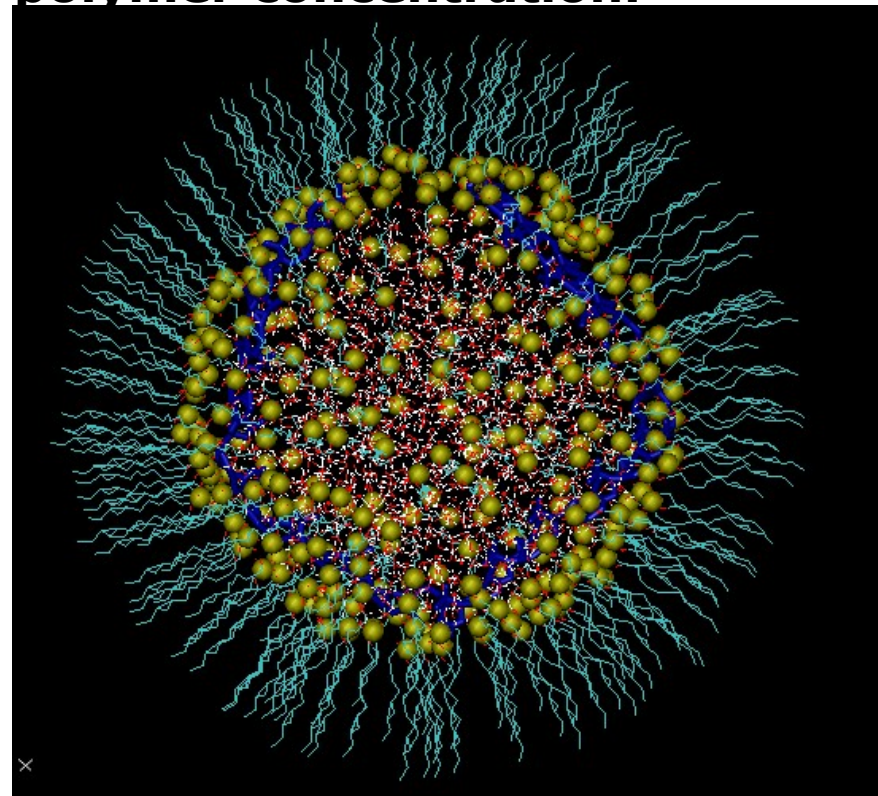
LS VRC – Selected Results



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- **Searching for novel miRNA genes and their targets tems**
- **Parallel molecular dynamics simulation of Sodium dodecylsulfate (SDS) – polymer systems (inverse micellar and lamellar) depending on the temperature and the polymer concentration.**
- **Scalability Achived: 4096 cores**
-



***Figure - Sodium dodecyl sulfate (SDS)/PalH/
water system in oil solute***

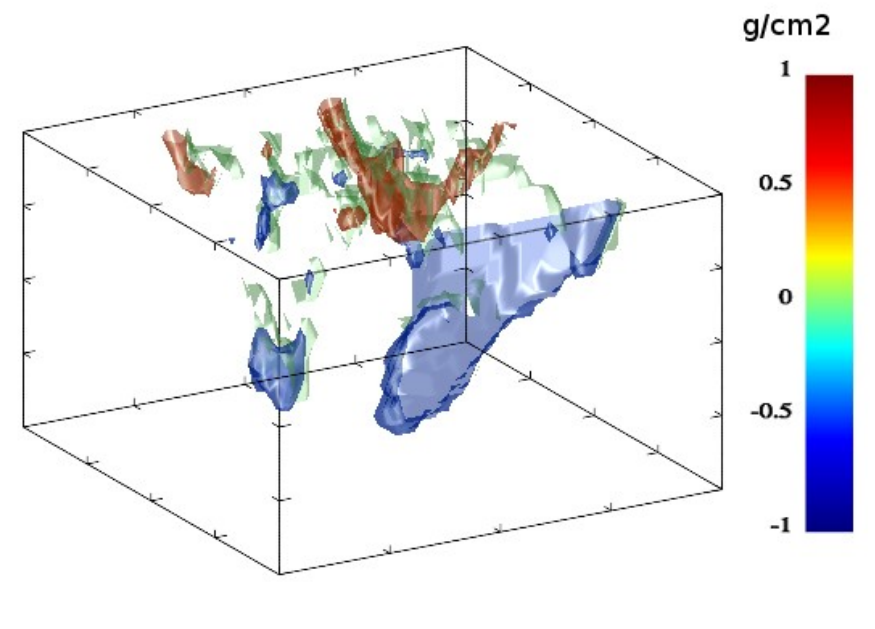
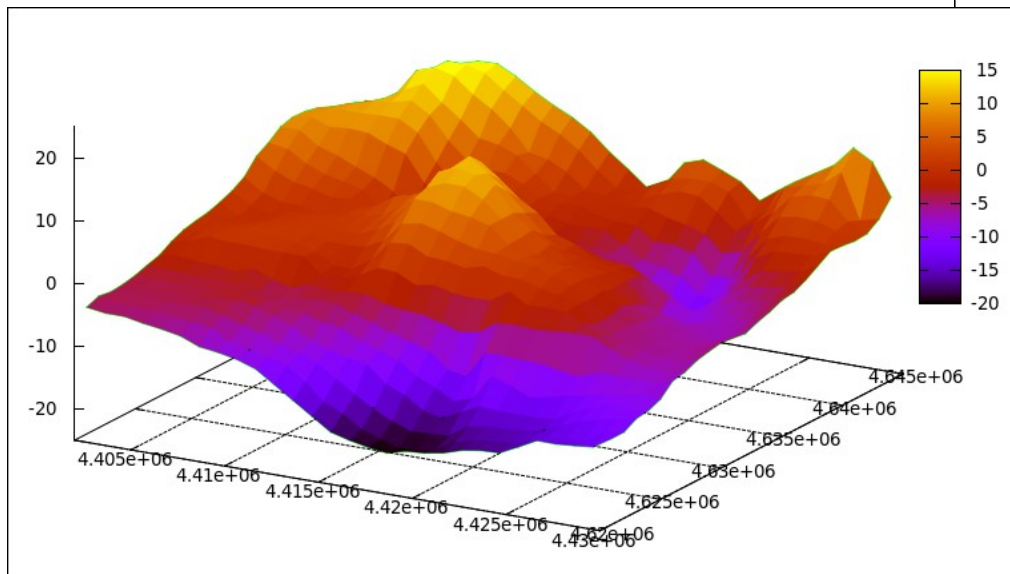
Albania - Gravity Inversion



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- Iterative approach for shaping of anomalous bodies based on ground surface surveys
- From 16 to 1024 cores with OpenMP in Bulgaria and Hungary
- Publications
 - 3 conferences, 2 submissions in journals

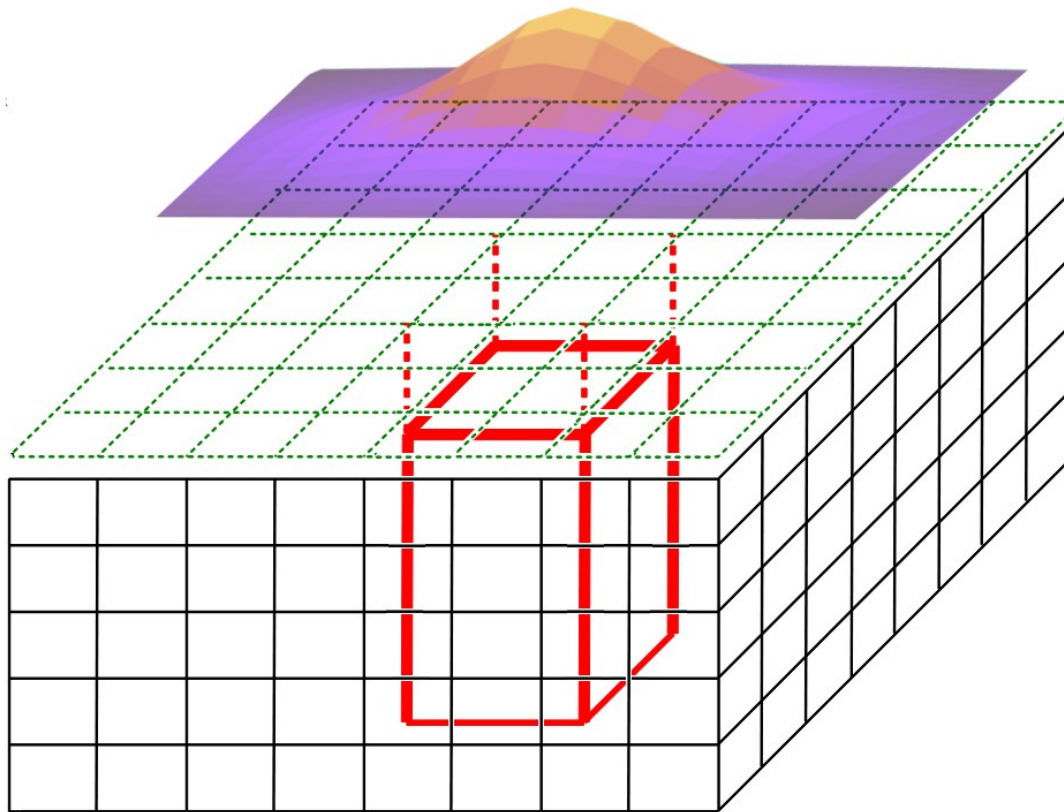


Gravity Inversion Model



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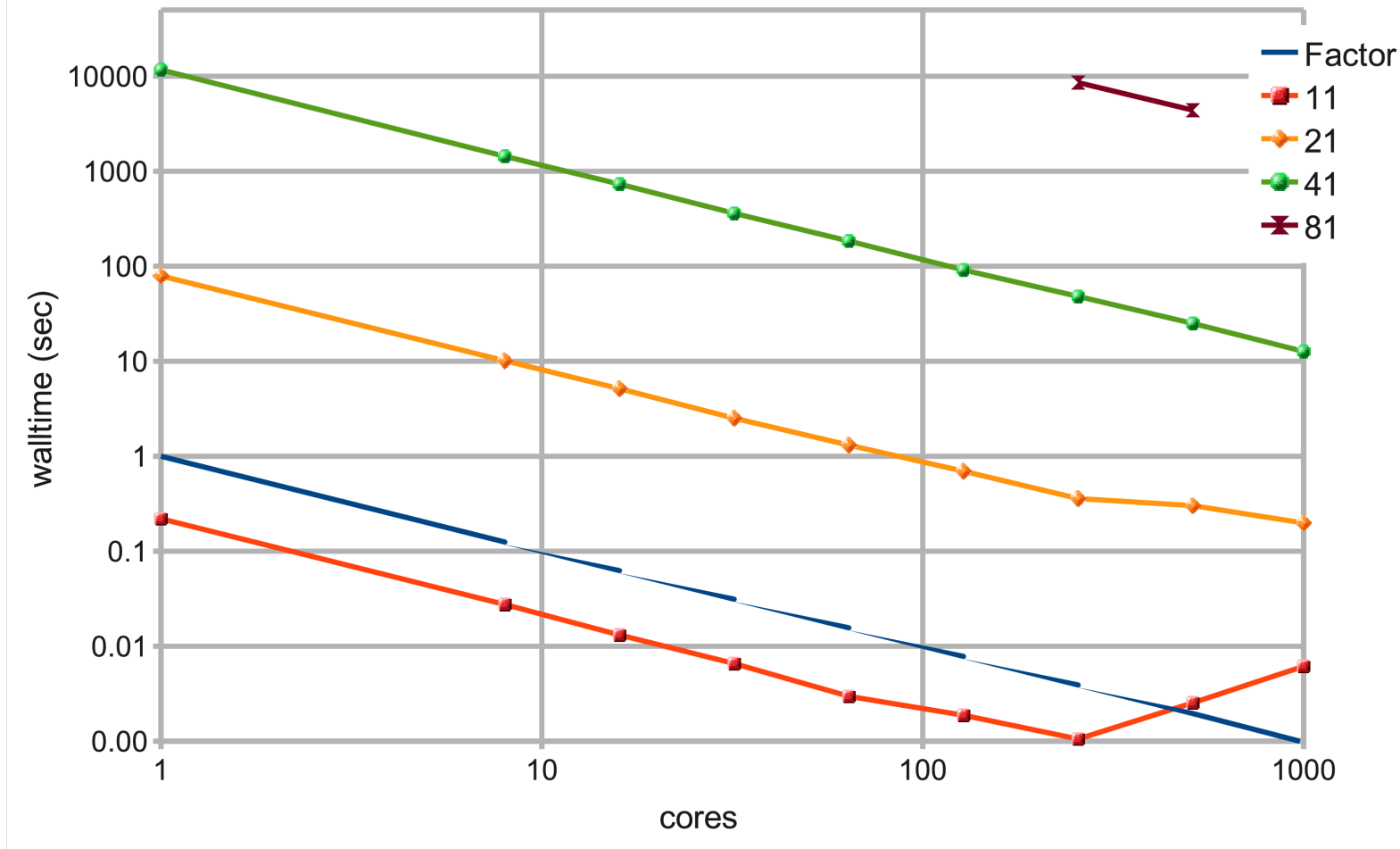
Gravity Inversion Convergence 1



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Usertime per Cores & Nodes



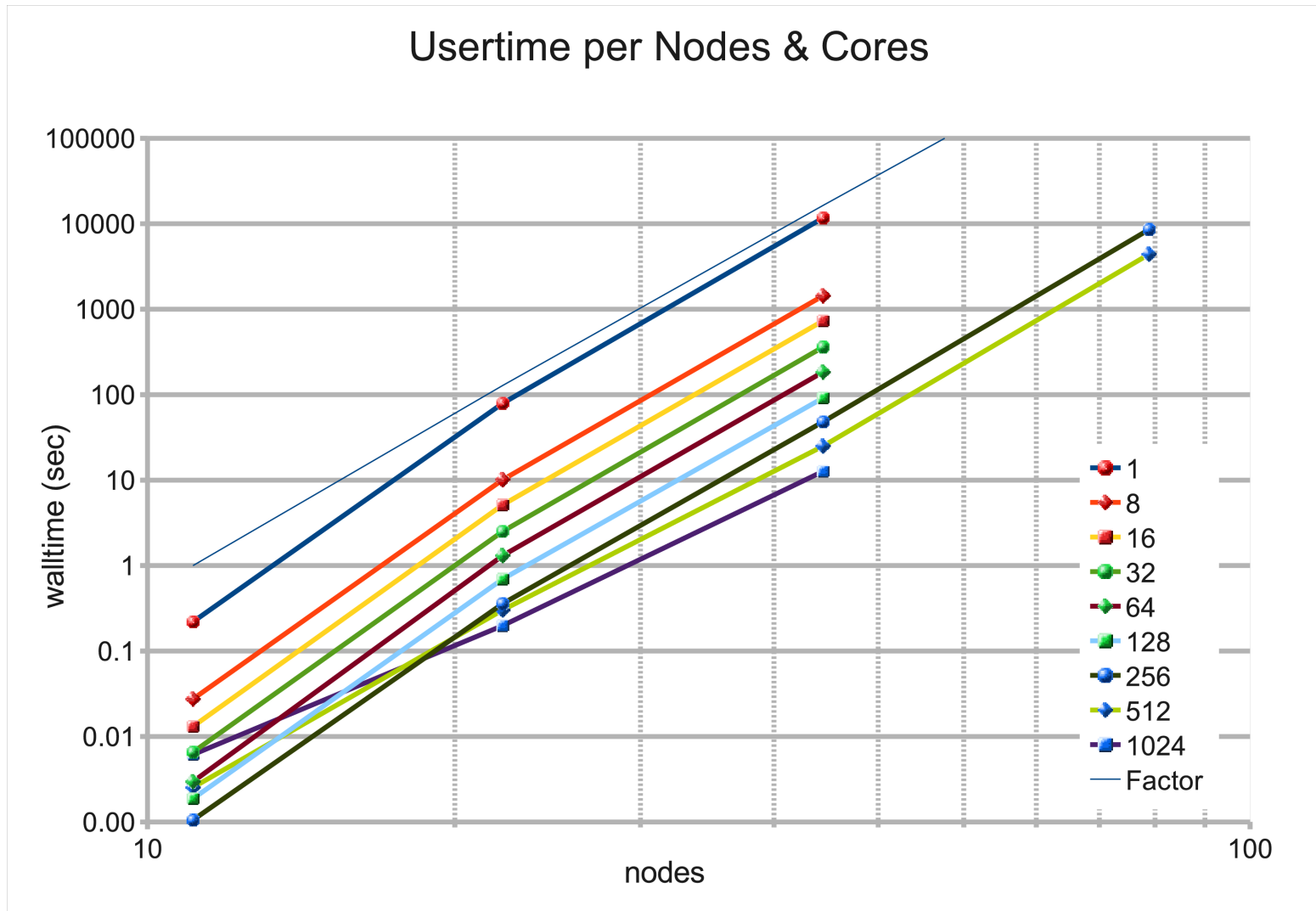
Gravity Inversion Convergence 2



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Usertime per Nodes & Cores

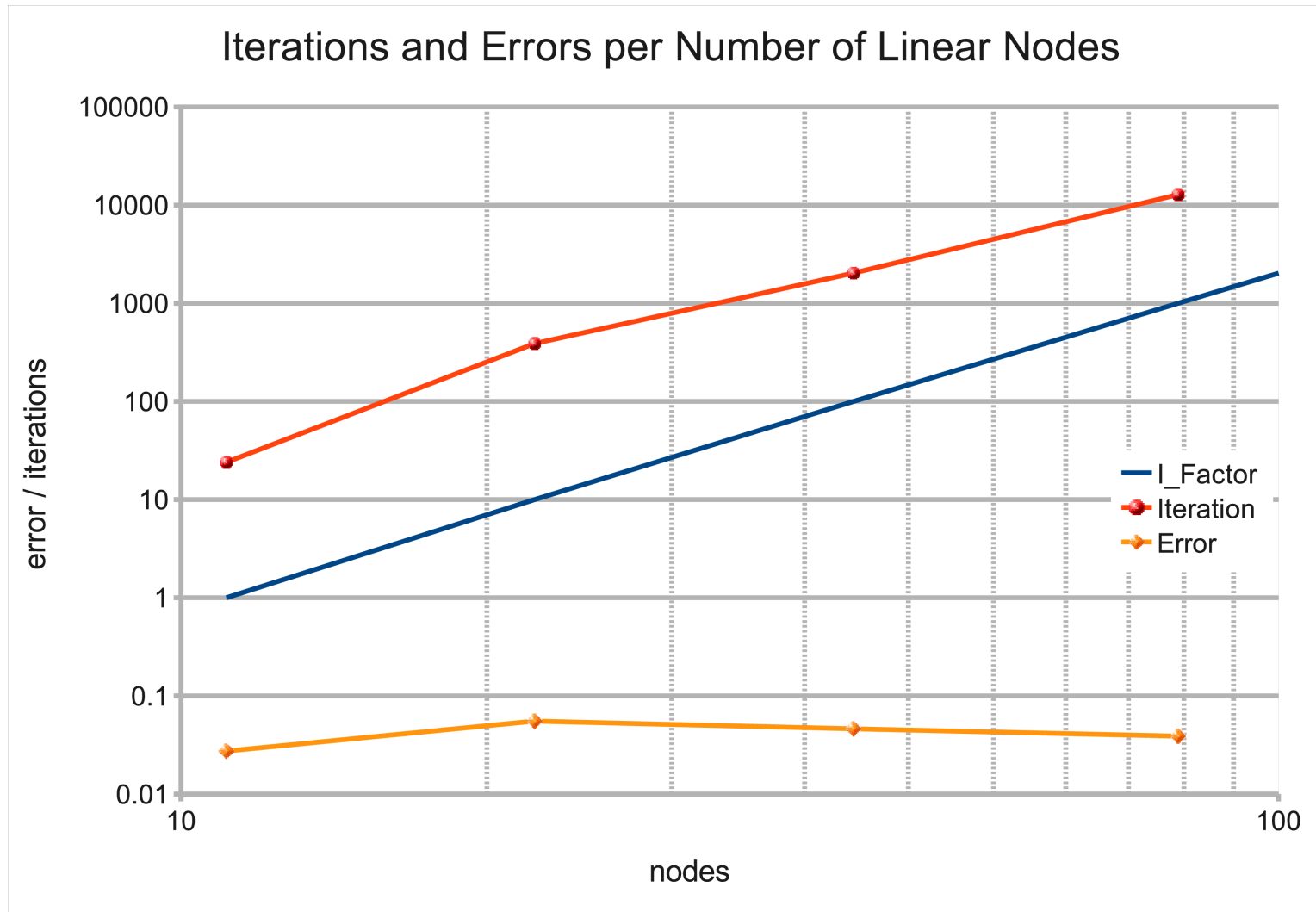


Gravity Inversion Convergence 3



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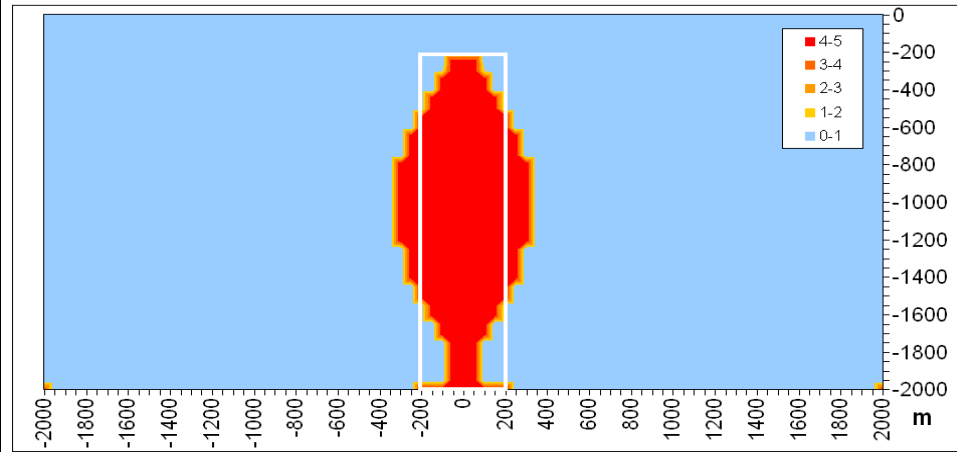


One & Two Bodies Gravity Model

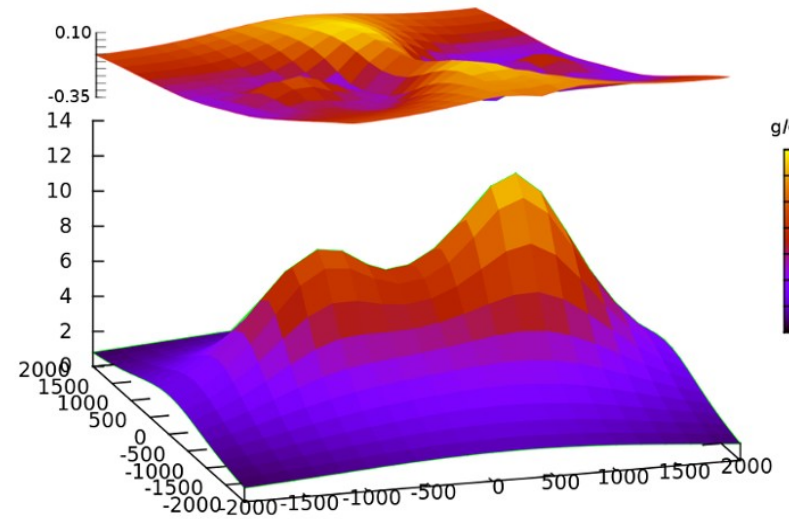
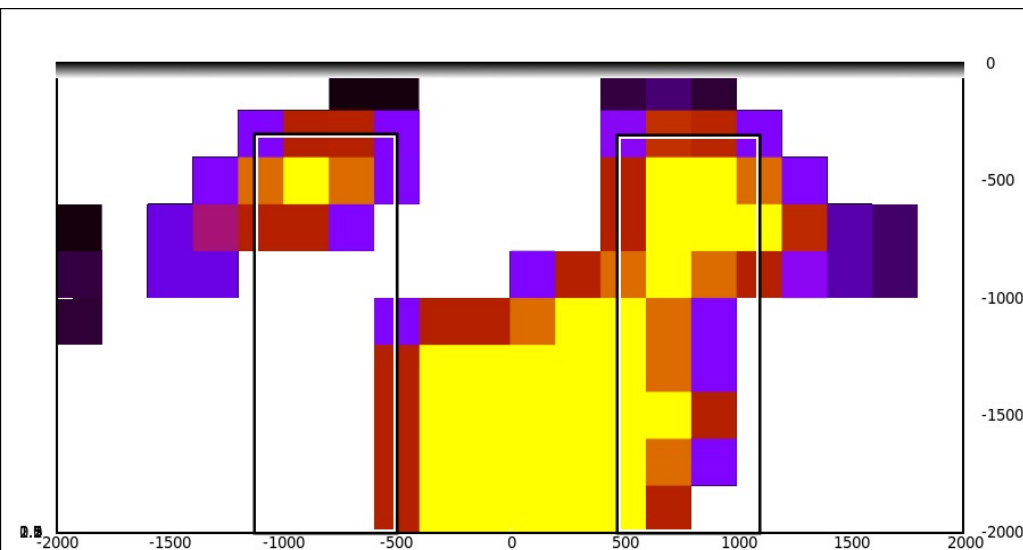
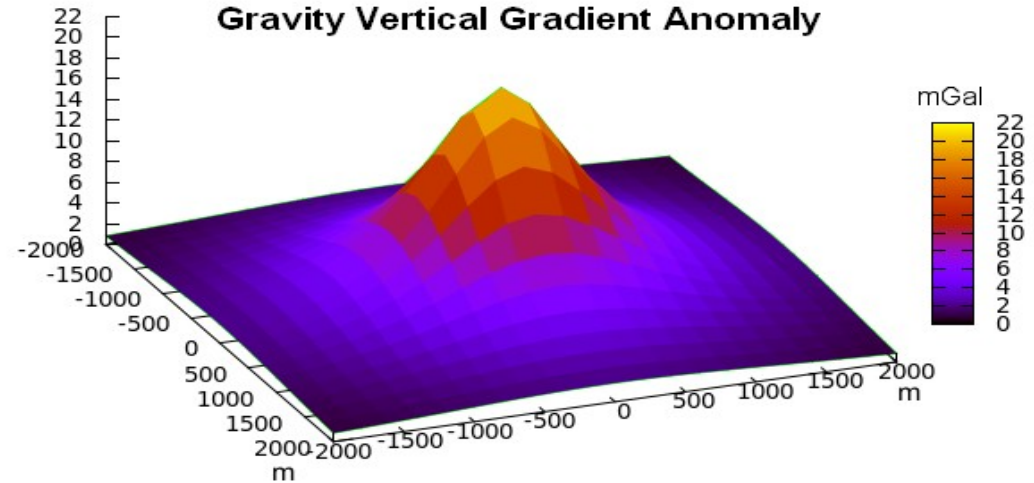


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Anomalous Body 5 g/cm³



Gravity Vertical Gradient Anomaly

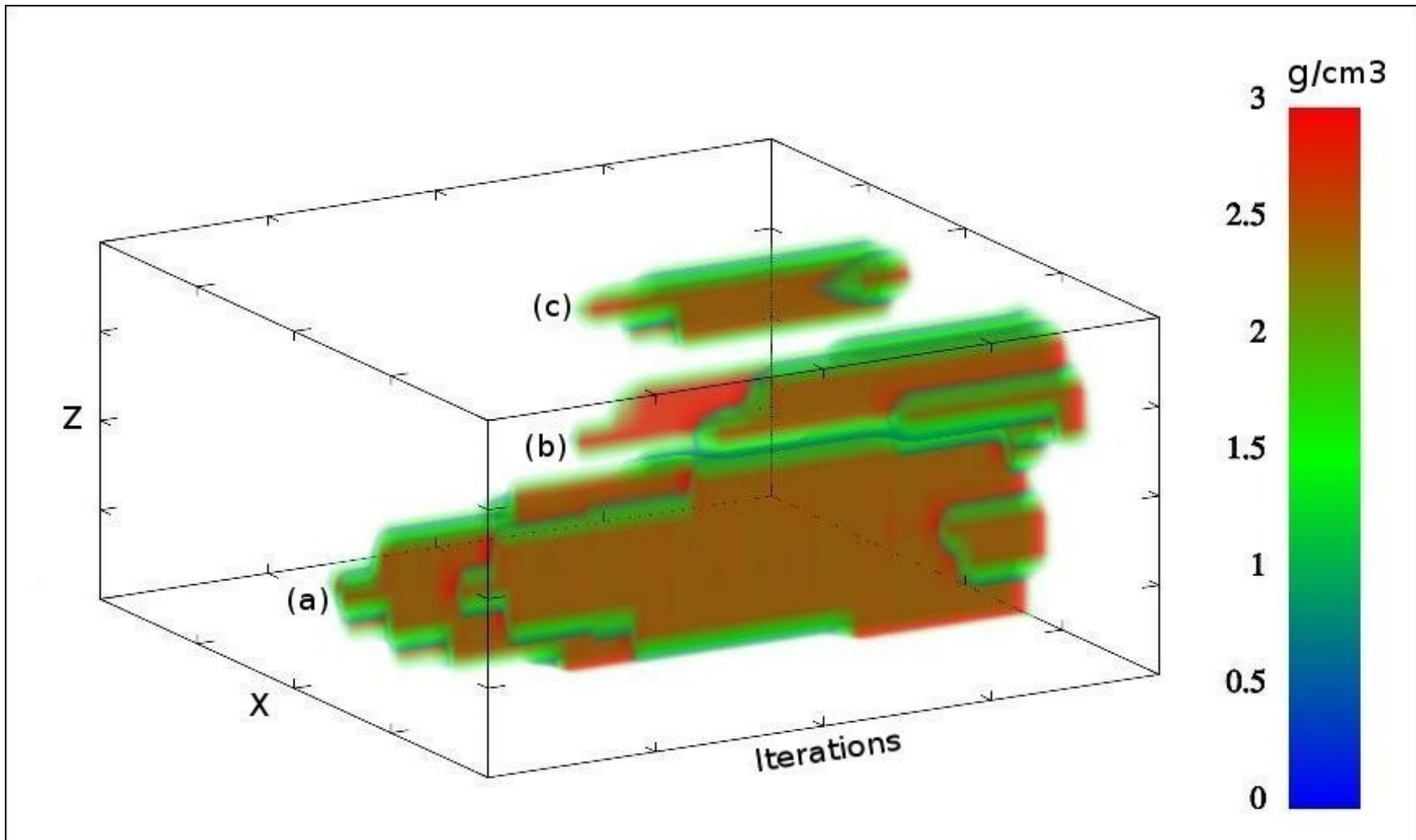


Two Bodies Gravity Inversion



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Gravity Inversion Future



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- ❑ **Until the date results based in OpenMP**
 - **Few shared memory systems available**
- ❑ **Actual work for implementation using MPI**
 - **Use of distributed memory systems**
- ❑ **Possible using GPU with CUDA / OpenCL**
 - **Porting in desktop systems**
- ❑ **Open for future research & development for the optimization of inversion algorithms in parallel systems**

Long-term Vision for HPC



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- ❑ **New parallel system of 256 cores for Albania**
 - **A donation of Chinese government**
 - **Will be available for the research community**

- ❑ **Being on the technological par with the rest of Europe**
- ❑ **Enabling local scientists to use their potential**
- ❑ **Integrating the region into pan-European HPC landscape**
- ❑ **Role-model for regional developments**
- ❑ **Leading the way in wider contexts**

Thank You



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