Distributed European Infrastructure for Supercomputing Applications

DEISA

SEVENTH FRAMEWORK PROGRAMME

Proposal

for a challenging project within the DEISA Extreme Computing Initiative (DECI-6)

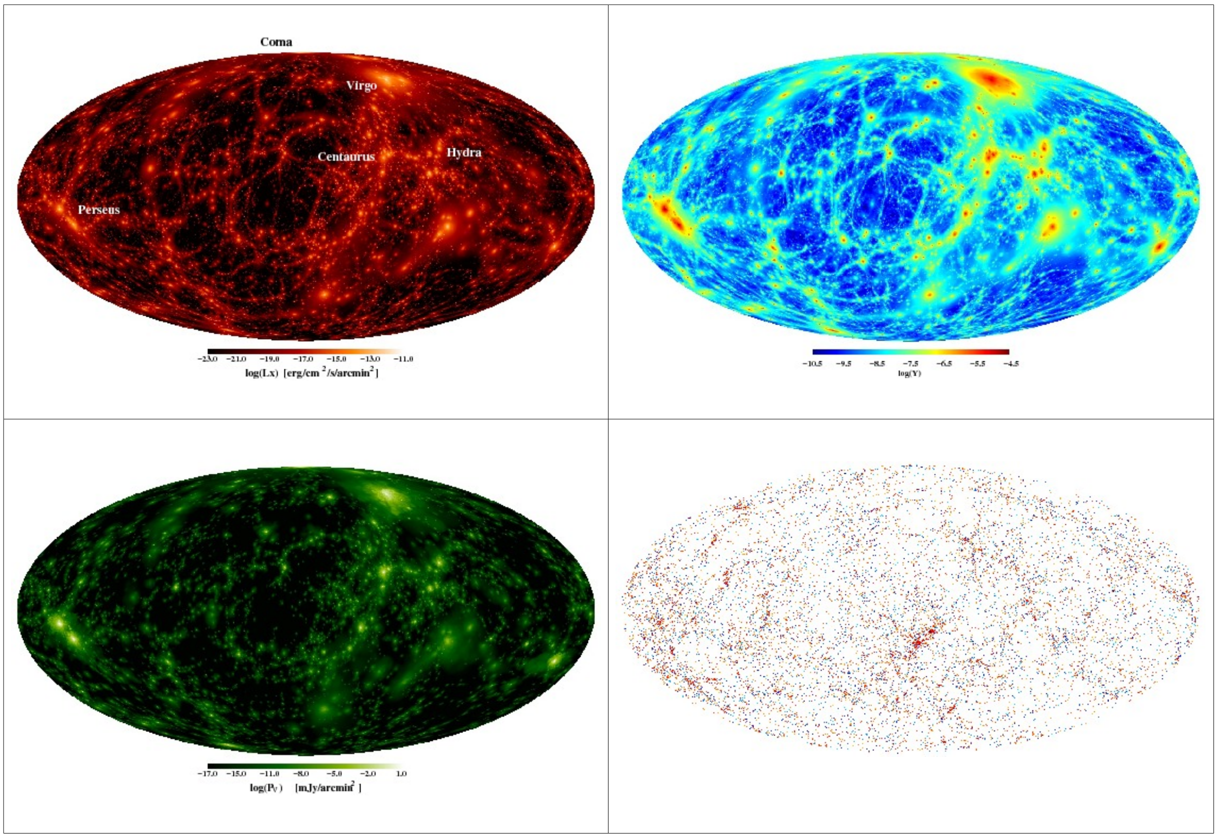
DEISA is an EU FP7 Research Infrastructure Project to advance computational sciences in the area of supercomputing in Europe.

The DEISA Extreme Computing Initiative is aiming at leading, ground breaking applications in selected areas of science and technology dealing with complex, demanding, innovative simulations with a label of excellence from at least one national evaluation committee.

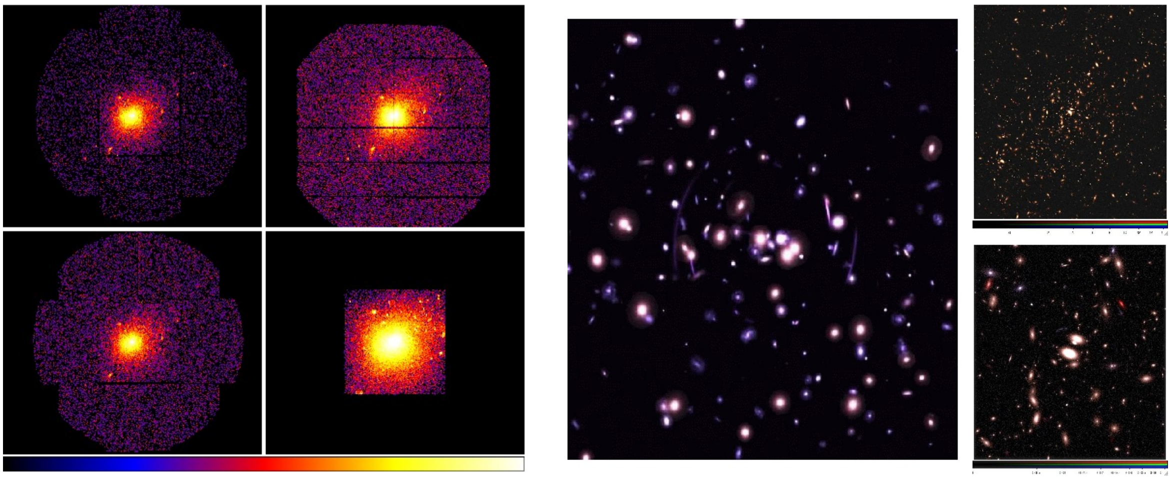
The initial focus on "Grand Challenge" applications with only little or moderate application enabling work for the DEISA environment has been expanded to include medium to long term support for important complex application enabling.

*Please mail this **Proposal** to the DEISA Executive Committee* execomm@deisa.eu *(and in cc to:* ataskf@deisa.eu*) not later than **February 16, 2010.***
For technical questions please contact the DEISA Applications Task Force ataskf@deisa.eu

Project Title	*Magneticum Pathfinder, towards the next generation of cosmological structure formation simulations*
Project Acronym	*MagPath*
Principal Investigator	*Klaus Dolag*



Synthetic multi-wavelength full sky maps of a low resolution MHD cosmological simulation using ***Smac*** (Dolag et al. 2005). From top left to bottom right: idealized X-Ray signal, Sunyaev-Zeldovich (SZ) signal and synchrotron signal (radio; from Donnert et al. 2010) and the distribution of galaxies, color-coded by their photometric colors (from Nuzza et al. 2010).



Synthetic maps of high-resolution simulations of galaxy clusters (Dolag et al. 2009a) produced by virtual telescopes. Left for different X-ray telescopes using ***X-MAS2*** (Rasia et al. 2008), right for different optical instruments and including the gravitational lensing signal from the cluster using ***SkyLens*** (Meneghetti et al 2009).

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DEISA Extreme Computing Initiative

Principal Investigator

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Benedetta Ciardi	*LOFAR*	MPA
Jochen Weller	*EUCLID*	USM

In case of further cooperating institutions, please extend the above table.

Research area: <please describe the research area here, and also tick one box only below>

Principle area	
Astrophysics	☒
Bio-Sciences	☐
Earth Sciences	☐
Engineering	☐
Materials Science	☐
Plasma Physics	☐
Particle Physics	☐
<if ‘Other’, specify here>	☐

DEISA Extreme Computing Initiative

Type of proposal with respect to resource requirements

	low	medium	high
Computing time requirements: **total number of core-hours**			1.6M
Computational resources requirements: **number of cores per job**			2048
Storage requirements within DEISA			10 TB
Requirements for **application enabling**		2 FTE	

Proposals with 'application enabling requirements only' will also be considered.

For the above table, examples for low, medium or high requirements are:

core-hours: low: < 300 k core hours; high: > 1 M core hours
number of cores: low: < 128 cores per job; high: => 1024 cores per job
storage resources: low: < 500 GB; high: > 5 TB
application enabling: low: < 1 FTE month; high: > 3 FTE months
where
FTE is a Full Time Equivalent of a single person;
low implies limited migration effort, else application requires specific fine tuning and optimization, and potentially includes eventual redesign (I/O redesign, scalability extension, workflow design, etc.);
medium: 1 FTE more than 1 month and less than 3 months;
high: 1 FTE more than 3 and less than 6 months.

Resource Requirements per Application

If you have more than one application, i.e. a pre-processor, post-processor, workflow of applications, etc., then please **copy this table for each application**

Total number of core hours *(elapsed time of a single run)* * *(number of cores used in a single run)* * *(total number of runs). Include a lower bound, if relevant.*	700k-900k 2048 2
*Type of core, clock rate and **architecture on which this Total number of core hours requirement is based** (i.e. IBM Power5/Power6/ PowerPC, SGI Itanium-2, NEC SX-8 or Cray XT4/XT5 Opteron)*	SGI Itanium-2
Requirements for a typical run	
Maximum number of usable cores	2048

Minimal memory per core (GB) at maximum number of cores	3GB
Total memory for smallest target problem	3.2TB
Total memory for largest target problem	5.5TB
Temporary disk space requirement during a single run (input, output, restart files, etc.)	10TB
Storage requirements for the total project (incl. mass storage)	20TB
Name of application and role (i.e. pre-processor, main application, etc)	**P-Gadget3(XXL)**
Pure MPI or mixed-mode (MPI + OpenMP) communication	MPI + pthreads
Own / 3rd party code	own
Own / 3rd party input files	own
Code commercial (yes/no)?	no
Code publicly available (yes/no)?	no
Commercial library requirements	no
Non-commercial library requirements	FFTW, gsl
Architecture(s) where application is already used in production, if any	P4/P5/P6/Intel/amd
Site name(s) where application is already used in production, if any	LRZ,RZG,CINECA
Preferred target architecture(s)	none
Data management tools requirements, i.e. if runtime access to remote databases is required, are they public or private?	
Application enabling work requirements (porting, code optimisations - single core and/or improved scaling)	
Any other requirements	
Physical problem simulated (e.g. MHD, CFD, Solid Mechanics, MD, weather, QCD, galaxy formation, etc.)	MHD, structure formation
Main computation kernel (e.g. SPH, T/DFT, FEM, FVM, Spectral, etc.)	N-Body Tree-PM+SPH
DEISA middleware requirements/preferences (UNICORE, DESHL, GridFTP, etc.)	

DEISA Extreme Computing Initiative

Project Title: Magneticum Pathfinder, towards the next generation of cosmological structure formation simulations.

Project Acronym: MagPath

Abstract:

This project aims to follow the formation of cosmological structures in a so far unaccomplished level of detail by performing one large scale plus one high-resolution simulation, taking into account many physical processes to allow detailed comparison to a variety of multi-wavelength observational data. We view this as a pathfinder simulation towards what will be needed as the ultimate theoretical counterpart of upcoming, large volume and multiple wavelength astronomical surveys from instruments like Planck, SPT, Pan-STARRs, LOFAR, eROSITA and many more. In combinations with datasets from these surveys, our proposed simulations will enable forefront studies of the formation and evolution of galaxies and galaxy clusters as well as the study of dark energy and the origin of cosmic acceleration.

Detailed Project Description and Relevance for DEISA

1. scientific objectives

Introduction:

It is now well accepted that the observed structure of our universe is best reproduced in the presence of cold dark matter and dark energy, within the framework of ΛCDM cosmology, in which structures form in a hierarchical bottom up fashion. The increased size, range and completeness of observational data obtained using the latest generation of astronomical instruments recently opened the so-called era of precision cosmology, meaning that the basic parameters describing the standard cosmological model can be in principle determined with a precision of ten per cent or better. Therefore, we have now entered the period where we need to understand the formation of structures in the universe with high precision, e.g. investigating large volumes by following in detail the internal structures of observable tracers of the underlying matter distribution, like galaxies and galaxy clusters. In our hierarchical picture of structure formation, small objects collapse first and then merge in a complex manner to form larger and larger structures. To a first approximation one can study the formation of cosmic structures using N-body simulations, which basically follow the evolution of collision-less particles under gravity. Such simulations have been performed with high resolution for individual objects, like galaxies and galaxy clusters as well as for very large-scale structures. However, with the possible exception of gravitational lensing, observations mainly reflect the state of the ordinary (baryonic) matter. Therefore, their interpretation in the framework of cosmic evolution requires that we understand the complex, non-gravitational, physical processes, which determine evolution of the cosmic baryons. The evolution of each of the underlying building blocks -- where the baryons fall into the potential well of the underlying dark matter distribution, cool, and finally condense to form stars -- within the hierarchical formation scenario will contribute to the state and composition of the inter-galactic and intra-cluster media (IGM and ICM, respectively), and are responsible for energy and metal feedback, magnetic fields, and high-energy particles. Depending on their origin, these components will be blown out by jets, winds or ram pressure effects and finally mix with the surrounding IGM/ICM. Some of these effects will be naturally followed within hydrodynamic simulations (like ram pressure effects), others have to be included in simulations via effective models (like star formation and related feedback and chemical pollution by supernovae). Further *components like magnetic fields and high-energy particles need additional modelling of their injection processes and evolution, and must also be self consistently coupled with the hydrodynamics. To fully exploit the potential of the upcoming large sky surveys for cosmology and for the study of the effects of Dark Energy, we need to improve the predictions of how the large-scale structure is traced by luminous matter. This requires a detailed description in simulation codes of the above-mentioned complex astrophysical processes and their impact on observational properties of cosmic structures. This project is aimed at providing an essential step forward for the overall ambitious programmes for precision cosmology.*

Limitations of current cosmological simulations:

Most current large-scale high-resolution cosmological simulations are based on pure gravitational physics (examples: Millennium, Springel et al. 2005; Millennium II, Boylan-Kolchin et al. 2009; Coyote Universe, Heitmann et al. 2008). These simulations are usually complemented by running the so-called Semi Analytic Models (SAMs) of galaxy formation. While SAMs provide a realistic description of the properties of galaxy populations, they provide at best indirect information on the properties of IGM and, nor do they properly include the dynamical effects of the baryons on structure formation, which is highly relevant for the study of environmental effects. Attempts have been pursued to perform large-scale (e.g. ~500 Mpc/h), hydrodynamical simulations, but they usually include only non-radiative physics (examples: The Marenostrum Universe, Gottlöber et al. 2006) or very crude description of star formation (example: Millennium gas project, Gazzola & Pearce 2007). All such simulations additionally suffer from their poor resolution (typically ~20 kpc/h). Simulations with higher spatial resolution and better treatment of cooling and star formation (examples: Borgani et al. 2004; CLEF simulation, Kay et al. 2004), can only be realized for relatively small simulation volumes (~200 Mpc/h) and still are performed with moderate resolution (typically ~10 kpc/h). Only relatively tiny volumes (~25 Mpc/h) are so far explored at high resolution (2 kpc/h) and with moderate inclusion of physical processes (e.g., Tescari et al. 2009; OWLS, Schaye et al. 2009). However, a more complete and refined description of physical processes, larger volumes and higher resolution are needed to produce a theoretical counterpart to interpret data coming from current and forthcoming astronomical surveys and instruments.

Current state of hydrodynamical cosmological simulations:

The most advanced simulations nowadays include the description of radiative cooling of the gas, sub-resolution prescriptin to follow the formation and evolution of the stellar component and the release of energy and metals from Type II and Type Ia supernova and AGB stars (e.g., Tornatore et al. 2007a, Fabjan et al. 2008, Wiersma et al. 2009). A self-consistent treatment of these processes is necessary for a comprehensive description of the observational properties of the IGM/ICM and of galaxies (e.g. Saro et al 2006, Nuzza et al. 2010). Furthermore, Additional modelling AGN feedback is required to obtain a more realistic description of the the X-ray properties of the ICM in central regions of galaxy clusters and to suppress low-redshift star formation within the most massive galaxies (e.g., Puchwein et al. 2008, Fabjan et al. 2010). Furthermore, transport processes, such as thermal conduction, also affect the structure of the ICM (e.g., Dolag et al. 2004). Including a self-consistent treatment of magnetic fields (Dolag & Stasyszyn 2009) allows one to extend comparison with observations towards radio wavelength (Donnert et al 2010) as well as towards astronomy with Ultra-Hig Energy Cosmic Rays (UHECRs; Dolag et al 2005b). The underlying, hydrodynamical treatment is now advanced enough to even capture additional effects like turbulence within the ICM (Dolag et al 2005a), which should be detected by the next generation of X-ray telescopes. Finally, advanced tools for post-processing of large simulations allow one to reliably detect multi-component substructures (i.e., galaxies; Dolag et al. 2009a) as well as to distinguish different dynamical components within the formed structures (e.g. intra-cluster stars vs. stellar populations in galaxies; Murante et al. 2007, Dolag et al. 2009b, Puchwein et al. 2010).

Aim and spirit of the project:

*The numerical description of all such processes, and a study of their interplay, have been only realized so far in simulations of individual galaxy clusters and groups, with the purpose of describing their effect on the ICM and on other global cluster properties. However, they have never been brought together in a large-scale, cosmological simulation, that would follow not only the evolution of galaxy clusters, but also of the properties of galaxies in different environments and of the inter-galactic baryons permeating the cosmic web. To this purpose, a large volume (1 Gpc/h) simulation with resolution comparable to that of the Millennium Run (10^9 $M_\odot$/h for the mass dark matter particles) would be needed, thus requiring 4096^3 DM particles and as many gas particles. Such a simulation is clearly out of range for current facilities, but in range for key projects on the next generation of European supercomputers. Therefore we here propose (in the spirit of a pathfinder) two simulations, one with the same high resolution but within a reduced volume, and one covering the large volume but with reduced resolution to be performed using **P-Gadget3(XXL)**. Table 1 list the parameters foreseen for the two simulations and the* *mass down to which hydro-dynamical quantities of galaxy clusters (col. 8) and directly simulated galaxies (col. 6) will give converged results as well as the mass limit for galaxies inferred from SAMs (col. 7). In combination, these simulations would:*

1. **shed new light on and enable unique insights into many current astrophysical aspects of structure formation;**
2. **help in the interpretation of observational results and the refinement of observational strategies for many of the current astronomical observatories;**
3. **drive the development and exploration of new simulation and post-processing infrastructure.**

Simulation	BoxSize [Mpc/h]	Resolution [$M_\odot$/h]	Softening [kpc/h]	N_{DM}	Galaxies (hydro) M* [$M_\odot$/h]	Galaxies (SAM) M_{vir} [$M_\odot$/h]	Cluster (hydro) M_{vir} [$M_\odot$/h]
Box1	1000	$2x10^{10}$	14	1536^3	$1.6x10^{10}$	$6x10^{11}$	$2x10^{14}$
Box2	310	$1x10^9$	5	1280^3	$8x10^8$	$3x10^{10}$	$1x10^{13}$

Table 1: Parameters and resolution of the two proposed simulations.

2. scientific and technical innovation potential

Included physics:

The proposed simulations will for the first time combine the description of a number of physical processes, which so far have been developed and tested only separately. Specifically, we plan to include the following modules:

1. *low-viscosity SPH to allow the development of turbulence within the ICM (Dolag et al. 2005a);*
2. *star formation and a detailed model of chemical enrichment (Tornatore et al. 2007a);*
3. *AGN feedback (Springel et al. 2005, Fabjan et al. 2010);*
4. *thermal conduction (Dolag et al. 2004);*
5. *passive magnetic fields based on Euler potentials (Dolag & Stasyszyn 2009)*

Depending on the progress of development and on the testing performance, we will also consider including the description of the following processes, which have been already developed and are currently in a testing phase:

1. *extension of cooling to include low-temperature cooling by molecules/metals (Maio et al. 2007);*
2. *transition of metal free Pop-III to Pop-II star formation (Tornatore et al. 2007b);*
3. *anisotropic conduction (work in progress);*
4. *non-ideal MHD effects, magnetic dissipation (work in progress)*

Primary scientific targets:

- ***Magnetic fields within the large scale structures [KD]***

These simulations will follow for the first time the evolution of magnetic fields within the large scale structures, filaments, galaxy clusters and groups simultaneously (Box1 + Box2). They will provide a self-consistent characterization of the magnetic field structure within large representative volumes of the universe. This will enable statistically meaningful studies of the magnetic field amplification in cluster mergers (Box1), the associated radio emission in the ICM (halos and relics; Box1 + Box2), and the propagation of UHECRs within the large-scale structures (Box2).

- ***Clusters as tracers of the large scale structures [JM,KD,SB]***

These simulations will allow us to predict X-ray and Sunyaev-Zeldovich (SZ) signals from galaxy clusters in so far unaccomplished fidelity (Box2) and for a very large set of simulated cluster (Box1). Individual clusters will be used as templates to improve extraction of cluster properties from joint X-ray and SZ observations (Box1 + Box2). Deep light-cones can be used to predict the performance of cluster finders applied to mock observations (Box1). Both will help to theoretically predict the significance to which cosmological parameters (especially dark energy parameters) can be extracted from current X-ray and SZ observations.

- ***Cluster X-Ray and SZ scaling relations [SB,KD,JM]***

Due to the large volume of Box 1, X-Ray and SZ scaling relations can be extracted for a fair sample of massive clusters, which was not possible given current limitations of hydrodynamical simulations. Making use of the high resolution of Box 2, it will be possible to study the observed transition of the scaling relations towards groups and characterize especially the effect of AGN feedback, which was not taken into account in previous studies using large, cosmological volumes. Moreover, studying the biases affecting the lensing measurements will allow us to verify whether lensing can be used as a powerful complement to X-ray and SZ observations to calibrate cluster masses.

Secondary scientific targets, which will be evaluated within the team of PIs and CoIs:

Box1:

- *Full-sky SZ maps to predict the diffuse SZ signal in the CMB power spectrum from PLANCK [KD]*
- *Full-sky X-Ray maps for eROSITA [KD,HB,JM]*
- *Appearence of massive clusters at high redshift [HB,SB,KD,GD]*
- *Morphology of massive clusters and its evolution [HB,KD]*
- *Distribution of Luminous Red Galaxies and application to measure baryon acoustic oscillations (BAOs) [HB]*
- *Galaxy properties and mock light-cones from SAMs [GD]*
- *Properties of Lyman-alpha transmitted flux and their cosmological application [MV]*
- *WEAK and strong lensing signal and production of mock optical observations using SkyLens [MM]*

Box2:

- *Detailed SZ maps of clusters and groups to study detectability with SPT [JM,KD]*
- *Morphology of groups [HB,KD]*
- *Protoclusters at high redshift [HB,SB,KD,GD]*
- *Physical and chemical enrichment of the high-redshift IGM and interplay with the galaxy population [SB,LT,KD,MV]*
- *Galaxy dynamics in clusters and origin of the intra-cluster light [GM,KD,GD]*
- *Evolution of the galaxy population within clusters [GM,SB,KD]*
- *Galaxy properties in different environments [SB,GD,KD]*
- *Magnetic field properties of groups and forecast of visibility for LOFAR [KD]*
- *Galaxy properties and mock catalogs from SAMs [GD]*

3. current profile and performance of code(s)

General Performance:

P-Gadget3(XXL) *is a highly optimised, MPI/pthread parallelized N-Body TreePM MHD-SPH code. It has already been used to perform several of the world's leading cosmological simulations (e.g. Millennium, MillenniumII, Aquarius and many more). It has been run on various platforms (IBM Power3,4,5,6 / Blue Gene, Linux based intel/amd clusters, SGI Altix, etc.). It shows a very good scaling with large numbers of CPUs, especially for cosmological boxes. From our code testing we expect less than 20% losses due to unbalanced workload effects, especially when using 2048 cores.*

CPU time estimation:

Our CPU time estimation is based on previous simulations of cosmological boxes performed on the ALTIX system at LRZ, as well as several simulations of individual galaxy clusters, carried out to test the additional memory and CPU requirement when including additional physical processes.

The following table compares the resolution and size of the test simulation compared to the proposed ones:

	N	m_{DM} [10^{10} $M_\odot$/h]	L [Mpc/h]		N	m_{DM} [10^{10} $M_\odot$/h]	L [Mpc/h]
Test1	2x960^3	14.1	1200	**Box1**	**2x1536^3**	**2**	**1000**
Test2	2x768^3	0.44	300	**Box2**	**2x1280^3**	**0.1**	**310**

The following table estimates, starting from the time needed by the test runs, how much CPU time will be needed according to the increased number of particles (dN), increased resolution (dm) and additional physical processes to be followed:

<table>
<tr><th></th><th>Test</th><th>dN</th><th>dm</th><th>Stellar evolution</th><th>conduction</th><th>Black Holes</th><th>Magnetic Fields</th><th>PopIII</th><th>CPU</th></tr>
<tr><td>Box1</td><td>50k</td><td>x4.4</td><td>x1.9</td><td rowspan="2">x1.4</td><td rowspan="2">x1.1</td><td rowspan="2">x1.1</td><td rowspan="2">x1.2</td><td rowspan="2">x1.05</td><td>900K</td></tr>
<tr><td>Box2</td><td>40k</td><td>x4.9</td><td>x1.6</td><td>700K</td></tr>
</table>

Therefore we expect the two runs to use ***1.6M*** *CPU hours. Note that the increased number of particles compensates roughly for the increased number of cores to be used. Therefore we expect losses that are mainly driven by imbalanced workload to be similar to losses observed in the test runs (e.g. <20%), which are already included in our estimation.*

4. computational objectives

Such large simulations require not only a substantial effort in terms of development of the simulation code, but also require the development of appropriate post-processing and analysis tools. Data management and access can be foreseen to be already quite demanding, and therefore such pathfinder simulations are an ideal testbed for improving algorithms and infrastructure of the whole simulation pipeline. A challenge is that for such large simulations these tools also have to be parallelized and optimized. Some of the basic post-processing tools have been already developed towards such large and complex simulations, others are currently under development as part of the preparation for the future, larger simulations. The most prominent post-processing tools needed and their current status are:

- *Visualization for static movies and time evolution.*
  (developed and tested, fully MPI/OpenMP parallelized, Dolag et al. 2008)
- *Map-making tools for flat maps, deep light cones and full sky maps.*
  (developed and tested, parallelized based on producing and combining partial maps, Dolag et al. 2005)
- *Detection of multiple component halos and sub-halos.*
  (developed and tested, fully MPI parallelized, Springel et al. 2008, Dolag et al. 2009b)
- *Photometric code to assign optical/near-IR luminosities to galaxies identified in the simulations.*
  (developed and tested, need to be parallelized, Saro et al. 2006, Nuzza et al. 2010)
- *Merger-tree construction and application to SAMs, to produce mock galaxy surveys.*
  (adapted and tested for hydro simulations, Saro et al. 2010)
- *X-ray telescope simulator for mock observations.*
  (Rasia et al. 2008, new, parallel version under development)
- *mock optical observations using SkyLens*
  (Meneghetti et al. 2009, currently beeing parralalized and ported to GPU)
- *Cluster and group properties extractor.*
  (under development, will be fully MPI parallelized)
- *Novel sub-data access scheme based on Peano-Hilbert sorting and look-up table.*
  (under development)

Besides the primary scientific targets, which will be reached by direct access of the team members to the data (we plan to have full copies of the simulation/postprocessing data at MPA, USM and Trieste), we also want to make simulation outcome (halo catalogues, maps etc.) available online. Prototype databases fed with small, test simulations are already available:

- *http://www.g-vo.org/HydroClusters/*
- *http://www.g-vo.org/hydrosims/*

5. specific benefits expected from DEISA

Of importance for this proposal is the infrastructure provided by DEISA. Especially as the computing time is concentrated to perform 2 complementary, outstanding cosmological simulations it would not be possible to have such simulations done (running on 2048 CPUs, using more then 5TB of main memory) without having access to significant fractions of large supercomputers.

6. summary

*We propose to perform two cosmological, magneto-hydrodynamical simulations of structure formation using the Tree-PM-SPH code **P-Gadget3(XXL)**. We will carry out one large-scale (Box1) plus one high-resolution (Box2) simulation, taking into account a variety of physical processes, which are expected to impact on the observational properties of the inter-galactic medium and on the evolution of the galaxy population in different environments. These simulations will allow us to carry out detailed comparisons to a variety of multi-wavelength observations. The combination of such two simulations will shed new light on and enable unique insights into many current, astrophysical aspects of structure formation. It will help in the interpretation of observational results and the refinement of observational strategies for many of the current and future astronomical observatories. This will be achieved by applying state of the art post-processing tools -- including virtual telescopes – to the simulation outputs as well as making data products publicly available to the community. This will in turn drive the development of post-processing and data handling infrastructure, which are of vital importance for the scientific exploitation of forthcoming large-scale cosmological simulations. Besides their large scientific return, we consider these simulations as pathfinders for a large simulation, to be carried out on next-generation European supercomputing facilities, which should combine the volume coverage of the large-scale simulation Box1, to the high-resolution of the Box2.*

Rererences:

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