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Production operation of distributed simulation code: status
report

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Table of Content

Table of Content	1
1. Introduction	2
1.1 Executive Summary	2
2. Environmental Sciences	3
2.1 Technical enhancements.....	3
2.2 Scientific results	4
2.3 Future works	5
3. Combustion project	6
3.1 Combustion / Radiation coupling.....	6
3.2 Technical enhancements.....	7
3.3 Scientific results	7
3.4 Future works	8
4. Astrophysical project.....	9
4.1 Technical enhancement	9
4.2 Scientific results	10
4.3 Future works	12
5. Conclusion.....	14
6. References and Applicable Documents.....	15
7. Document Amendment Procedure	17
8. List of Acronyms and Abbreviations.....	18

1. Introduction

1.1 Executive Summary

The main objective of JRA6 is to facilitate scientific research projects based on coupling methodology using distributed objects software technology. Coupling codes deal with multi-physic or/and multi-scale simulations and are more especially well-suited for interdisciplinary projects in which several legacy codes have to cooperate.

In previous report D-JRA6-1, we introduced the 3 scientific projects and described the general organisation of each coupling. In a second time, we introduced the basic CORBA knowledge need to understand the main mechanisms involved in the coupling. We finished this first report by the description of the migration phase on the DEISA platform.

In this document we are presenting the 12 month status report of the three scientific projects. For each project we are describing the technical enhancements and summing up the main scientific results. On the technical point of view, we are going to focus on how we are able to take advantage of a large number of processors in coupling context.

This document is public.

2. Environmental Sciences

<i>Title</i>	Hydrological cycles over West African continent (HYCYMAC)
<i>Scientific leader</i>	Michel Vauclin and Christophe Messenger, Laboratory LTHE (Laboratoire d'études des transferts en hydrologie et environnement) Grenoble, France.
<i>Partner Laboratories</i>	LGGE (Laboratoire de glaciologie et géophysique de l'environnement), Grenoble, France. HSM (Hydro sciences Montpellier), Montpellier, France. IRM (Institut Royal de Météorologie), Bruxelles, Belgium. LEGOS (Laboratoire d'étude en géophysique et océanographie spatiale), Toulouse, France. LEGI (Laboratoire des Ecoulements Géophysiques et Industriels), Grenoble, France. Lancaster University, Bailrigg, United Kingdom.
<i>Links with other scientific projects</i>	AMMA (African Monsoon Multidisciplinary Analysis) International project on West African monsoon

2.1 Technical enhancements

In D-JRA6-1, we described briefly the general architecture (see Figure 1) of the Atmosphere-Hydrologic coupling, in which we noticed the possibility to add new hydrological basins (extensible architecture).

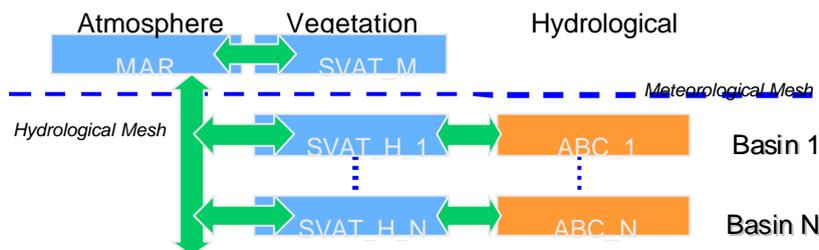


Figure 1: Description of the Atmosphere-Vegetation-Hydrology coupling.

In order to optimize this architecture, the main technical objective for these last 6 months was to be able to run simultaneously several SVAT invocations (SVAT on meteorological or hydrological mesh) from MAR. This problem is a consequence of the fact that the basic CORBA invocations block the client until the server replies, so running several simultaneous invocations are not directly possible. CORBA offers different possibilities to run the invocation mechanism asynchronously; in order to have more flexibility we choose to use *pthreads* technology.

The main idea consists in creating a thread at the beginning of the program, dedicated to handle the legacy code (see **Erreur ! Source du renvoi introuvable.**). Managing the

synchronisations between this *computing thread* and those handled by the CORBA implementation are done without difficulties with the *Mutexes* and the *Conditional Values* mechanisms. CORBA invocations have to be split into two pieces: one for input arguments and the other for output arguments (i.e. results of the remote service).

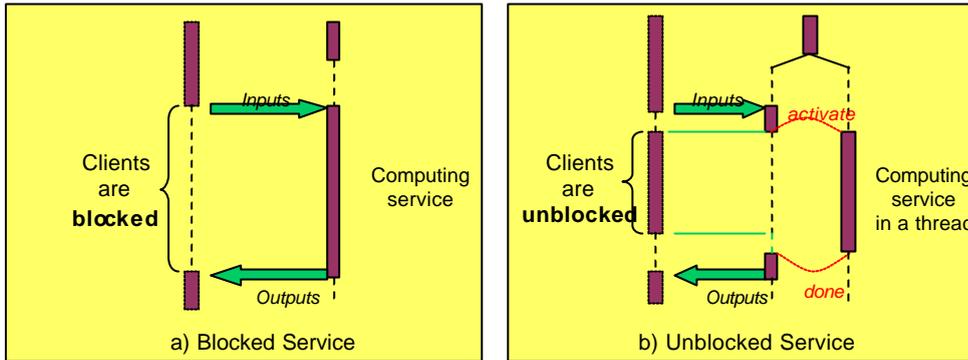


Figure 2: Description of an unblocked service (or CORBA invocation):

- a) the client waits the end of the entire remote computation,
- b) the client can compute simultaneously with the server.

These changes have been done without difficulties and without modifying the legacy codes (MAR, SISVAT, ABC).

2.2 Scientific results

The coupling area has been chosen so that the ocean has no major influence on the regional climate (i.e. continental processes like vegetation, soil and orographic should be dominant). Concerning the hydrologic part, the ABC code is known as a well suited for dry catchments and the availability of hydrodynamic datasets lead to choose the Sirba catchment (39 000 km² — see Figure 3).

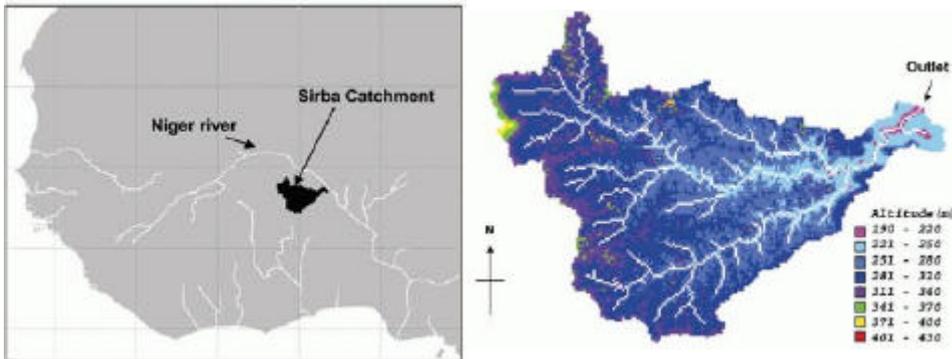


Figure 3: West Africa domain (left picture) on which the atmospheric model (MAR) run. The Sirba hydrological basin studied here is located near the Niger River. The Sirba hydrologic mesh, on which the infiltrated or runoff water part is computed at each time step, is represented on the right picture.

First the RCM-MAR (Regional Climate Model) has been validated on the West Africa, more particularly the spatial and time variability has been reasonably simulated. Nevertheless, the results show that the moister soil field (ECMWF ERA15) used in input

of numerous climate models are overestimated. Consequently, the RCM MAR has to be run 4 months to take off this excess of soil moisture in the model. All these have been submitted for publication on January 2005 to Climate Dynamics [6].

On the hydrologic part, forced simulations have been done with both observed rainfall and simulated rainfall by MAR. They show that these hydrologic experiments are more sensitive to temporal than spatial distribution of the rainfall. This shows the importance of the temporal sampling for infra-daily precipitation, as this has rarely been emphasized. For more details see [6] and C. Messager PhD thesis [8].

After this preliminary calibration and validation, coupling has been achieved with the 3 models: RCM (MAR), SVAT (SISVAT) and hydrologic one (ABC) during the dry year 84. The results, which have been submitted for publication [7] in January 2005, mainly show that the flows between the atmosphere and the continental surfaces are sensitive to the soil moisture and land use. These later directly influence the albedo and in this way the energy budget which, in its turn, modifies the water balance. This first experiment on one catchment can be extended to multiple catchments because of the modular and extensible architecture (see D-JRA6-1).

2.3 Future works

Our coupling approach and our previous studies on the Sirba, have been well appreciated by researchers involved in the AMMA international project (African Monsoon Multidisciplinary Analysis see [9]) which is funded in part by the European Community (12 M€).

Consequently the choice of the new catchment has been done in collaboration with them. More particularly, a part of the AMMA project focuses on the entire Ouémé catchment (38000 km²) on which is planned international observational campaigns and associated modelling studies. Thus our future works are associated with several AMMA work packages:

- ? WP1.2 The Water Cycle,
- ? WP1.3 Surface-atmosphere feedbacks,
- ? WP4.1.2 WAM (West Africa Monsoon) in regional and global climate model.

Since the new basin is located in a humid area, it is not suitable to make this study with the ABC model which is, as we have already said, a dedicated model for arid regions. So the Ouémé catchment choice imposes to us the use of the well known hydrologic model TOPMODEL.

Our coupling architecture is, once again, completely justified by adding the new hydrologic model in the previous simulations. So we are going to add to the previous runs one SVAT module dedicated on Ouémé catchment and the TOPMODEL hydrological model.

3. Combustion project

Title	Large eddy simulations (LES) of turbulent combustion including pollutant species prediction and radiative heat transfers.
Scientific leader	Denis Veynante, Laboratory EM2C (Laboratoire d'énergie moléculaire et macroscopique, combustion), Chatenay Malabry, France.
Partner Laboratories	- CERFACS/IMFT (Institut de mécanique des fluides de Toulouse), Toulouse, France.

3.1 Combustion / Radiation coupling

The coupling between the codes "Combustion" and "Pollutant", both based on AVBP, the Navier-Stokes solver developed by Cerfacs, has been successfully carried out and validated. The coupling between "Combustion" and "Radiation", developed by EM2C, is now presented.

As in the case of Combustion / Pollutant coupling (work introduced at the 10th International Conference on Numerical Combustion, see [10]), the time scales involved in the combustion process and the radiative heat transfer process are drastically different (the radiation characteristic time, associated with large scale motions of the flow, is typically several times higher than the combustion characteristic time). This means that the two modules must be synchronized every N_R iterations of the combustion process (the number N_R has to be defined):

$$t_R = N_R * t_C,$$

where t_C and t_R are respectively the physical times for one iteration of the code "Combustion", and the code "Radiation". As presented in **Erreur ! Source du renvoi introuvable.**, Combustion sends the temperature field T and the mass fraction fields Y_i of radiative species (H_2O and CO_2) every N_R iterations. Radiation, based on a ray tracing algorithm combined with the Correlated-K method (to solve the equations governing the emission/absorption processes), computes the radiative transfers and returns to Combustion the radiative power P field emitted by the radiative species. Then this power field is reinjected as a source term in the energy balance equation which is solved in Combustion.

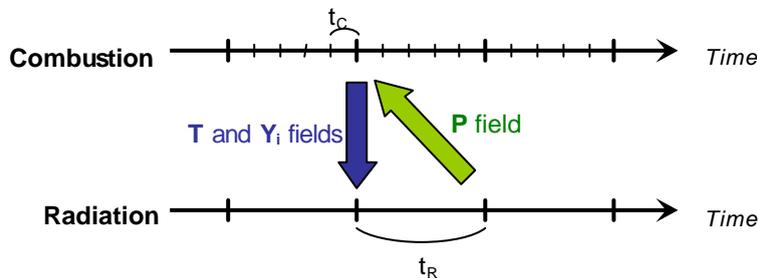


Figure 4: Combustion / Radiation coupling time description. Input fields are in blue and output fields are in green.

3.2 Technical enhancements

Since Combustion and Radiation are parallel codes, it is important that the 2 codes do not wait for each other. To avoid this issue, we have planned to implement very soon the same asynchronous mechanism with *pthread* as described in the environmental sciences project (see section 2.1). Thus when Combustion invokes Radiation, the first one sends the temperature and the mass fractions at t and receives, without waiting for it, the radiative power already computed at $t - N_R * t_C$ (see Figure 5).

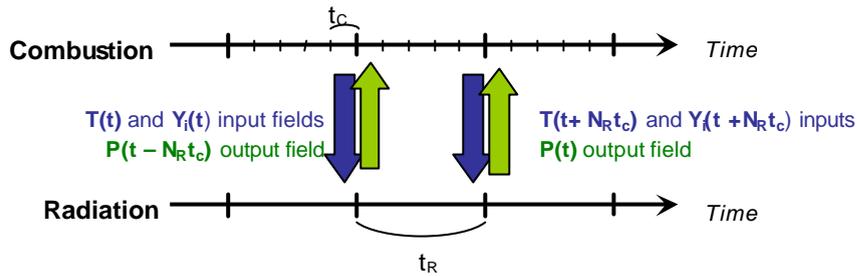


Figure 5: Time description of an asynchronous Combustion / Radiation invocation. Input fields are shown in blue and output fields in green.

This new feature has been successfully implemented. The load balance between the two coupled codes can be tuned by choosing the CPU number for each module. It is not necessary to redistribute the CORBA arguments (see paragraph 4.1 for more details about the redistribution mechanism) because the Radiation code has been parallelized (with OpenMP) over the absorption/emission frequencies and the whole fields T and Y_i are known by each thread.

3.3 Scientific results

To validate the Combustion/Radiation coupling, numerical simulations have been carried out by the researchers at EM2C laboratory (see M. Lecanu thesis [13]) in which only the CFD and the radiative aspects are considered (no reactive flow in Combustion). This validation, based on previous works done by Soufiani and Taine, consists in studying the evolution of a water steam 2D-flow in a channel of 3 meter long. Two temperature configurations were achieved for 2 channel widths (20 cm and 2.5 cm) :

- ? the steam is injected at 1200 K in the channel and the channel edges (2 walls) are set at 400 K,
- ? the steam is injected at 400 K in the channel and the channel walls are set at 1200 K.

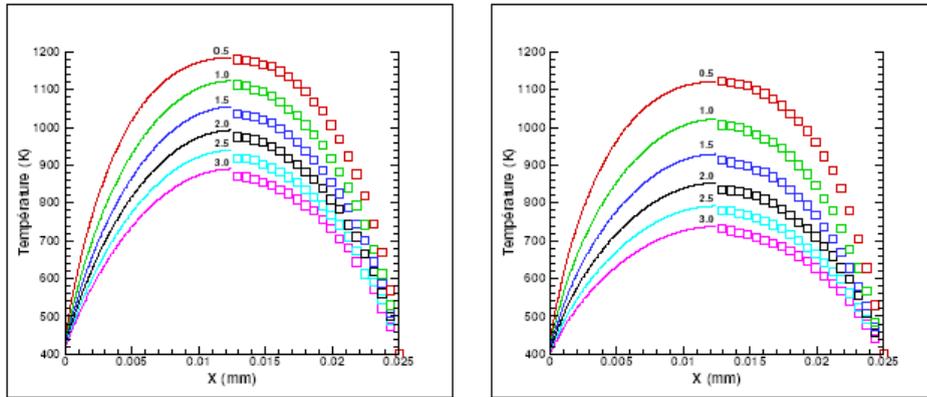
(a) Without H_2O radiation(b) With H_2O radiation

Figure 6: Temperature profiles at different lengths in a channel of 2.5 cm width (0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 meters) The wall temperature is set to 400 K and the water steam is injected at 1200 K. The curves (—) represent the numerical values coming from the Combustion application (without the radiative process) or for the coupled application (Combustion/Radiation — with the radiative process). The symbols (?) represent values obtained by *Soufiani and Taine*.

For all these cases, numerical simulations have been done with and without the radiative heat transfer (i.e. with and without the coupling module Radiation). Here (see Figure 6) we present one of these results, in which the impact of the radiative process is clearly shown for different profiles in the channel (the temperature in the channel decreases from some 10 to more than 100 degrees Kelvin). Slight differences are observed with the results from *Soufiani and Taine* results, M. Lecanu thesis [13] explains these differences by the fact that more physical aspects are considered in the Radiation code (like axial radiative flow dissipation and the influence of far hot areas).

3.4 Future works

Following the Combustion / Radiation validations experiments, we have decided to implement the asynchronous mechanism to the whole coupled application (3 modules). Thus, in the next 6 months we plan to run a Combustion / Radiation coupling to study, this time, a reactive and turbulent flow and, to complete the work planed in this JRA, a whole coupled simulation (Pollutant / Combustion / Radiation). These coupled last experiments simulations have been announced in the ECCOMAS Computation Combustion Conference [12] and in a brief communication submitted to Combustion and Flame [11].

4. Astrophysical project

<i>Title</i>	From origin of galaxies to stars.
<i>Scientific leader</i>	Jean-Michel Alimi, LUTH (Laboratoire de l'Univers et de ses Théories), Meudon, France
<i>Partner Laboratories</i>	Miguel Hernandez University, Elche, Spain. Astrophysical department in CEA (Commissariat à l'Energie Atomique), Saclay, France.
<i>Links with other scientific projects</i>	Horizon project: French astrophysical project which federates the research efforts of several laboratories in numerical simulations to understand the complex physical mechanisms which organize the galaxy distribution.

4.1 Technical enhancement

Recently we have incorporated a new parallel gravitation module, which was developed at the LUTH laboratory. This module uses the FFTW Fourier transform library which is well known as a fast FFT parallel library and the asynchronous message passing of the MPI library to hide communication with computing by overlapping the two steps.

We took advantage of implementing this new module in the distributed architecture, to add the asynchronous mechanisms. The same kind of structure as in Environmental Sciences project in 2.1 (see **Erreur ! Source du renvoi introuvable.**), has been used for all the modules of the distributed application.

Since the physical fields are distributed on spatial domains (i.e. that one process manages its own spatial sub-domain) and the natural CPU time of the 3 modules are naturally imbalanced, the improvement due to the asynchronous mechanism is not sufficient. In order to balance the coupled application we have to adapt the different number of processors for each module so that one module will not wait for another one. Consequently we have to redistribute parts of field. For example the space sub-domain managed by the Hydrodynamics component could spread on several processes in Gravitation and could be a part of the sub-domain managed by Chemistry. More precisely, when a CORBA invocation calls a remote service (as for example the computation of the potential in the Gravitation module), the implemented service splits the fields received and redistributes the pieces with the MPI library to the adapted processes (of the Gravitation module in our example).

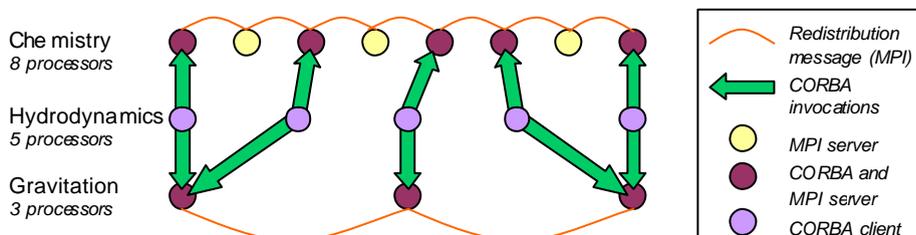


Figure 7: Redistribution mechanism diagram — CORBA servers redistribute part of the field received to MPI servers.

4.2 Scientific results

The thermodynamic properties of the baryonic gas, such as non equilibrium processes in the primeval Hydrogen-Helium plasma, have a crucial influence on the process of galaxy formation. Reproducing numerically the appearance of very first galactic objects is a challenging question in this field as it imposes to consider several different physical processes - in the present case, gravitation, hydrodynamics and chemistry, altogether with a very high number of particles to reach the level of accuracy needed to reproduce observations. Here, we illustrate how increasing the resolution of the simulations allows to reproduce earlier formation of galactic objects.

From the simulations including gravitational, hydrodynamic and chemical processes, it is possible to consider a simple yet realistic model of galaxy formation based on the identification of converging dense cold gas regions (see [14,15] and references therein). A galaxy-like object can be identified in a discretization cell of the volume under consideration if the gas in this cell exhibits the following properties:

1. The most important condition for galaxies to form is that the gas cloud from which they originated cools down faster than it collapses. The typical cooling time is computed from the internal energy loss undergoes by the gas in the considered cell while the dynamical time of gravitational collapse is computed from the total mass density (including dark matter) contained in the cell.
2. To ensure that gas regions giving birth to galaxies are correctly identified, three other criteria are added. First, the size of the gas cloud (typically which of the cell itself) must be less than the Jeans length, which ensures the region is gravitationally unstable.
3. Then, the gas must be in a converging flow (the divergence of the velocity field in the cell is negative).
4. Finally, the baryonic density contrast is sufficiently high to ensure a non-linear gravitational collapse.

Each of the discretization cell that satisfies all of the previous criteria is identified to a galactic particle with mass, position and velocity given by some physical criteria such as energy and momentum conservations. These galactic particles can therefore be considered as building blocks of galaxies and they can be used to identify so-called galaxy-like objects that will partly reproduce the observable properties of galaxies (cf. [15]).

Within this model, the question of the formation of the very first galaxies, or galactic embryos, is related to the early appearance, in the simulations, of the galactic particles we have just defined. The formation of very first galactic object in the Universe is a discriminating property of different competitive cosmological models. They should become within reach of observations in few years with large observational projects like Atacama Larger Milimeter Array (ALMA).

Actually, the production rate of such particles is closely related on the efficiency of the cooling mechanisms in gravitational potential wells dynamically built during the simulation. Therefore, increasing resolution allows obtaining earlier galactic particles and embryos of galaxies. Figure 8 to 10 show the first galactic objects formed in Λ CDM models with different resolutions (in this model the universe contains 30% of ordinary pressureless matter amongst which 4% of baryons, 70% of cosmological constant to

account for cosmic acceleration and has a value of the Hubble constant of 70 km/s/Mpc. The Λ CDM is the concordance model of the physical cosmology). Figure 8 illustrates the temperature of the neutral species in the plasma for a resolution of 512^3 particles in a volume of $(16h^{-1} \text{ Mpc})^3$. The x-y axes indicate the position normalised to this length of the box. With this resolution, the first galactic particles, associated with galactic embryos, appears at $z=14$ (290 million years after the Big Bang, in agreement with WMAP results with a mass of about 80000 solar masses. A lower resolution of 256^3 and 384^3 show them appear only later at $z=10$ and 12 (470 and 360 million years after the Big Bang), respectively, and with a higher mass (see also reference [15]). Increasing the resolution not only allows seeing deeper into the gas distribution, but the lighter and younger galaxy-like objects it exhibits cannot be reproduced with a lower resolution. To prove this, Figure 9 shows the isocontours of the gas temperature in the same region of Figure 8 in a simulation with only 256^3 grid cells: the gas has remained cold and less dense as the low resolution did not allow catching up the small scale processes. Finally, Figure 10 presents one of the first galaxy-like object formed at $z=10$ in a simulation with 256^3 grid cells. The galactic particle recovered (indicated by a cross in the figure) has a mass of about 6 million solar masses. It is also important to notice the different sizes of the galactic embryos found in the simulations: in Figure 8 (high resolution of 512^3 particles), the size of the galaxy-like object is about 30 000 parsecs while in Figure 10 (lower resolution of 256^3 particles) it is 1.3 Mpc.

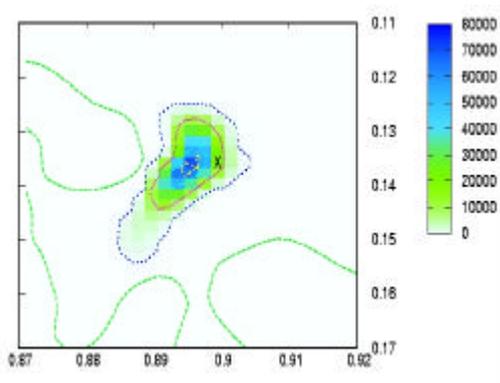


Figure 8: Isocontours of the gas temperature in a simulation with 512^3 particles at $z=14$, 290 Millions Years after the Big Bang ($T=70000, 50000, 10000, 100, 30$ K). A cross indicates the position of galaxy like object as defined in the text.

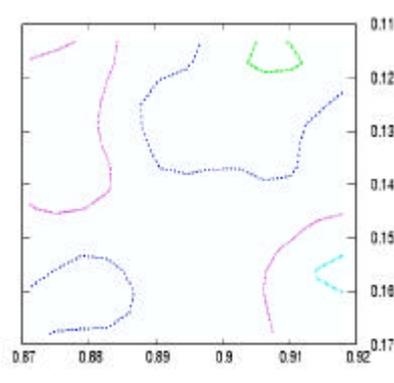


Figure 9: Isocontours of the gas temperature in a simulation with 256^3 particles in the same region of Figure 8 and at the same time $z=14$ ($T=28, 25, 23, 22$ K). We do not observe at all any galaxy like object formation.

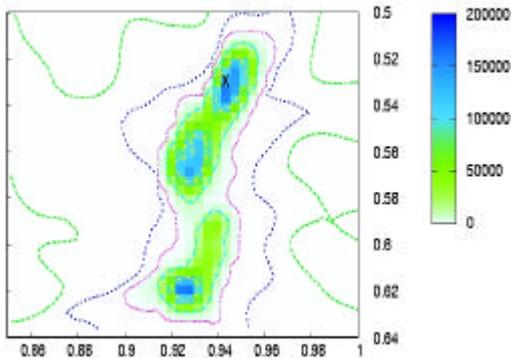


Figure 10: Isocontours of the gas temperature in the simulation with 256^3 particles at $z=10$, 470 Millions years after the Big Bang ($T=500\ 000, 100\ 000, 10000, 100, 20, 15$ K). The cross indicates the position of galaxy like object as defined in the text.

4.3 Future works

The very high resolution ($1024^3, 2048^3$ and even more) that can be reached thanks to the numerical techniques of parallel and distributed computing will open exciting perspectives in the field of galaxy formation by reproducing the very first objects formed in the universe with a level of details never reached before. One of these perspectives is to test new cosmological models inspired by high energy physics. Indeed, one of the most puzzling point in modern cosmology is the characterisation of the cosmic acceleration, which seems to be unavoidable to explain the distance-redshifts measurements obtained by observations of far-away supernovae as well as the fine properties of the cosmic microwave background. The origin of this acceleration is still unknown and a lot of models coming from various considerations of modern theoretical physics have arisen to tackle this problem. However, galaxy formation is expected to bring more insights on this question. An analysis of the clusterization of dark matter within the framework of different accelerated universes has shown that the properties of dark matter halos are quite sensitive to the cosmological scenario considered, especially at high redshifts (see [16, 17] and references therein). This makes particularly interesting

to pursue this analysis to see the influence of cosmic accelerations, and the different theoretical reasons advanced to explain it, on the very first galaxy-like objects formed in the universe. This exciting perspective offers the possibility to constraint very recent and interesting theories of gravitation and cosmology with the properties of the first objects formed.

5. Conclusion

For these first 12 months, we have migrated and transformed the 3 coupled applications coming from the Eurogrid project [5], which were more especially adapted to run on heterogeneous platforms with a low parallelism level. The use of the asynchronous and, if needed, redistribution mechanisms, allow us to have a higher parallelism level than before and to be able to take advantage of the DEISA infrastructure. These main technical features to adapt our 3 coupled applications are now finished. In the next months we are going to focus our activities on the production of the 3 projects and on the optimization of the whole coupled applications.

On the scientific point of view, the new recent results and the involvement of researchers in these projects, in these 3 cases, corroborate the fact that the coupling approach is an effective way to “produce” new science” by making cooperate legacy codes.

6. References and Applicable Documents

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7. Document Amendment Procedure

8. List of Acronyms and Abbreviations

ABC	Name of the hydrologic model well-suited for arid catchments.
ABVP	CFD code for numerical simulation of unsteady turbulence for reactive flows (developed by the CERFACS).
ALMA	Atacama Larger Milimeter Array — International astronomy facility — www.alma.nrao.edu .
CFD	Computational Fluid Dynamics.
CORBA	Common Object Request Broker Architecture is the OMG's specification which defines the middleware to allow remote computer applications to work together over networks.
FFTW	Fast Fourier Transform in the West (Massachusetts Institute of Technology).
IOR	An Inter Operable Reference is a reference on a CORBA service. This reference is a kind of “universal pointer” in which the hostname and the port on which the service is running are coded. Once created by the application which delivers this service, it can be used by any CORBA application which invokes it.
OMG	The Object Management Group is a consortium that produces and maintains computer industry specifications for interoperable enterprise applications. The other well-known specifications are UML (Unified Modelling Language) and MDA (Model Driven Architecture).
NS	A Name Server is a CORBA utility which works as an IOR's database and which can be remotely inquired.
RCM	Regional Climate Model.
SISVAT	Sea Ice Soil Vegetation Atmosphere Transfer.
SVAT	Soil Vegetation Atmosphere Transfer.
WMAP	Wilkinson Microwave Anisotropy Probe — map.gsfc.nasa.gov