Research Topic b3:
GW, Cosmology, and Astroparticle

Coordinator: B. Giacomazzo

UNICAL

Luigi Delle Rose (3 mo/yr), Alessandro Papa (3 mo/yr *)

1. Development of numerical methods for the description of the out of equilibrium dynamics of a plasma during a first-order phase transition in the early universe: (a) design, validation and release of parallelized algorithms for the numerical solutions of the **Boltzmann equations** for massive and massless particle species, using **iterative and/or spectral methods**; (b) determination of the speed and thickness of the phase-transition front in the steady-state regime.

2. Study of the properties of the confinement and the chiral first-order phase transitions, at finite temperature, in dark QCD-like theories (pure SU(N) Yang-Mills and Yang-Mills with fermion and/or scalar matter content). Exploitation of **lattice simulations** and the PNJL description for the determination of thermodynamics quantities.

3. Application of **Monte Carlo Markov Chain** techniques for the exploration of the parameter space of suitable benchmark models aimed at identifying regions in which first-order phase transitions are realized. The results obtained in tasks 1 and 2 will be used for the characterization of gravitational wave spectra in the early universe.

* *shared across other use cases in WP1*

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- The research team has longstanding expertise on numerical methods, development of algorithms for high-energy physics, simulations, as well as on theoretical modelling, as proven by several publications on the subject. A RTD-a will be hired to work on the projects of WP1. A second RTD-a position, with focused expertise on software development and HPC management, to be shared across the working packages of spoke 2 in UNICAL, will assist in addressing the more technical issues of the project, thus guaranteeing a high level of success. Tasks 1 and 2 will require, approximately and including testing and code release, 16 months each. Task 3 will require approximately 4 months.

- For the achievements of the objectives of the project we will develop software in C++, Python and Fortran that will heavily exploit parallelization techniques to be run on high-performance computing clusters with several CPUs (we will use ReCaS at UNICal and Cineca). During the development phase of the algorithms, according to the performance achieved by those, we will assess the necessity of porting the codes to GPU architectures.

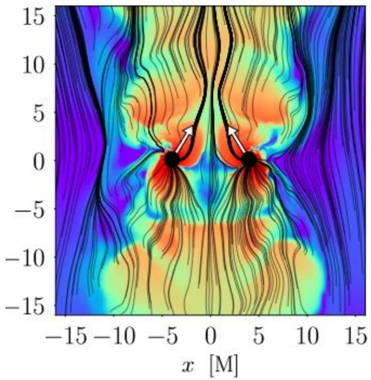
UNIMIB

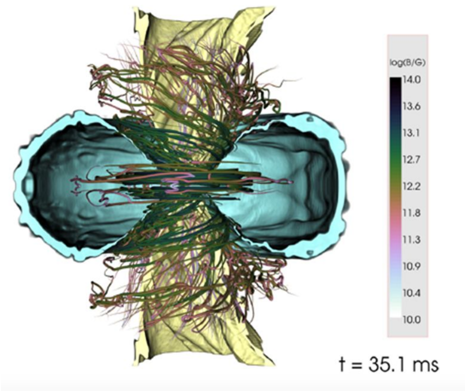
Staff: Giacomazzo (3 mo/y at 70%), Lupi (3 mo/y at 70%), Dotti (⅔ of mo/y at 70%), Sesana (⅓ of mo/y at 70%), Gerosa (⅓ of mo/y at 50%), Colpi (⅓ of mo/y at 50%)

Use cases:

- Development of numerical relativity codes for the study of compact binary mergers
- Numerical Relativity simulations of compact object binaries (GW and EM signals)
- Mesh-free/moving-mesh Newtonian simulations of formation and evolution of massive black holes

Our codes solve fluidodynamics equations in Newtonian physics or General Relativity (GRMHD).





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Personnel and Resources Required

- 1 RTDA will be hired on PNRR money
- We have access (via INFN) to CINECA clusters Marconi A3, Marconi 100, and Galileo 100 that are used for production runs. We have also an in-house cluster with ~1000 cores (funded with Sesana's ERC).
- We need hours dedicated for code development and testing. Our typical simulations requires a few hundreds of cores, but they may be scaled up to ~1000s of cores.
- We need debuggers and profilers for both CPUs and GPUs. Assistance on the selection and use of these softwares will be useful.

UNIBA

Antonio Marrone (3 mo/y), Alessandro Mirizzi (2 mo/y), Giuseppe Lucente (0 mo/y), Francesco Sivo (0 mo/y), PhD student XXX (6 mo/y)

- Development of numerical algorithms to study neutrino oscillations in dense environments. The non-linear flavor dynamics in a supernova core, associated with neutrino-neutrino interactions, requires deep numerical studies to assess the impact on the observable neutrino signal and on the supernova explosion.

- Development numerical algorithms to characterize the signatures of axion-photon conversions in cosmic magnetic field on gamma and X-ray observations.

UNIBA

- Large-scale numerical simulations will be performed on the local cluster at the RECAS-Bari data center, that consists in 128 servers, each with 64 core and 256 GB RAM

UNIFI

Dimitri Colferai (3 mo/y), Aldo Lorenzo Cotrone (1 mo/y), Giuliano Panico (1 mo/y), PhD student (12 mo/y)

Numerical methods in high energy theoretical physics and astrophysics. The research concerns the development and application of advanced numerical methods to the study of theoretical aspects of high energy physics and cosmology. In particular:

- Simulating the dynamics of bubbles of true vacua in cosmological first order phase transitions in hidden (dark) sectors. The dynamics is crucial to accurately estimate the spectrum of produced gravitational waves to be searched for in experimental facilities.
- Simulating the dynamics of bubbles of true vacua in extensions of the Standard Model that modify the properties of the electroweak phase transition. The domain wall dynamics is important to assess the possibility of obtaining successful baryogenesis and to study possible experimental signatures (eg. gravitational waves).
- Solving equations for computing the spectrum of gravitational waves in transplanckian collisions. This study is important for determining the features of gravitational waves produced by collisions of ultrarelativistic objects.

UNIFI

The numerical simulations and the determination of the solution of the Boltzmann equation require the use of a cluster of CPUs. Some of the used algorithms could be easily rewritten implementing parallel computation, with this approach a speed-up could be obtained by running the code on GPUs.

UNIFE

Use cases

Walter Boscheri (1 mo/yr), Lorenzo Pareschi (1 mo/yr), Giacomo Dimarco (1 mo/yr), Giulia Bertaglia (3 mo/yr)

1. Development of numerical schemes for plasma physics in the context of general relativity. We will consider the general relativity magnetohydrodynamics equations (GRMHD) . Design and validate new algorithms to properly address multiple time scales (IMEX methods) as well as high order spatial discretizations (**finite volume, discontinuous Galerkin**) able to capture wave patterns of the fluid structures with high accuracy.

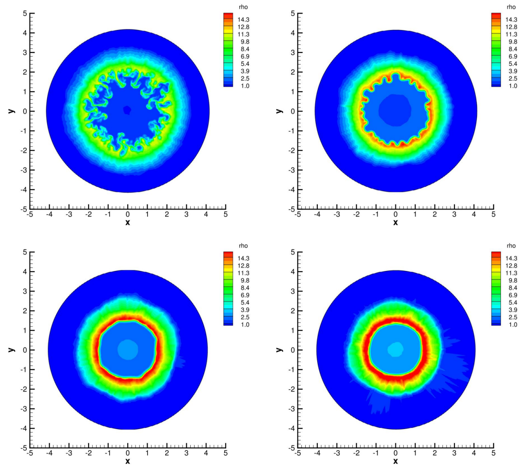


Fig. 20. Density distribution for the spherical implosion problem solved using the ideal MHD equations with a magnetic field of intensity B_0 applied on the horizontal plane x–y. From top left to bottom right: $B_0 = 0$ at output time $t_f = 2.77$, $B_0 = 1$ at output time $t_{f,1} = 2.70$, $B_0 = 2$ at output time $t_{f,2} = 2.63$ and $B_0 = 3$ at output time $t_{f,3} = 2.55$. All simulations stop when the external radius of the domain reaches $r_e = 4$.

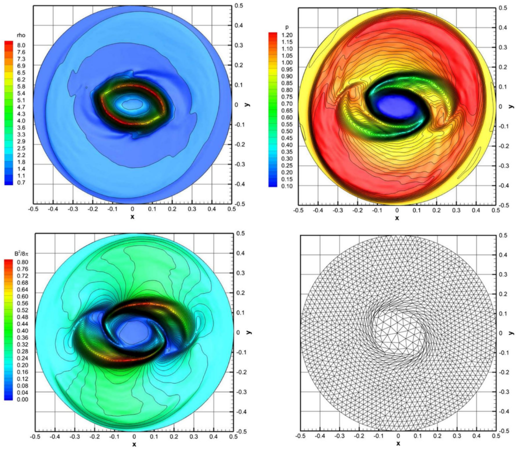


Figure 17. Numerical results for the ideal MHD rotor problem: density, pressure, magnetic pressure, and a coarse mesh configuration at time $t = 0.25$. A fourth-order Lagrangian WENO scheme has been used with the rezoning stage and the multidimensional node solver $\mathcal{NS}_b$.

UNIFE

Use cases

2. Development of numerical methods for plasmas out of equilibrium. Design new schemes for the solution of Vlasov-Fokker -Planck models and to connect these methods to the solution of MHD models. The case of collisional plasmas as well as the case of quasi neutrality will be considered by means of **spectral methods and Monte Carlo schemes**. Applications to space plasma, thrusters and magnetic fusion will be considered.

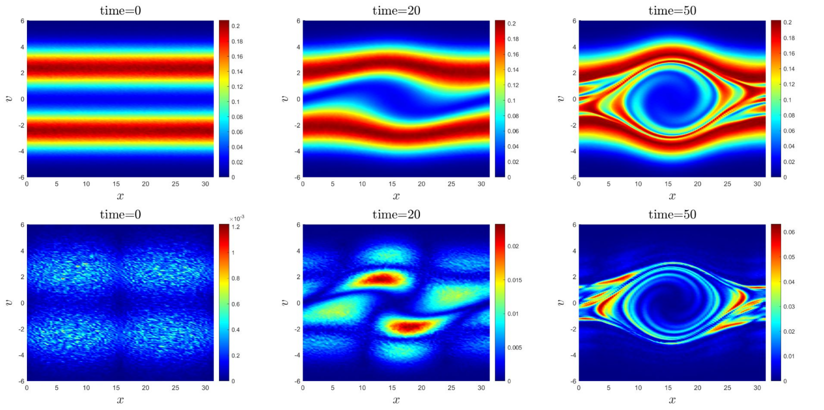


Figure 7: **Test 3: linear two stream instability**. We report $\mathbb{E}_{\mathbf{z}}[f(x,v,t,\mathbf{z})]$ (top row) and $\text{Var}_{\mathbf{z}}[f(x,v,t,\mathbf{z})]$ (bottom row) at fixed times $t = 0, 20, 50$, in collisionless linear two stream instability. We choose $k = 0.2$, $N = 5 \cdot 10^7$ particles, $M = 5$ and $\Delta t = 0.1$. We considered the initial condition (34) with $\alpha(\mathbf{z}) = 3 \cdot 10^{-3} + 4 \cdot 10^{-3}\mathbf{z}$, $\mathbf{z} \sim \mathcal{U}([0,1])$.

3. Numerical methods for the transport of neutrinos in core-collapse supernovae and neutron star mergers. We will focus on the truncated-moment formalism, considering the first two moments (M1 scheme) within the grey approximation, which reduces Boltzmann equation to a system of 3+1 equations. To solve the interaction of radiation and matter in several regimes we will develop IMEX methods overcoming time-step restrictions.

UNIFE

Personnel and resource requirements

- The accomplishment of the task requires approximately 2 years of work carried out by two junior researchers under the supervision of a senior researcher for each task. Due to the previous experience of the research team about modeling and numerical methods the project has a very high probability of success.

- Due to the complexity of the physics and of the numerical schemes which will be faced during the three tasks, we would need to hire two junior researchers, thus we primarily foresee **two RTD-a positions** which will be supported by two PhD positions hired on other grants (MSCA doctoral network “DATAHYKing”).

- **We need access to a supercomputer with thousands of CPUs**, to massively parallelize our codes (Fortran, Python,...). We will apply to national and international calls for getting access to supercomputers, like Cineca (Bologna-Italy), HLRS (Stuttgart - Germany) and SuperMUC (Munich - Germany). Our research team had already experienced these architectures in the past through ISCRA-type projects and the PRACE program at the European level.

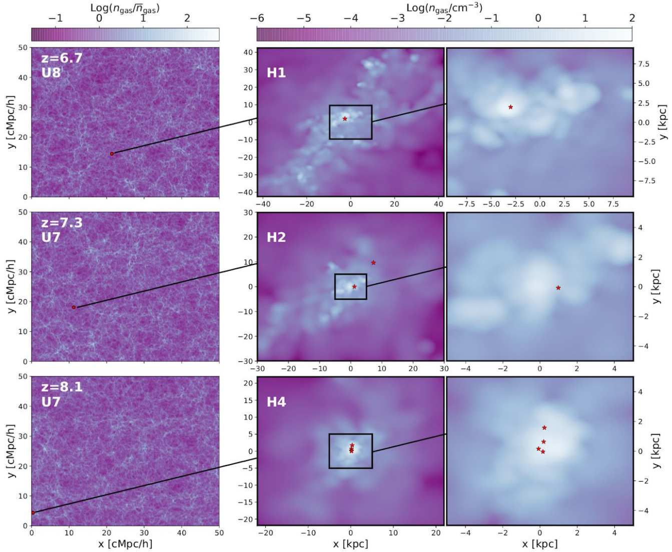
UNISAPIENZA

Staff*: Graziani (1 mo/y at 100%), Masi (1 mo/y at 100%), Melchiorri (1 mo/y at 100%, Contact Person), Pani (1 mo/y at 100%), Piacentini (1 mo/y at 100%), Schneider (1 mo/y at 100%), Urbano (1 mo/y at 100%)

* (Pending Sapienza PNRR resources allocations)

Usecase 1: **Simulating BH formation environment** (Graziani, Schneider + RTDA):

- SPH multi-scale cosmological simulations of the formation environments of compact binary systems and of supermassive black hole seeds and their evolution (mass growth, mergers) through cosmic time.
- Development of new zoom-in algorithms to couple star forming regions with large databases of evolving stellar binary systems and to predict the associated electromagnetic and gravitational wave signals.



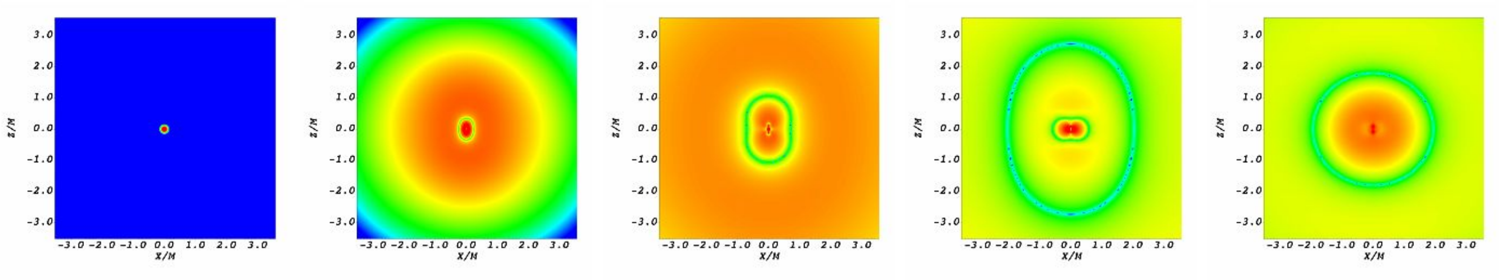
Our simulations adopts cosmological hydrodynamical solvers to follow low-metallicity star formation in high-redshift galaxies.

UNISAPIENZA

Usecase 2: **Numerical Relativity beyond general relativity** (Pani, Urbano, +RTDA)

Scientific Goals: (1) perform simulations of black-hole binary coalescences in motivated nonperturbative extensions to GR and produce gravitational-wave signals to be used in current and future tests of GR. Study the nonlinear collapse of fundamental matter fields in an expanding primordial universe in order to better characterize the formation of primordial black holes (PBHs), their abundance and properties. (2) Exploration of (single- and multi-field) inflationary models that are consistent with measurements of the cosmic microwave background (CMB) anisotropy and generate a sizable abundance of PBHs during the early Universe. An accurate understanding of PBH formation requires i) a motivated and simple parametrization of the inflationary dynamics beyond the usual slow-roll paradigm ii) a full exploration of the associated parameter space iii) dedicated simulations of gravitational collapse in numerical relativity with the inclusion of non-gaussian effects and iv) a statistical analysis of the expected observational signals in comparison with gravitational-wave data.

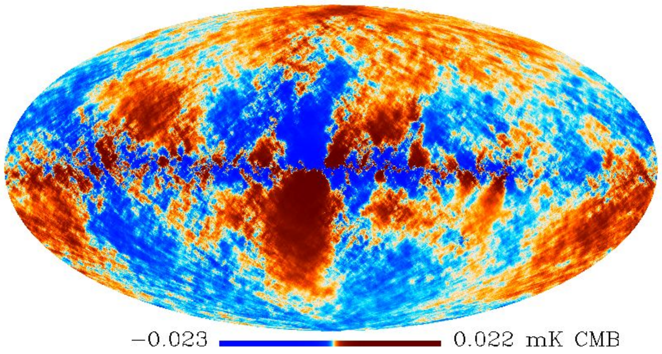
Technical Goals: (1) To develop and extend new formulations of the initial value problem in modified gravity in order to study binary simulations beyond GR, in particular gauge issues related to loss of hyperbolicity. Produce thornes and modules to be implemented in the **Einstein Toolkit and in the GRChombo infrastructures**; (2) Perform 1+1 and 3+1 simulations of fundamental fields in the early universe to study the critical collapse and gravitational-wave signals. (3) Extension of the available likelihood code for the comparison of inflationary models beyond slow-roll with CMB data; computation of PBH mass function and threshold for gravitational collapse in the presence of primordial non-gaussianity; inclusion of these effects in a **Markov-Chain Monte Carlo** for fitting models to gravitational-wave data.



UNISAPIENZA

Usecase 3. **Improving theoretical modelling in data analysis of large cosmological datasets** (Melchiorri, Masi, Piacentini, +RTDA)

Measuring the large scale features of the Universe ranks as one of the most critical open problems in modern astrophysics. Improved information from cosmological observables as Cosmic Microwave Background anisotropies or galaxy surveys would shed light on the physics of the early universe as well as offer insight into the physical properties of dark matter that remain largely unconstrained. This project aims to analyse current and future cosmological data using novel state-of-the-art Bayesian pipelines, directly improving our current knowledge of the universe and of its structure. Novel theoretical models will be investigated, especially in view of current cosmological tensions. It will have the dual advantages of identifying possible and still undetected systematics in the data and it will provide an independent measurement of several key cosmological parameters. The new algorithms and the considerable amount of data that we plan to analyze (several TB) make it necessary the use of new HPC pre-Exascale and Exascale systems.



Simulation of CMB polarisation B-Modes

UNISAPIENZA

- We forecast the need for (at least) 2 RTDA positions.
- we have an in-house cluster with 200 cores (funded with the Amaldi research Center Excellence Department), which needs to be extended with:
    - 768 CPU cores x84 based (1TB RAM/node);
    - storage space with 3 dedicated NAS servers with 350 TB HDD space;
    - GPU graphic cards for the new nodes.

Adopted HPC Technologies:

- Parallelization: standard MPI/OpenMP/CUDA/P-THREADS
- Programming languages: C++ / Python /Julia/Java/Fortran-2008
- Intel/GCC/Portland Compilers

Adopted Software Technologies:

- Codes: Einstein Toolkit, CACTUS, CARPET (for AMR), GADGET, COBAYA
- Data Analysis: MCMC, pyCBC, BILBY,

SALENTO

Daniele Montanino (1 mo/yr), RTDA (12 mo/yr), PhD (?) (12 mo/yr)

- Conversion of Axion-Like Particles (ALPs) in realistic astrophysical magnetic fields coming from 3D magnetohydrodynamic simulations
- Neutrino oscillations in matter and analysis of forthcoming experiments
- Numerical relativity and simulations of compact object coalescence (presumably will be carried out by a RTDA and/or PhD student)

SALENTO

An access to supercomputer is necessary to evolve the ALP-photon system in a large 3D magnetic field environment. Our code needs to be parallelized.

Moreover any calculation involving numerical relativity requires a large computing power to be performed. However, at the moment it is not possible to quantify the necessary amount of computing power

UNIPD

Raccanelli, Bartolo, Liguori, Matarrese

Improved Methods for New Physics from LSS observables

Adaptation of existing codes that calculate Large Scale Structure observables in standard cosmology, to allow for new physics effects, including integration with **Markov Chain Monte Carlo** packages. Development of user interface taking the linear cosmology evolution as input

Summary

Overlaps:

- Numerical Relativity (UNIMIB, UNIFE, UNISAPIENZA, SALENTO). Moreover, UNIMIB and UNIFE both working on GRMHD+neutrinos.
- Neutrino Oscillations and Axion-Photon Conversions (UNIBA, SALENTO)
- Simulating Black Hole Formation Environment (UNIMIB, UNISAPIENZA)

Resources:

- UNIFE and UNISAPIENZA need RTDAs (they did not get any from PNRR?)
- Everyone needs access to computing time
- Many would work on porting their codes to GPUs