Romanian Reports in Physics **72**, 114 (2020)

SIMULATIONS AND ANALYSIS OF THE FIRST BLACK HOLE POPULATIONS

R. A. BALAȘOV[1,2], L. I. CARAMETE[2]

[1] University of Bucharest – Faculty of Physics, 405 Atomiștilor Street,
RO-077125, Măgurele, Romania
[2] Institute of Space Science, 409 Atomiștilor Street,
RO-077125, Măgurele, Romania
E-mails: *rabalasov@spacescience.ro; lcaramete@spacescience.ro*

Received November 14, 2019

Abstract. We simulate various black hole populations using the GIZMO code package for cosmological N-body/Smoothed-particle hydrodynamics (SPH) problems. The objective of this analysis is to use the results of the simulations in order to compare them with the present black hole mass distribution. In doing this, we can predict the initial population of black holes, the mass distribution and the black hole merger rate, which will be a direct contribution to the future gravitational waves observatories (such as the LISA Space Mission).

Key words: massive back holes, mergers, simulations.

1. INTRODUCTION

Our current understanding of the Universe places supermassive black holes (SMBHs) in the center of most galaxies [1]. These compact astrophysical objects play an important role in galaxy formation and tracing cosmological structures [2]. In order to meet the scientific requirements for studying black holes (BHs), a growing number of ground-based and space gravitational waves (GW) observatories are either in use or development: LIGO (*Laser Interferometer Gravitational-Wave Observatory*) [3], Virgo interferometer [4], GEO600 [5], and CLIO (*Cryogenic Laser Interferometer Observatory*) [6] as a prototype for KAGRA (*Kamioka Gravitational Wave Detector*) [7] and LISA (Laser Interferometer Space Antenna).

At present, there are approximately 50 black hole merger candidate events [8] detected by LIGO's Scientific Collaboration (LSC) [9] third observing run (O_3), which was active between the 1^{st} of April 2019 and the 27^{th} of March 2020. This detection rate is considerably higher compared to the one of the first two runs (O_1 and O_2) [10], that highlighted 10 mergers in approximately 1-year time. The near future paves the way for another type of observatory: space-based detectors [11, 12], which will allow comprehensive SMBH investigations by enlarging the frequency domain of observations (thus expanding the mass spectrum of the BH detections).

The year 2034 will mark the launch of the first space-based gravitational wave detector: LISA (*Laser Interferometer Space Antenna*) [13], as part of the European Space Agency (ESA) Cosmic Vision program [14]. The detection of SMBH mergers and the study of the early Universe will be made possible using an entirely different tool. In order to provide requirements for this particular space mission, predictions regarding the black hole populations are essential. That is to say, investigating early Universe black hole distributions will produce a higher chance of LISA observations. The results presented in this paper anticipate future simulations which will, in turn, provide merger rates that directly involves LISA detections.

Although there are various proposed mechanisms based on which the BHs grow [15–20], it is believed that the main growing mechanism is based on past generations mergers, with the differences of evolution related to the initial ("seed") BHs. The seed BHs scenarios can be categorized as *light* or as *heavy*. In the first case, the light seed scenario, the sources are the Population III stars which form in a low-metallicity Universe [21, 22] and explode forming a black hole with a mass of 2/3 of the original mass, on the order of a few hundred solar masses ($M_\odot$) [23–27]. In the second one, the heavy seed scenario, the black holes are already massive and were formed, for example, by collapse of protogalactic disks and they have masses with orders of 10^4 to 10^6 $M_\odot$ [28].

In this paper, we use an N-body/Smoothed-particle hydrodynamics (SPH) code package named GIZMO [29], with the help of which we explore different scenarios for the first black hole populations. We investigate the properties of the resulted population from realistic BH growth mechanisms (gas accretion and merging). In section 2, we describe the software package and, in section 3, the initial conditions alongside the physics of the models. Afterwards, the simulation results are analyzed. Section 4 is reserved for further development of the initial conditions files and necessary parameters in order to obtain a similar present BH mass distribution [30].

2. SIMULATION SETUP

GIZMO is an open-source software package developed by Philip F. Hopkins [29], with code descendancy from the GADGET (*Galaxies with Dark matter and Gas interact*) [31] program series. More specifically, it draws a part of its codebase from P-GADGET, which itself is a successor of GADGET-2 [32]. For reasons of similarity, we will briefly describe GADGET-2 (emphasizing only on the differences or modifications brought up by GIZMO).

Written by Volker Springel, GADGET-2 represents a code package that provides the possibility to simulate collisionless particle interactions and smoothed particle hydrodynamics (SPH) using parallel programming. Periodic boundaries may or may not be taken into consideration. The program may be used for simple Newtonian dynamics or for cosmological frameworks. MPI (*Message Passing Interface*) libraries are used for data exchange. Therefore, one of the requirements is to use an *mpi* (1.0 or higher) library when compiling. Other resource requirements include non-standard libraries like *gsl* (*GNU scientific library*), *fftw* (*Fastest Fourier Transform in the West* – 2.0 or higher) and *hdf5* (*Hierarchical Data Format* – 5.0 or higher). When installing *fftw*, the user must activate the parallel support option by adding the "--enable-mpi" command during the process otherwise the library will not be used.

When running the code, the number of processors can be specified and the simulation will run based on the parameters file. The parameters file includes details such as memory allocation, computer time limit, formats and output names, cosmological parameters, etc. Also, this file will make use of the *initial conditions* (ICs) file, which can be generated in any programming language, as long as the *hdf5* extension is recognized by GADGET/GIZMO. For example, GIZMO includes in its scripts folder a basic ICs makefile written in *Python*. The ICs file controls the initial number of particles, their type and characteristics (distribution, masses, velocities and so on). Based on their type, the output files will record different parameters. For example, if *black hole* particles are generated in the ICs file, those type of particles will have a recorded *black hole mass*, different from the dynamical mass used in various interactions [33]. GIZMO uses identical ICs files as GADGET. The snapshot format is also the same. Snapshots are output files that can be exported at different simulation time intervals (that can be adjusted in the parameters file).

Major differences between GADGET-2 and GIZMO are linked to the modules they provide. GIZMO offers a considerable higher number of physics options (*e.g.* magnetic fields, conduction, turbulent diffusion, models for galaxy and star formation, feedback, coupled dust-gas physics, nuclear reaction networks, cooling, exotic dark matter, black holes, etc.). For more information, please consult *Table 1*, which is an extract of the GIZMO user guide [32]. Adding to that, GIZMO has the option of non-SPH hydro solver, besides various SPH methods that are not included in GADGET.

In order to run GIZMO, the user must configure its different compile-time options in the *Config.sh* file, after which an executable is generated. The configuration file offers the user an ample number of options (*flags*) that can be turned on or off. There are also flags that can be assigned different values (in addition to turning the default option on). These flags are basically calling functions that simulate different particular aspects of the physics modules. Running GIZMO requires all of the earlier mentioned files: the executable (dependent on the *Config.sh*), the parameters file and the ICs.

Table 1

GIZMO physics modules

Physics module name	Notes
Hydrodynamics	Lagrangian, SPH, or fixed-grid Eulerian methods
Magnetic fields	Ideal or non-ideal MHD
Cosmological integrations	On-the-fly group finding enabled
Radiative heating/cooling & chemistry	Various cooling packages
Galaxy/Star/BH formation and feedback	Explicit sub-grid models
Star/Planet sink-particle formation	Individual particles
Non-standard cosmology	Arbitrarily time-dependent dark energy, Hubble expansion, gravitational constants, etc.
Self-gravity with adaptive gravitational resolution	Fully-Lagrangian softening for gravitational forces, with optional sink particle formation and growth, and ability to trivially insert arbitrary external gravitational fields
Subgrid-scale turbulent diffusion models	And the ability to run arbitrary shearing-boxes
Anisotropic conduction & viscosity	Fully-anisotropic kinetic MHD
Dusty fluids	Explicit evolution of aerodynamic particles
Degenerate/stellar equations-of-state	Helmholtz equations of state and simple nuclear reaction networks
Elastic/plastic/solid-body dynamics	Arbitrary equations-of-state with pre-programmed modules for common substances
Radiation-hydrodynamics	Variety of modular solvers
Cosmic Ray transport and magneto-hydrodynamics	Including full coupling to gas
Other in-development features	nuclear networks, relativistic hydrodynamics, and more

3. BH POPULATION STUDY

Henceforth we will consider the results of the “heavy/light seed” scenarios (regardless of the seeding mechanism) by presenting different simulations constructed in GIZMO. The differences will be represented by the initial conditions frameworks. The purpose is to compare the generated results with the current massive black hole (MBH) mass distributions. This “calibration” will generate the baseline upon which more complex situations can be built. We generated two main situations: two-dimensional and tridimensional.

I. 2D case

The reasoning behind the two-dimensional case is the need for preliminary testing and benchmarking. GIZMO amounts to a considerable number of methods, therefore the code package provides a great deal of modules. After successfully configuring GIZMO in the Linux environment, we used this situation to testcase, verify and accommodate with the simulation codes.

The benchmarking consisted of a defined volume in which we generated black hole “particles” (as we mentioned beforehand, this type of particle being already defined as such in the GIZMO libraries). Considering the software’s time units (by default, one internal time unit equals 9.8×10^8 yr/h, where h = 1 for non-cosmological runs [32]), we let the system evolve from a gravitational point of view for 13 Gyrs. The BH particles have been assigned random values for the initial velocities (using a Gaussian distribution). It is worth mentioning that, for this step in particular, no growth mechanisms (accretion or merging) were used, therefore no gas particles were generated as well (Fig. 1 and Fig. 2).

a) BHs case (without the gas particles)

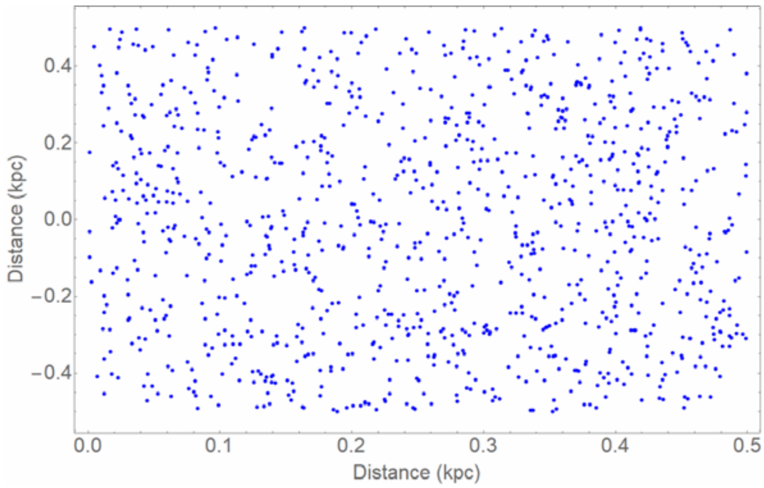

Fig. 1 – (Color online) Initial conditions for the 2D case with BHs alone (blue).

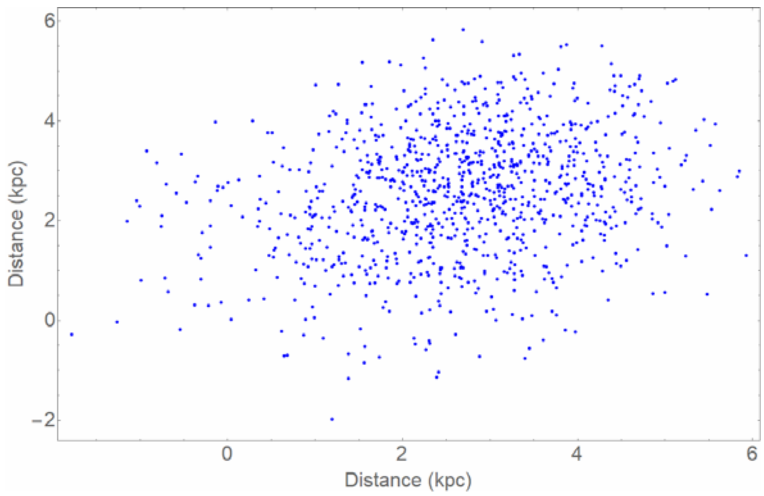

Fig. 2 – (Color online) Final snapshot of the 2D case with BHs alone (blue).

As expected from a simple gravitational interaction, at the end of the simulation, we get a clustering of black holes.

b) BHs placed in a uniform gas background

Inside this system, rather than generating a high number of gas particles (in red, in Fig. 3 and Fig. 4) with low masses, we generated a lower number, but with masses comparable to the BH particles (in blue) in order to have the same gravitational influence one would have in the first case. Thus, the particles play a collective role (*i.e.* gas concentration) rather than exhibiting the particle distribution itself. Every gas particle was assigned null values for the velocity components, as opposed to the BH particles which had started with random values for the initial velocities (using a Gaussian distribution). The end time was set to a higher value (t_{end} = 20), for testing purposes, with no physical meaning and we let the system evolve.

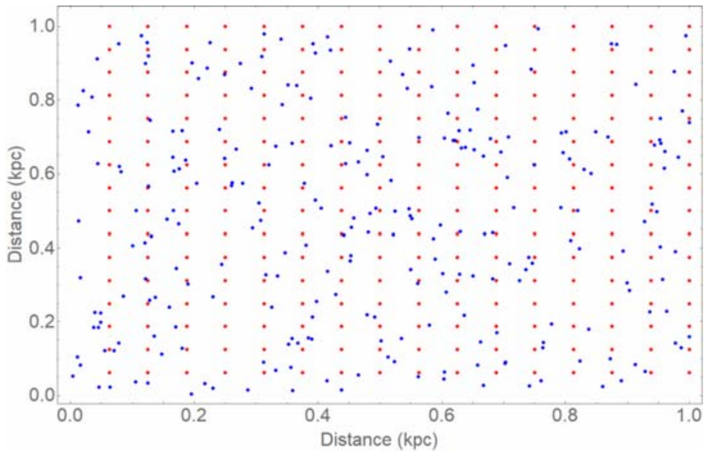

Fig. 3 – (Color online) Initial conditions for the 2D case with BHs (blue) placed in a uniform gas background (red).

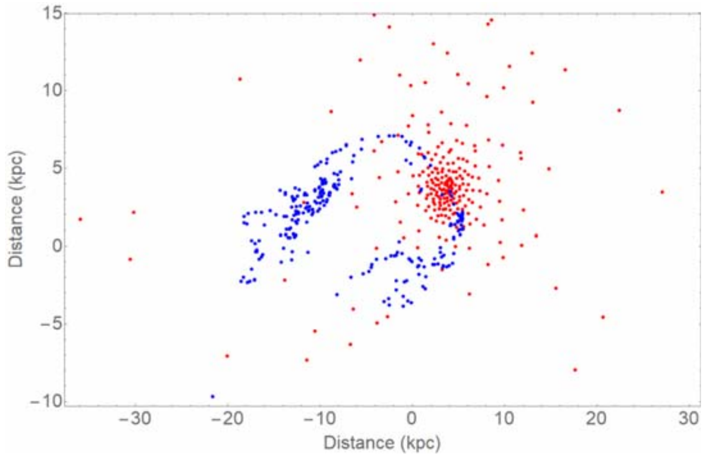

Fig. 4 – (Color online) Final snapshot of the 2D case with BHs (blue) placed in a uniform gas background (red).

This case was done with flags for merging turned on in the *Config.sh* from the GIZMO setup. The same values for the masses were kept from the previous simulation. The resulted behavior was an expected one: due to the high number of BH compared to the space given, all the BH particles merge following a classic “merger tree” resulting in one MBH.

II. 3D case

The purpose of the tridimensional case is to get as close as possible to the full distribution of the black holes as inferred from observations. As we are using the results from the “heavy seed” scenarios, the initial values of the mass of the black holes are $\geq 10^4$ M$_\odot$ [34]. We decided to test the 10^5 M$_\odot$ case to begin with and observe the subsequent numerical behavior across the span of 13 billion years (as well as the final results after this set time interval). The desired results were correlated with a concentration of 350–2200 of BHs per kpc^3 derived from observations [30], each having masses of 10^8 M$_\odot$. Considering an extreme case, where BHs grow by accretion at Eddington limit, a simple computation estimates an approximate growth of one order of magnitude per maximum of one billion year. Also, taking into account that a black hole can’t be in the Eddington limit for too long (new material for feeding is provided only after a new bulge/galaxy merger) and that the main gravitational effects end after the first billion year, we place a limit of maximal accretion (Eddington limit) at one billion year. That is to say that, by not taking into consideration accretion, the simulations should provide a growth from 10^5 M$_\odot$ to 10^7 M$_\odot$ by merging only (at which we can add the remaining accreted mass and obtain the expected results).

The other parameters used here were “inherited” from the two-dimensional case (with the exception of adding one more spatial dimension). This resulted in no mergers at all. It is also worth mentioning that GIZMO requires a smooth background in order to enable the merging of BHs [33]. Therefore, gas particles were spread uniformly across the initial volume with negligible masses, in order to not influence the growth of BHs. Even so, GIZMO’s *hdf5* output files allow recording of the BH mass growth related to mergers only. To this extent, we can track the BH masses without any other growth mechanism interfering.

This first inconclusive result showed that a simple linear extension from a simple scenario with a generic black hole mass and concentration to the real observed black hole mass distribution is not feasible. In what follows, we describe a complex iterative procedure to find the most suitable initial parameters, for instance, the concentration of black holes.

Also, the way we search for the above-mentioned concentration, is illustrated in Fig. 5. We start from an “elementary cell” that we let evolve through time and space. After the end of the timesteps, we compute the resulted BH concentration (taking into consideration only the masses with values over the 10^7 M$_\odot$ limit and the total spread volume). That resulted concentration will be associated with the “elementary cell” volume (*e.g.* a cube with a side length of 10 pc) and then multiplied until it reaches a volume of 1 kpc^3 (Fig. 6), thus scaling our result from the simulations, without the need for more computing power that would match that exact same case.

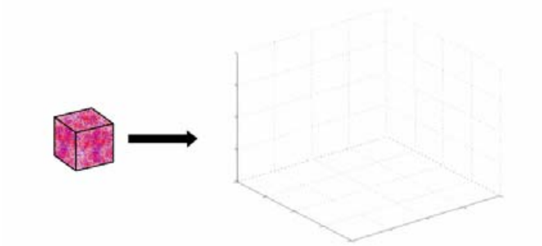

Fig. 5 – "Elementary cell" placed in the 3D space (concept). The scale differs depending on the starting elementary cell volume. For example, an elementary cell cube with a side length of 10 pc has to be multiplied until it fills the space generated by a cube with a side length of 1 kpc (*e.g.* 10^4 elementary cells).

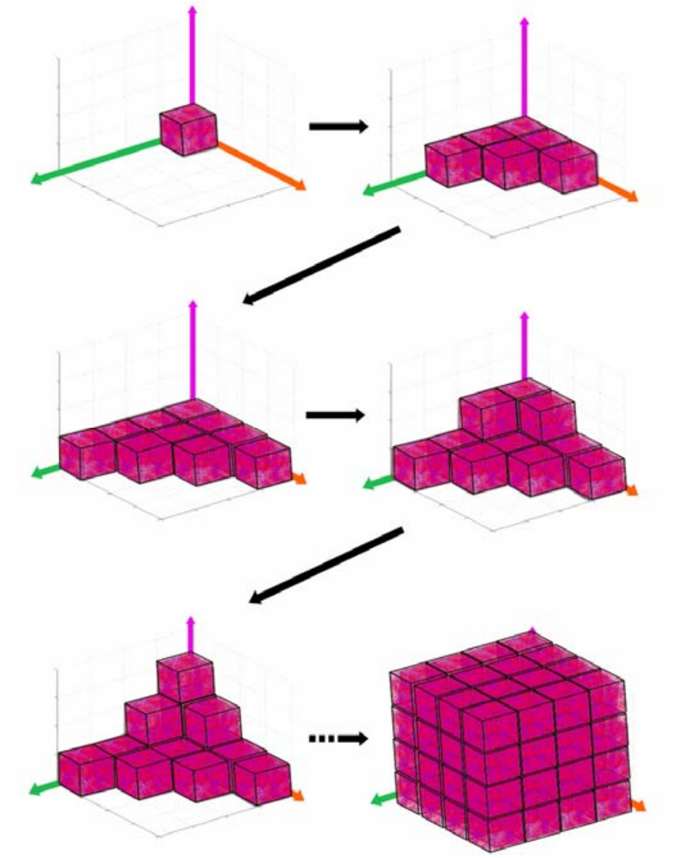

Fig. 6 – Scaling from the "elementary cell" volume to the final one (concept).

For a number of 13 500 BHs, distributed randomly across a volume of 0.125 pc^3 (*i.e.* a cube with the side length equaling to 0.5 pc), we obtained a growth of two orders of magnitude from 10^5 $M_\odot$ to 10^7 $M_\odot$. However, the resulted concentration of BHs was 0.6/kpc^3 (well below the desired value). Consequently, we increased the number of initial BHs for a higher concentration value. One direct effect was a mass increase of the merged BHs and not on their actual number. Another difficulty emerged when looking at the final volume of occupied space: a higher number of initial BHs meant a larger volume of space for the final timestep. Accordingly, the concentration would change as well. These were all obstacles related to the simulation parameters. Due to the non-linear BH evolution processes, they could not be determined *a priori*. The lack of analytical behaviors forced an iterative analysis of the parameters.

In the end, setting up 4 000 BHs (Fig. 7) as initial conditions, in a volume of space equal to 1×10^{-6} kpc^3 (*i.e.* a cube side length of 10 pc), took the end results to a concentration of 650 BHs/kpc^3 (Fig. 9a).

Placing 17 280 initial BHs (Fig. 8) provided a final concentration of 1 800 BHs/kpc^3 (Fig. 9b). Both results are well within the desired interval (obtained from observations).

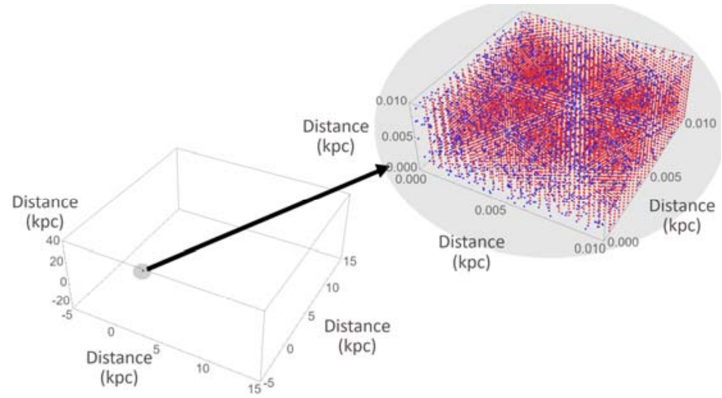

Fig. 7 – (Color online) Initial conditions for 4000 BHs (blue) placed in a uniform gas background (red) in a cubic volume with a side length of 10 pc. The figure on the right represents the zoomed in volume.

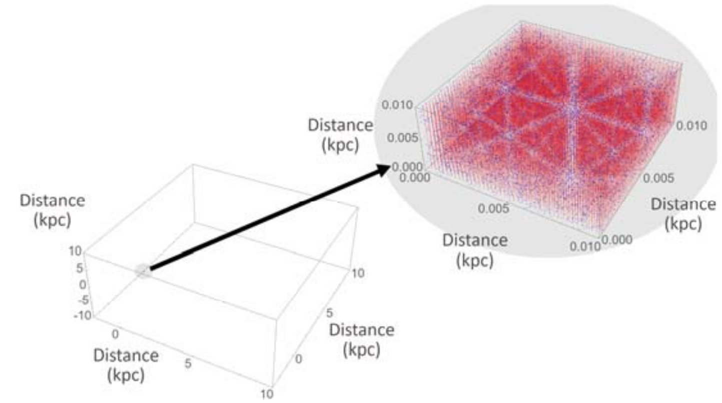

Fig. 8 – (Color online) Initial conditions for 17 280 BHs (blue) placed in a uniform gas background (red) in a cubic volume with a side length of 10 pc. The figure on the right represents the zoomed in volume.

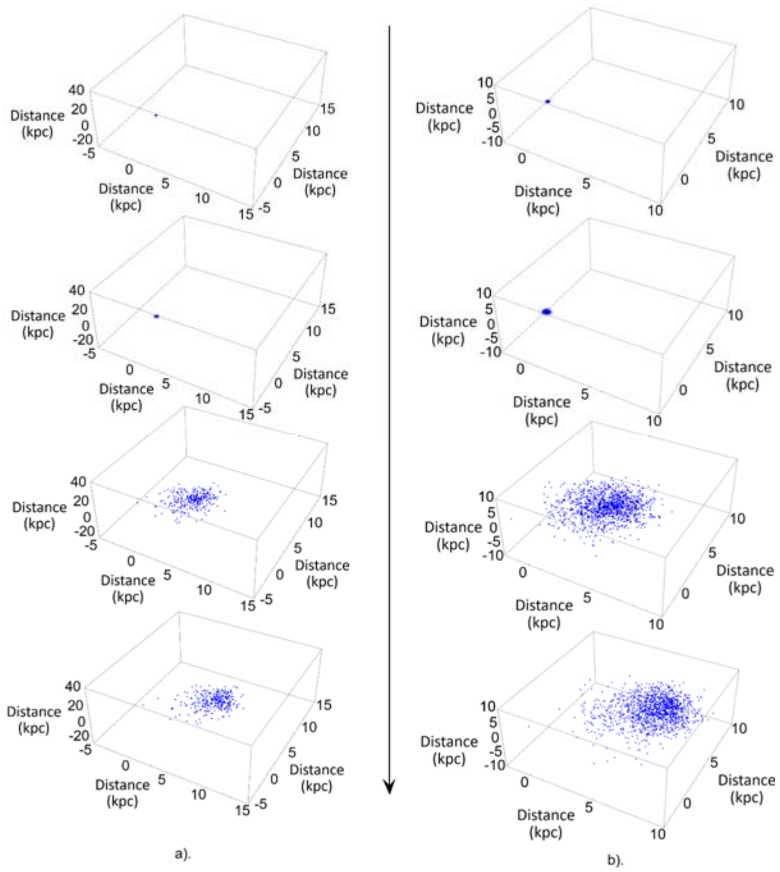

Fig. 9 – (Color online) Evolution for: a) 4000 BHs (blue); b) 17200 BHs (blue).

4. RESULTS

The next figure presents the evolution of the merger rate cumulated number, for both cases, modelled with a power function that has a slope of 0.54, for the 650 BHs/kpc^3 concentration (blue), and one of 0.66, for the 1800 BHs/kpc^3 case (red). It can be noted that, in the first case, the slope is much closer to the ideal value of 0.5 (resulted from normal evolution of cosmological scale structures).

Although both results are well beyond the limits of the BH mass concentration interval resulted from observations, they will be analyzed separately. Therefore, in the next figure, mass distributions are presented for both cases. The left distribution is the one resulted from the 650 BHs/kpc^3 concentration, and the one on the right is the 1800 BHs/kpc^3 concentration. These graphical representations demonstrate that the first case is closer to a Gaussian distribution, suggesting a normal evolution, whereas the second one displays an exponential growth, followed by a quick descent, in a mass interval that is larger than the observational data suggest (thus indicating a non-physical behavior).

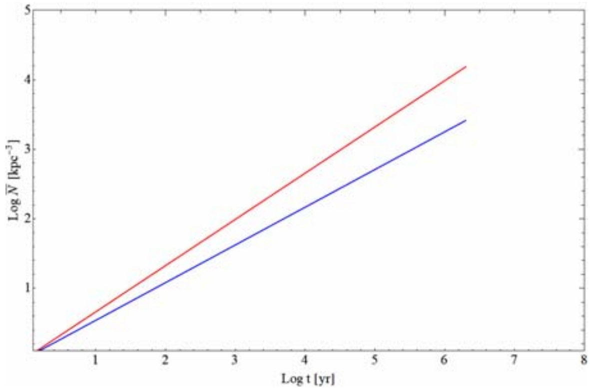

Fig. 10 – (Color online) BH growth rate fit plots, for both cases, the 650 BHs/kpc^3 concentration (blue – 0.54 slope), and the 1800 BHs/kpc^3 one (red – 0.64 slope).

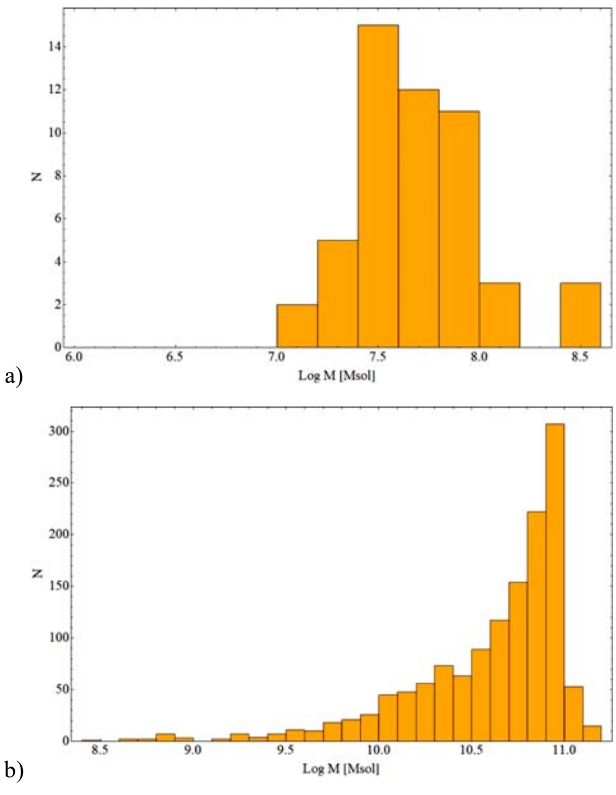

Fig. 11 – BH mass distributions: a) resulted from the 650 BHs/kpc^3 concentration; b) resulted from the 1800 BHs/kpc^3 concentration.

In this way, we managed to find the initial BH concentration, that generated the present distribution, as well as the merging rate for growth, which is a very important result for the LISA Space Mission. This result will be used in the LISA collaboration for detection rate estimations and for a better preparation of the acquisition and data processing systems. Further improvements regarding the simulations will also be part of the same process.

5. CONCLUSIONS

We have simulated MBHs populations, using the GIZMO code package, both for test-case and growth evolution purposes. We started from a primordial Universe paradigm and let the entire system develop and expand, taking into account gravitational interactions and merging processes, for the duration of 13 Gyrs. We then applied an iterative procedure to generate BH concentration for final masses $\geq 10^7$ $M_\odot$ in order to place our simulation results inside the 350–2200 BHs/kpc^3 interval, as extracted from observations. Note that the observations interval is related to BHs with masses of 10^8 $M_\odot$, but we assumed BHs accrete at Eddington limit in the first 1 Gyr. This specific assumption accounts for the gap in orders of magnitude.

After the iterative process of numerical simulations due to the non-linear evolution process of the system, we were left with two candidate situations, one with 4000 initial BHs, and the second one with 17200. Both resulted in concentrations that situate themselves inside the observations interval: 650 BHs/kpc^3 and 1800 BHs/kpc^3, respectively.

We showed that the evolution of the merger rates, for both cases, modelled with a power function, had a slope of 0.54 (for the 650 BHs/kpc^3 scenario), and one of 0.66 (for the 1800 BHs/kpc^3 one). We noted that the 0.54 slope is very close to the ideal value of 0.5, associated with cosmological scale structure evolution. We eliminated the second case, by considering that it resolves around a non-physical process, a conclusion also supported by the black hole mass distribution that showed many black holes with masses equal or greater than 10^{11} $M_\odot$, a result not supported by observations.

In conclusion, we succeeded in finding the initial BH concentration, that, in turn, generated the present distribution. This result will be used by the LISA collaboration to estimate the detection rate of MBH mergers.

An introductory part of this article was communicated at the *Atomic and Molecular Physics. Astrophysics. Applications* session of the “Bucharest University Faculty of Physics 2019 Meeting”.

Acknowledgements. This work is supported in part by research grant LAPLAS VI and ESA PRODEX program. The numerical results reported here were obtained using the Scientific Computing Cluster of ISS (Institute of Space Science).

REFERENCES

1. L. Ferrarese and H. Ford, Space Science Reviews **116**, *3–4*, 523–624 (2005).
2. A. Sesana, F. Haardt, P. Madau, and M. Volonteri, ApJ **623**, 23–30 (2005).
3. LIGO working group, https://www.ligo.caltech.edu/
4. Virgo working group, http://www.virgo-gw.eu/
5. GEO600 working group, http://www.geo600.org/
6. CLIO working group, http://www.icrr.u-tokyo.ac.jp/gr/GWPOHPe/clio-e.html
7. KAGRA working group, https://gwcenter.icrr.u-tokyo.ac.jp/en/plan
8. Grace Database, https://gracedb.ligo.org/latest/
9. LSC https://www.ligo.org/
10. B. P. Abbott *et al.,* Phys. Rev X **9**, 031040 (2019).
11. S. Kawamura *et al.,* J. Phys.: Conf. Ser. **122**, 012006 (2008).
12. LISA L3 Proposal, https://www.elisascience.org/files/publications/LISA_L3_20170120.pdf
13. LISA Space Mission, https://www.elisascience.org/
14. Cosmic Vision, http://www.esa.int/Science_Exploration/Space_Science/ESA_s_Cosmic_Vision
15. S. Hawking, Mon. Not. Roy. Astron. Soc. **152**, 75 (1971).
16. B. J. Carr and S. W. Hawking, Mon. Not. Roy. Astron. Soc. **168**, 399 (1974).
17. G. F. Chapline, Nature **253**, 251 EP (1975).
18. A. M. Green, Fundam. Theor. Phys. **178**, 129 (2015).
19. M. Sasaki, T. Suyama, T. Tanaka, and S. Yokoyama, Class. Quantum Grav. **35**, 063001 (2018).
20. M. Rees and M. Volonteri, Proceedings of the International Astronomical Union 2(S238), 51–58 (2006).
21. Volker Bromm *et al.,* ApJ **527**, L5 (1999).
22. Tom Abel *et al.,* ApJ **540**, 39 (2000).
23. Ya. B. Zel'dovich and M.A. Podurets, Astronomicheskii Zhurnal **42**, 963 (1965).
24. Ya. B. Zel'dovich and I. D. Novikov, *Relativistic astrophysics*, Vol. 1: *Stars and relativity*, University of Chicago Press, Chicago, 1971.
25. S. L. Shapiro and S.A. Teukolsky, ApJ **292**, L41–L44 (1985).
26. G. D. Quinlan and S. L. Shapiro, ApJ **356**, 483 (1990).
27. P. Madau and M. Rees, ApJ **551**, L27 (2001).
28. M. Begelman, M. Volonteri, and M. Rees, Mon. Not. Roy. Astron. Soc. **370**, *1*, 289–298 (2006).
29. P. F. Hopkins, Mon. Not. Roy. Astron. Soc. **450**, *1*, 53–110 (2015).
30. L. I. Caramete and P. L. Biermann, A&A **521**, A55 (2010).
31. V. Springel, Mon. Not. Roy. Astron. Soc. **364**, *4*, 1105–1134 (2005).
32. GIZMO user file, http://www.tapir.caltech.edu/~phopkins/Site/GIZMO_files/gizmo_documentation.html
33. P. F. Hopkins correspondence, https://groups.google.com/forum/#!forum/gizmo-code
34. F. Pacucci *et al.,* ApJ L **850**, L42 (2017).