Program Title Computational Astrophysics and Cosmology

Program Acronym ASTROSIM

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Abstract

This program aims to bring together European computational astrophysicists working on a broad range of topics from the stability of the solar system to the formation of stars and galaxies. Understanding our origins and the formation of structure in the universe is a challenging multi-disciplinary research activity that brings together observational, experimental and theoretical researchers with a broad range of expertise. The systems that we attempt to model are complex and involve a range of physical processes operating over enormous lengths and timescales. Computational techniques developed by researchers in Europe since the 1960's have played a central role in advancing this subject, developing theories for structure formation, testing cosmological models and solving the complex non-linear problems inherent to gravitational and hydro-dynamical astrophysical processes. Understanding the strong interplay between different scales is essential for a complete theory and true understanding of structure formation. Our aims are to strengthen the existing European activities in computational astrophysics, avoiding fragmentation as this field grows in strength and to exchange expertise through an active program of conferences, workshops, training schools and exchange visits. Our scientific objectives are to refine our computational techniques and multi-scale modelling in order to develop and test theories of structure formation in readiness for the grand challenge European projects planned by ESO and ESA over the coming decades.

Keywords Astronomy, Cosmology, Computational Techniques, Numerical Simulation

Computational Astrophysics & Cosmology: Context and Status Report

In the past decade a combination of satellite and ground based observational experiments have mapped and quantified the observed universe to an unprecedented precision. The fundamental parameters that govern the evolution and future of the universe have been measured. We know the matter and energy densities and primordial fluctuation spectrum – the initial conditions for cosmic structure formation - to a few percent. However, only a small fraction of the universe has been physically identified and understood - the dominant components of matter and energy remain a mystery. We believe that most of the mass in the universe is a new fundamental particle that links astrophysics with particle physics and super-symmetry, whilst the dark energy may be some property of the vacuum or extra dimensions. Furthermore, even processes where only the well known physics of baryons operate are not very well understood, such as in the formation of stars and planets. Central to this proposal is to understand how the material in the universe arranges itself into the wide range of observed structures from planets to stars to galaxies.

Observations of structures in the universe span the entire range of wavelengths, from the present epoch to proto-galaxies at $z \sim 6$ when the universe was just 10% of its present age. An inspiring picture is building up that reveals how cosmic structures form and evolve. Forthcoming instrumentation will enable astronomers to look further back in time to when the first stars and supernovae lit up and re-ionised the universe, and to explore in detail systems on smaller scales such as star-forming regions and proto-planetary disks. Star formation and the subsequent stellar evolution play a central role in understanding both the origin of galaxies on larger scales, and planetary systems on smaller scales. This latter topic has seen intense activity through the detection of extra-solar planetary systems and the coming decade is likely to see the detection of earth mass planets and even the possibility of carrying out spectroscopy on their atmospheres.

On galactic scales and above we observe a single snapshot of the universe – nothing changes on human timescales. We piece together the history of the universe through observations at different epochs, or in the case of our own Milky Way, by deciphering the fossil record imprinted in the different properties of its stellar populations. Computer simulations are a unique tool that let us “observe” the evolution of model universes. With full three dimensional data, simulations allow us to disentangle observational biases, to test different cosmological models and to understand the origins of cosmic structures as the universe evolves from its nearly smooth initial conditions to its present “ordered state”. Accurate modelling of astrophysical processes requires advanced computational techniques and specialised supercomputing resources that have only recently become widely available to academic research groups.

The relevant physical processes can involve the comparatively simple gravitational evolution of a collisionless dark matter fluid that can be solved via n-body simulation of the Boltzmann equation. In this case particle-particle interactions can be ignored and we follow the collective effects by approximating the mass distribution using Monte Carlo techniques. Collisionality adds an additional degree of complexity to self-gravitating systems but plays an important role in the evolution of dense star clusters and the formation of central black holes. Close encounters can drive the evolution and thus accurate symplectic integrators and collision detection routines are necessary. Special purpose hardware such as GRAPE and FPGAs are being employed to speed up these calculations – other areas of computational astrophysics could benefit from these techniques.

Once we consider the baryonic component of the universe we enter a new level of sophistication since the full hydrodynamic equations must be solved alongside the gravitational forces. Astrophysics has contributed a new technique to this field which is now used in many diverse areas from simulating car crashes to protein folding. Smoothed particle hydrodynamics is a Lagrangian technique for modelling gaseous processes that is different from the Eulerian approach. These techniques are complimentary and each has its drawbacks and strengths. On stellar scales, one must follow hydro- and magneto-hydrodynamical turbulence in the ISM during the formation and collapse of a molecular cloud core to the point at which nuclear burning may start. The evolution of proto-stellar and proto-planetary disks might also involve transport of angular momentum by both gravitational and magneto-rotational instabilities (MRI). Similar physical processes may apply to studies of galactic nuclear disks and AGN accretion disks whose evolution is essential to understand the growth of super-massive black holes. Often 3D radiative transfer is required to compute the thermal evolution of such structures and is especially important for studying processes responsible for re-ionising the universe.

Numerical simulations have played a central role in understanding observational phenomenon. They are the theorist's tool for solving complex non-linear problems. Notable success of simulations have included an understanding of how galaxies can undergo morphological transformation by merging and interactions, the structure of dark matter halos within a collisionless hierarchical cosmology, the large scale pattern of galaxy clustering, the formation of galaxy clusters and the global properties of the intra-cluster medium (ICM). On smaller scales, simulations have helped us to understand the dynamics of self-gravitating galactic systems, the flow of gas in galaxies and the fuelling of nuclear black holes, the formation of the first stars and instabilities in self gravitating disks on different scales. Stellar evolution is now almost a closed subject, solved by complex numerical modelling of stellar structure and the appropriate physical processes. Notable problems await solution, including the final stages of stellar evolution, the origin of earth-like planets, the long term stability of the solar system, black hole formation and the interplay between black holes and accretion disks, the central evolution of dense stellar systems, star-formation and the formation of galactic disks and the detailed properties of the intra-cluster medium in galaxy clusters. Whilst theoreticians are still trying to understand how galaxies assemble themselves from the dark matter and baryons in the Universe, observers are acquiring exquisite multi-wavelength data for over a million galaxies. They have high resolution spectral information, colour maps, element abundances and kinematical data for individual galaxies. Theorists have not yet succeeded in making a realistic disk galaxy from first principles via direct simulation. Similar problems exist on other astrophysics scales. Whilst astronomers are cataloging the properties of numerous extra-solar planetary systems, theorists have yet to form a single realistic solar system via computational techniques. Despite these difficulties, theorists are not so far behind and we believe that many of these problems will be solved in the coming decade if sufficient resources and support are provided for this community.

Objectives and envisaged achievements

Our ultimate scientific objectives are to construct and test theories of structure formation that are powerful enough to compare with forthcoming observational data, and to make predictions for the grand challenge European Southern Observatory (ESO) and European Space Agency (ESA) programs that will take place over the next decade. We aim at building a large-scale coordinated effort amongst European computational astrophysicists that should match the notable efforts of the large teams typically involved in the large observational programs that characterise this decade. Only such a balance between resources and organisational level in theory and observations can produce a truly outstanding performance of European research in this field and thus justifying the funding given to either of the two activities. Several major barriers remain and we face the following difficulties:

- The range of scales in mass, length and time is vast. Important physical processes that are occurring below the resolution limit of our simulations are included in a phenomenological way.
- Initial conditions are often quite idealised and can influence the final results.
- Astrophysical fluid codes are extremely sophisticated yet different techniques are often not rigorously examined through comparative tests.
- Researchers working within one area rarely collaborate with other groups working on different scales, even though the physical processes can be very similar.
- Research can be fragmented, with no European wide forum for discussion and collaboration.

This program aims to overcome these problems by bringing together computational astrophysicists and cosmologists working on a wide spectrum of problems in astronomy. A platform for funding will be provided for exchange visits with emphasis given to interdisciplinary collaborations. A bi-yearly computational astrophysics conference will be organized that will bring the entire community in Europe together. Several focussed workshops will be held each year and graduate training schools will be organised.

A successful ESF Exploratory workshop was recently held to discuss some of these aspects of our research. We brought together several of Europe's leading computational astrophysicists (and several international experts) working on a diverse range of problems to discuss the above issues. The seminars from this workshop are published on the following webpage: http://www-theorie.physik.unizh.ch/~moore/wengen/
One of the major scientific goals of this ESF program is to create collaborations between astrophysicists working on the scales important to each other's problems. For example, a theory of star formation requires knowledge of large scale processes in galaxies such as gravitational driven turbulence in the ISM. The final stage of star formation provides the initial conditions for the onset of planet formation. Star formation and feedback processes are all included as unresolved sub-grid processes in current cosmological simulations. Europe has leading experts on each of these scales and by combining our expertise we can create realistic initial conditions; the end state of one simulation may be the starting point top grid model for another group. The processes resolved in one simulation, might be used to motivate a sub-grid model in a simulation on a different scale.

Communication and collaboration are essential to ensure that our physical modelling is as accurate as possible. This implies a rigorous testing phase in similar spirit as started by several of us as a discussion point at the exploratory workshop. We devised and distributed several simple test problems related to processes that many of us routinely face. Carrying out the test simulations were four independent adaptive mesh refinement (AMR) codes, five smoothed particle hydrodynamics codes (SPH), several grid codes and a unique re-meshable SPH code. The web page describing the tests and some of the results is here: http://www-theorie.physik.unizh.ch/~moore/wengen/tests/
This ESF program will allow us to follow up and extend these tests to include additional problems, such as radiative transfer and MHD. We will use the program to publicise and involve the entire community of researchers who are developing and using algorithms for simulating astrophysical fluids. Our aim is to stress the codes and ensure that we understand the systematic numerical effects whilst learning the strengths and weaknesses of different techniques.

Expected benefit from European collaboration in this area

The main benefit of carrying out this proposal at the European Community level is to:

- Forge new collaborations between researchers that do not currently exist.
- Train young researchers in the field of computational astrophysics & cosmology.
- Bring together the ideas and resources of top European research groups.
- Promote at a European and world level outreach from computational research.
- Enable European researchers to stay at the forefront of research in this field.
- Utilise the existing and planned supercomputing resources to their full extent.
- Support the grand challenge science projects of European astronomy by constructing detailed theoretical models of astrophysical systems.

The broad objective of the ESF programs is to support high quality science and act as a catalyst for its development through planning and implementation. We believe that it is a timely period to invest resources in computational astrophysics. European investment in observational astrophysics and cosmology is at a record level due to the impact of this field in the public sector, its role in training people for jobs outside of academia, motivating the next generation of scientific researchers and facilitating the fundamental goal of understanding our origins and place in the universe. Computational astrophysics is a research topic that attracts many young researchers which helps reverse the trend in Western countries that fewer and fewer young people are attracted by research in the sciences. The overall European capacity to train and transfer knowledge will be increased by bringing together the expertise and skills of the entire community, sharing and combining resources and knowledge, disseminating results and tools including analysis and visualisation software and coordinating a combined attack on understanding the multi-scale physics relevant to astronomical systems.

Computational astrophysics is a research area where European scientists are well established and are highly prominent. In order to maintain this position and to tackle the complex scientific problems discussed earlier, it is essential that strong collaborations exist within the European community. These research goals will not be solved by an individual, nor a single institute, but rather by the concerted effort of groups of experienced researchers. On a longer term, we specifically plan that long term collaborations between the different nodes will be forged during the network that will continue beyond the funded period. This is especially important since when the network closes there will be intense activity as GRID based computation will begin and we anticipate promoting collaboration with the European Grid programs such as GEANT. The scientific output of the community should eventually be linked to the European virtual observatory via a dedicated database. Several of our participants already have strong connections to these programs. We envisage that the students and young researchers we train will play a major role in the future of high performance computing and computational astrophysics in Europe.

European Context

Europe is investing billions of euros in astronomical instrumentation designed to survey, catalogue and study structures in the universe. From extra-solar planetary systems to the epoch of re-ionisation, a wealth of new data is flowing into European research institutes. Extracting the most useful information from the data, helping to guide and plan new missions and making predictions for the next generation of observational missions are amongst the key goals of our research. Europe currently benefits from powerful computing hardware on a national level at focused centres such as UK Astrophysical Fluids Facility or the various national supercomputing centres. Many individual institutions have access to their own large scale supercomputing resources, such as the Max Planck research centres or the 288 processor supercomputer in the computational cosmology group in Zurich. Furthermore investment in such facilities is rapidly growing. In 2005 Spain will install a large 4564 processor, 40 Teraflop machine as powerful as the world's fastest supercomputer, the earth simulator in Japan, which will be used solely for scientific research. It is important to stimulate activity in computational astrophysics on a European scale to develop the links between different research groups which are predominantly working alone or within bi-lateral collaborations, so as to utilise these expensive resources to their full capabilities.

In addition to the existing ground based observational facilities such as the VLT, the European Southern Observatory (ESO) will soon complete ALMA (a large millimeter array for a range of astronomical projects from solar system studies to star and galaxy formation) and has ambitious plans for the next decade through the construction of a 100m telescope (OWL). The European Space Agency (ESA) is developing several missions that will greatly increase our understanding of astrophysical systems. The James Webb Space Telescope (infra-red satellite to study the first structures in the universe), Corot (optical earth-like planet detector), Planck (cosmic microwave background studies) and Herschel (infra-red and sub-millimetre satellite for probing star formation and galaxy formation) will all be launched during the operation of this proposed program. The following decade will see further advancement of space instrumentation with many new missions in the planning stage, including GAIA (an astrometry mission for mapping a billion stars within our Galaxy), Darwin (extra-solar planet finder and interferometer for studying their atmospheres), LISA (gravity wave detector), XEUS (X-ray telescope two orders of magnitude more sensitive than XMM-Newton, for studying black holes and the ICM of groups and clusters). Unfortunately, our ability to make realistic predictions for these missions is minimal – for example no group has been able to create a rocky planet from first principles thus we have no idea if earth like planets are expected to be rare or ubiquitous. Predictions for the gravitational wave signals that LISA should see as a result of coalescing supermassive black holes are based on poorly constrained models of the formation and merging of such objects while hierarchical structure formation proceeds. In order to extract the most scientific knowledge from ongoing and forthcoming missions it is essential that Europe invests in theoretical modelling and computational astrophysics is central to this activity. We believe that this ESF program is the ideal platform for coordinating activities in this theoretical domain and to act as a unified forum for motivating new, more focussed networks, such as the EU Marie Curie research and training activities.

Small working groups do exist in this field, for example the MODEST collaboration studying the evolution of dense star clusters. However, this proposal will be the first large scale European initiative in computational astrophysics. This is surprising given the number of world class researchers in this field in Europe today and the fact that these researchers have played the lead role in developing this field to its current status. Since the 1960's, soon after the first computers became available for research, European researchers were tackling problems ridiculously small by today's standards, but extremely challenging at that time. Sverre Aarseth's first 50 particle simulation in the 1960's has recently been pushed to 10 billion particles by researchers at the MPA, Garching. Computational astrophysicists push the boundaries of supercomputing resources, such as CPU power, data storage and analysis and visualization. Large astrophysical simulations are often used to showcase the performance of today's supercomputers. It is important to maintain and even improve the world class research in this area through this program.

Europe is beginning to feel the technological feedback from scientific researchers demanding more and more performance from computers. One of the world's lowest latency communications network for parallel supercomputing is developed in Norway by SCI. Researchers in Mannheim are pushing the network performance using ATOLL and in collaboration with computational astrophysicists are developing FPGAs for n-body calculations. The Zurich group has created a spin-off company developing supercomputer hardware based on a novel new design for optimising performance and stability within a high density system. The past decade saw a significant number of researchers in this field leaving Europe for the USA which is still ahead of Europe in computing resources and commercial enterprises. The above examples are just a few of the cases of innovation occurring in Europe.

Proposed activities

Our methodology is to promote collaboration through training and stimulation of ideas by mobility of human resources in addition to training schools and workshops. Two or three showcase conferences in computational astrophysics will bring together European researchers through this ESF initiative and overseas researchers by matching grants from other sources. In order to sustain the impact of this ESF program, EU research and training networks and other large scale collaborations will be encouraged.

Major European conferences in computational astrophysics in years 1, 3 & 5
These meetings will be a showcase for the diversity and excellence that already exists in this research area. We anticipate that these major conferences will gather well over 200 people each year and we suggest that they should be open to international researchers for which additional funding may be sought. These conferences will span the entire remit of computational astrophysics, from the three body problem to the origin of large scale structure in the universe.

Focused scientific workshops
Workshop themes that have already been suggested by the program participants include: chaos in n-body systems, 3d radiative transfer, stability and origin of planetary systems, turbulence in the interstellar medium and the formation of stars, collisional dynamics in dense star clusters, specialist hardware for astrophysical computation, the physics of accretion disks and the connection to super-massive black holes, galaxy formation and the origin of the Hubble sequence, galaxy clusters and the connection to large scale structure in the universe. We will also host two workshops devoted to the continued comparison and testing of the various astrophysical fluids codes from program members. US participants will be invited to participate through the equivalent NSF grant scheme.

Graduate and postgraduate training schools
Experts in Europe will hold training schools in many areas including the following topics: n-body dynamics, astrophysical fluid dynamics, particle methods for fluid simulation, adaptive mesh methods for fluid simulation, galactic dynamics, visualisation and analysis techniques for astrophysical computation. In year two we will organise a Saas Fee school on computational astrophysics. These are well known schools attended by between 50 and 100 young researchers to hear lecture series by three distinguished researchers. The lectures will be written up as a graduate level textbook.

AstroSim information database.
We propose the formation of a sophisticated and informative website for the entire computational astrophysics community – a forum for information, discussion and dissemination of results. Such a database/website does not exist but would be a

remarkable resource for the European and worldwide community, firmly establishing the European leadership in this field. Pictures, movies and scientific results from computations are frequently used for education purposes yet a centralised data base does not exist. We can use this tool to archive "virtual observations" from theoretical models which will be linked to the virtual observatory. The ESF program will be highly publicised through this extensive resource. Our code comparison website resulting from the Wengen exploratory workshop is already a significant database and will grow over the next year as more tests are carried out and results archived and analysed. We anticipate that this database will be a significant resource and possibly become a standard reference for groups who wish to compare existing or new codes under development. The majority of the funds requested will be used to design and configure the database and website interface during the first and second years, and thereafter to pay for constant updates to the site.

Short term collaborative training visits, fellowships

A central activity that is essential for the interdisciplinary scientific program is to actively promote the transfer of skills across the different sub-fields within this domain. On the AstroSim site we will keep a database of researchers in computational astrophysics with details of their particular skills and interests. Young researchers will be able to apply for funding to visit groups with expertise outside of what they can achieve locally. Postdoctoral students will be encouraged to collaborate with research groups around Europe. Six month fellowships will be granted for young researchers in order to broaden their skills and maximise knowledge transfer. The European community of interested researchers in this program is in the several hundreds of scientists. We will encourage applications from researchers seeking to collaborate with research teams outside of their specialist interest area.

Internships at Industrial and Government Laboratories

Astrophysicists already have a culture where scientists have been at the forefront of the development of numerical methods. As a result, many of the top computational scientists in fields as diverse as aeronautics (for example van Leer) and climate modelling (for example Killian the current head of NCAR) started as computational astrophysicists. Many of the techniques that we are developing have even broader applications to fields as diverse as protein folding, the radiosity problem and panel methods for antenna design. We will start a program of internships for young scientists at Industrial and Government laboratories. In addition to providing unique training for these scientists, it will ensure that "best of the breed" developments are shared by scientists in different fields.

Program Coordinator

For the duration of the program, the steering committee proposes to employ a program coordinator at the 40% level. This person will be an experienced researcher at the postdoctoral level who has a broad experience in computational astrophysics, preferably in a range of different areas. The remainder of this person's time will be devoted to research in computational astrophysics funded by the University of Zurich. The role of the coordinator is to attend and help organise steering committees, help with organisation of workshops, schools and conferences, maintaining and coordinating the astrophysics code comparison tests, compiling and disseminating information through the website and program brochure, be a contact point for enquiries and assisting the chair to achieve the program aims and objectives.

Duration 5 years