Community paper „Computational Astrophysics“

T. Naab, R. S. Klessen, W. Kley, F. Röpke, with input from the computational astrophysics community

Executive summary

How does the large-scale structure of the Universe emerge? Which astrophysical processes govern the dynamics of the interstellar medium, and how do stars form and evolve in galaxies? What determines when and where planets build up, and how can we explain the large diversity of the planetary systems observed today? What happens when black holes accrete matter? How do black holes merge and emit gravitational waves? High-performance supercomputer simulations have become the primary theoretical tool to answer essential astrophysical questions. Using about 25% - 30% of the German supercomputing time, computational astrophysics is exemplary for high-performance computing, technical excellence and technology transfer driven by fundamental science. With access to world-class computing facilities many strong research groups in Germany have reached world-leading excellence over the past decade. However, the field will face unprecedented challenges in the next decade. Progress in our theoretical understanding of the Universe requires more complex and computationally demanding simulations. This challenge - in a highly competitive international environment - requires new research and funding strategies. The rapidly increasing effort for the sustained and innovative development of parallel simulation codes, which can make efficient use of upcoming supercomputers, is beyond the scope of typical astrophysical research projects. Efficient simulation codes are the basis for excellence in the field. They serve the same purpose and should be treated and funded similarly to observational instruments for telescopes. New and innovative funding schemes can provide the necessary support for the development, validation, and dissemination of astrophysical simulation tools. It is also essential for the field that German funding agencies continue their high-level support for upgrading the German tier-0 supercomputing facilities at a world leading level.

1. Introduction

High-performance numerical simulations on supercomputers have become a major tool in theoretical astrophysics driving our understanding of complex nonlinear systems. Ultimately, high-performance computing (HPC) is the backbone of theoretical progress in astrophysics. With access to world leading tier-0 supercomputer infrastructure, supported by smaller tier-1 and tier-2 facilities, and with the development of innovative and efficient parallel simulation codes the German community has made significant scientific progress with high international impact in the last decade. By now high-performance simulations are used in almost any area of astrophysics for answering fundamental theoretical questions, for the interpretation of observational data, and for designing upcoming observational programs.

Major research areas of computational astrophysics in Germany include:

- Gravitational interaction of dark matter, galaxies, stars and gas in galaxies, stars in star cluster, and astrophysical many-body systems
- Magneto-hydrodynamic evolution of intergalactic gas, gas in galaxies, and the interstellar medium
- Magneto-hydrodynamics of star forming regions, accretion disks around stars and black holes, formation of planets and planetary systems
- Relativistic hydrodynamics for the evolution of neutron stars and black holes, mergers and gravitational wave emission, and relativistic shocks
- Radiation transfer for cosmic re-ionization, radiation from stars and black holes, stellar evolution models, line and continuum radiation transfer in stellar and planet atmospheres
- Plasma simulations, acceleration and impact of relativistic charged particles (cosmic rays)
- Stellar nucleosynthesis, hydrodynamics, instabilities and neutrino transport in supernova explosions
- Extensive efforts for direct comparison to observations (i.e. radiation transfer post-processing)
- Efficient handling, analysis and interpretation of large data volumes, both from numerical simulations as well as from wide-field astronomical survey

A wide range of theoretical questions in any of these fields can now be addressed with numerical simulations. However, due to limited computational power and/or complex algorithms, which are difficult to parallelize, the predictive power of the simulations is sometimes limited. Important physical processes have to be implemented as empirical rather than accurate numerical models. The most complex processes even might be too computationally demanding to be included at present. A prominent example is simulations of galaxy formation. Here the energetic processes from massive stars (radiation, winds, supernovae) are expected to regulate galaxy formation by controlling the gas flows in galaxies. These processes act on such small scales in the galaxies that they cannot be directly followed (and their effect is only approximated) in current cosmological simulations, which at the same time have to follow the large-scale environment. These approximations (sub-grid models) might capture the overall effect on galaxy evolution but they conceal the underlying physical origin. With novel and improved simulation techniques and more powerful computers it will be possible to abandon empirical models and numerically resolve the physical process on small scales. We will then understand in detail the impact of massive stars on the structure of the interstellar medium, on the driving of outflows and on the large-scale evolution of galaxy populations over many orders of magnitudes on spatial and temporal scales with a single set of simulations.

This example can be applied to many fields and the scientific impact of German astrophysics as a whole will depend to a significant degree on the sustained and improved support for high-performance computational astrophysics.

2. Upcoming Facilities in the Coming Decade

Germany has three national tier-0 supercomputing facilities: the High Performance Computing Center Stuttgart (HLRS), the Jülich Supercomputing Centre (JSC), and the Leibniz Supercomputing Center in Garching near Munich (LRZ). These facilities are regularly ranked in the top ten of the fastest supercomputers worldwide (HRLS is currently Nr. 8). A particular strength of the German facilities is the diversity of architecture with a mixture of general purpose CPUs and many core accelerators (e.g. Intel Xeon Phi, Nvidia Tesla GPU). Access to such world-class systems has enabled German research groups to conduct innovative and competitive simulations at unprecedented complexity and numerical resolution and is therefore a prerequisite for the international success of computational astrophysical sciences in our country.

For the coming decade continued scientific success of the German astrophysical community relies on sufficient funding for national supercomputing facilities. The upgraded facilities have to be competitive with other world-leading institutions and should strengthen their role as global players. The supercomputing centers should also keep their diversity in architecture and therefore support different high-performance simulation strategies, which can optimally handle various physical processes in the most efficient way. In the future the simulations will become more complex with an increasing number of degrees of freedom. The ever growing computational demand will have to be matched. Upcoming computing facilities do not only require enhanced computing power and memory but also improved communication networks (with reduced latency and enhanced bandwidth). It also is important that the computing centers provide sufficiently large disk systems for storing the simulation data and long term archival systems allowing research groups to keep their data for scientific validation and reproducibility of published results. The interaction between supercomputing centers and the respective research groups should be lively and enable the efficient transfer of knowledge and technology.

3. Main Achievements of German research groups over the past decade

A number of strong German groups have reached international excellence in several areas of computational astrophysics. Prominent examples for scientific success are computations of the explosion mechanisms of supernovae, new models for the formation of proto-planetary disks, realistic simulations of the relativistic astrophysics of accretion disks, the merging of neutron stars and black holes, realistic simulations of star formation and interstellar medium with clearly distinct chemical phases, simulations of star clusters resolving the full stellar and dynamical evolution, as well as converged simulations of cosmic structure formation and the first successful simulations of the formation of disk galaxies and the evolution of galaxy populations. In these fields the simulations have reached the level of realism required to provide reliable model predictions and to test theoretical models with direct observations.

It is important to note that the German community has a leading role in bringing astrophysical simulations closer to the observational domain. Mock observations of simulated galaxies or the generation of synthetic emission maps or of high-fidelity model spectra with high predictive power, for example, are key prerequisites for the one-to-one comparison between numerical simulations and multi-frequency observations, and thus for the successful astrophysical interpretation of computational results.

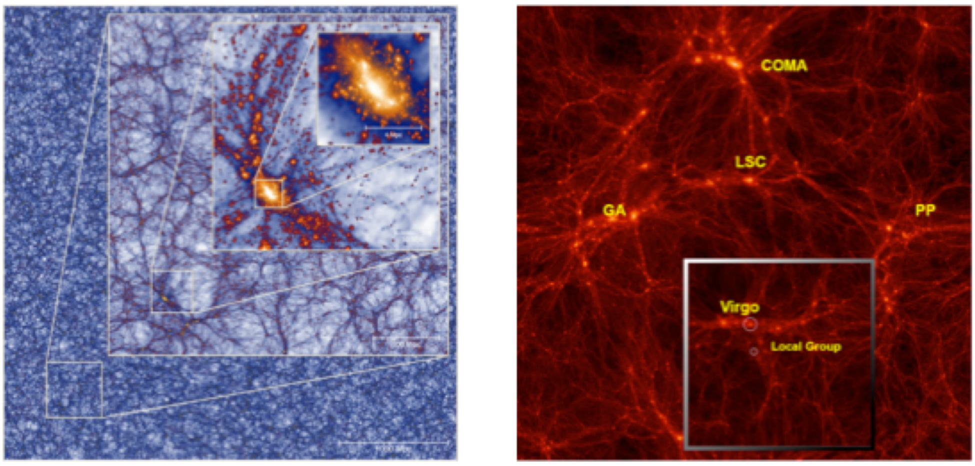
The basis for success in each of the computational astrophysics areas lies ultimately in access to supercomputing facilities and in methods development. Only groups investing significantly in the design of simulation codes and analysis tools, in one way or another, are competitive internationally. Germany has a significant number of such strong groups. In addition to excellent scientific work, the groups have trained outstanding students and postdoctoral researchers with special skills in software development. Many of these students and postdocs have moved on to research positions at top ranked universities worldwide, or they have made successful careers in industry. Overall, Germany has become one of the leading countries in high-performance computational astrophysics. The availability of state-of-the-art computing facilities is a prerequisite for this success and Germany's position has improved internationally over the past decade. At present computational astrophysics is using about 25% - 30% of the total German tier-0 supercomputing time, and the field has become exemplary for high-performance computing and technical excellence driven by fundamental science. Increasing support and funding is required to maintain and further improve this leading position.

4. Particular Role/Strengths of Research Groups in Germany

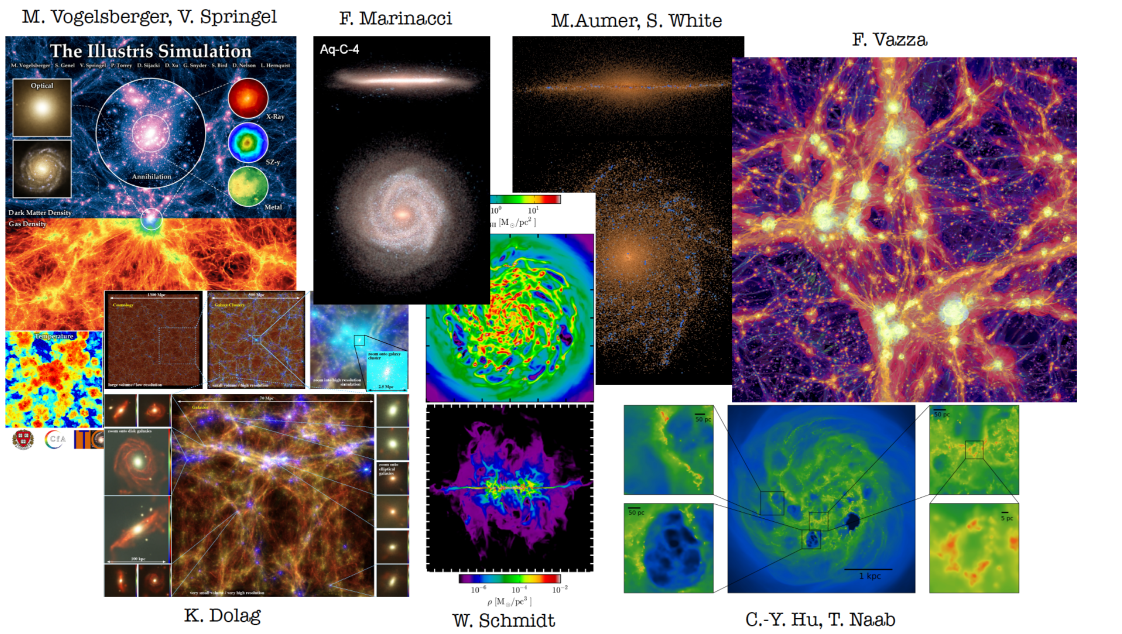
The German computational astrophysics community has reached international excellence in several research areas covering a large variety of astrophysical topics. German research teams have published a significant fraction the most highly cited publications in theoretical astrophysics worldwide (with direct HPC connection) over the last decade. This particular strength is rooted not only in scientific excellence but also in the important role of the German community in inventing (e.g. Gadget, Arepo, Vertex, Cactus, Leafs) and improving (e.g. FLASH, N-Body6, Nirvana, Pencil) major parallel simulation codes. As an example for the high impact it is worth noting that in the large field of structure formation and galaxy formation computational astrophysics groups in Germany have produced scientific publications which are in the top 20 most cited publications in all astrophysics worldwide in the years 2005, 2006, 2008, 2010, 2011, and 2013. In 2014 and 2015 the highest impact astrophysical publications based using high-performance simulations are the Illustris simulations (top 20 in 2014) and the Eagle simulations (Nr. 1 in 2015), which are based on codes (Arepo and Gadget, both by V. Springel) originally developed (and partly made publicly available) by German groups at MPA and HITS.

In the following we these and other particularly successful examples of HPC based astrophysical research together with the respective groups and the names of the codes used.

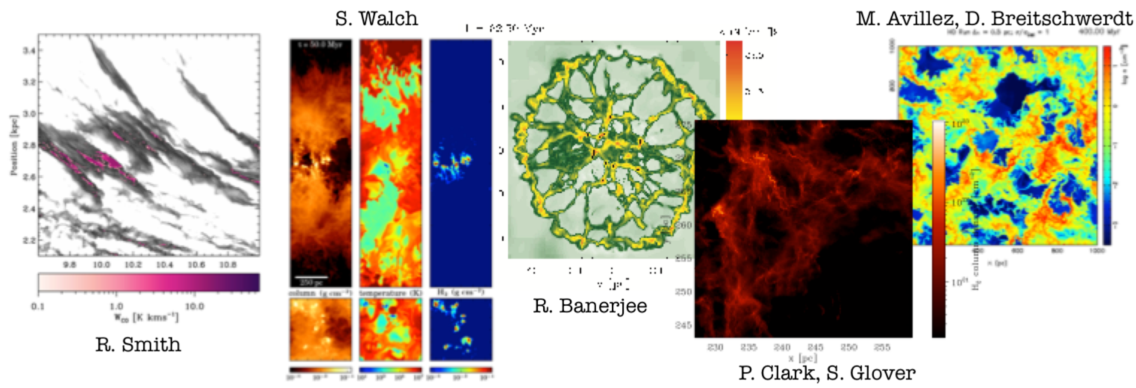
V. Springel, R. Angulo S. Gottlöber



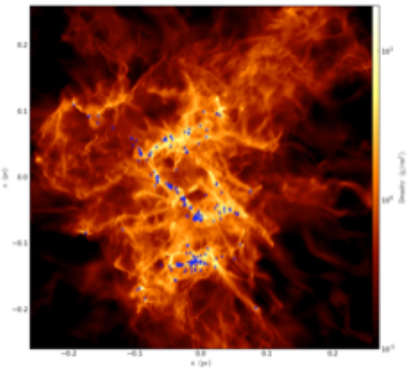
Dark matter simulations on structure formation, tests for cosmological models, tests of theories for gravity, calibration for observational surveys, origin of our cosmic neighborhood [left: the large scale structure of the Universe (Springel, Angulo et al., MPA, Garching / HITS, Heidelberg), right: the matter distribution on our Galactic neighborhood (Gottlöber et al. AIP, Potsdam); used codes: Gadget, ART]



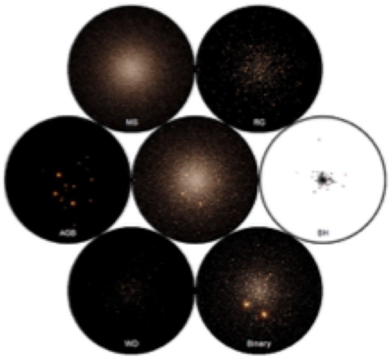
Magneto-hydrodynamical simulations of the formation of individual galaxies, galaxy clusters, and galaxy population on cosmic timescales. Tests of models for the impact of massive stars and accreting supermassive black holes on galaxy evolution, and direct comparison to observations [from left to right: cosmological simulation of the evolution of galaxy populations (Vogelsberger, Springel et al, Harvard, HITS, Heidelberg), Dolag et al. (USM, Munich), the cosmological formation and evolution of spiral and dwarf galaxies (Marinacci et al., HITS, Heidelberg; Schmidt et al., University of Göttingen; Aumer, White et al., MPA; Hu & Naab et al., MPA, Garching), the distribution of gas in galaxy clusters (Vazza et al., Hamburg University); used codes: Arepo, Gadget, FLASH, Enzo, Nyx]



Magneto-hydrodynamics, turbulence, non-equilibrium ionization, star formation, impact of stellar radiation, winds, supernovae, cosmic rays, magnetic fields on the structure of the interstellar medium, mock observations, continuum and line radiation transfer [from left to right: the filamentary structure of molecular clouds (Smith et al., ZAH, Heidelberg), the multi-phase structure of the ISM (Walch et al., University of Cologne), molecular cloud formation (Banerjee et al., Hamburg University; Clark & Glover, ZAH, Heidelberg), the magnetized interstellar medium (Avilles & Breitschwerdt, TU Berlin); used codes: Gadget, Arepo, FLASH]

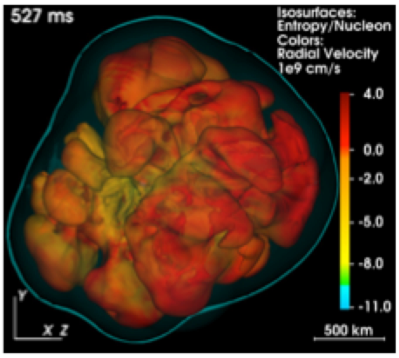


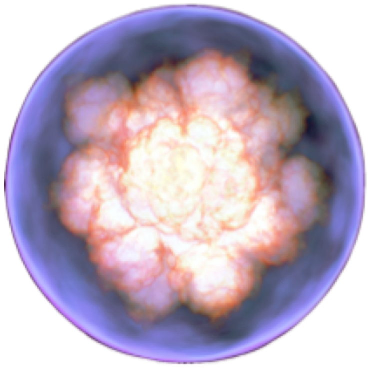
P. Girichidis



L. Wang, R. Spurzem

Initial conditions and evolution of star clusters, realistic simulations of globular clusters including stellar evolution with efficient use of special hardware (GPUs) [left: formation of a star cluster (Girichidies et al., MPA, Garching); right: evolution of a globular cluster (Wang , Spurzem et al, NOAO, Beijing, ZAH, Heidelberg); codes: FLASH, Gadget, Arepo, N-body6++GPU]





H. T. Janka, M. Rampp

F. Röpke

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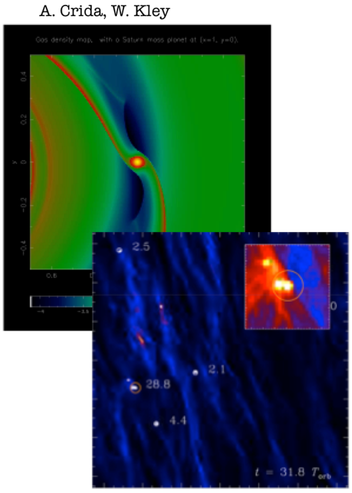
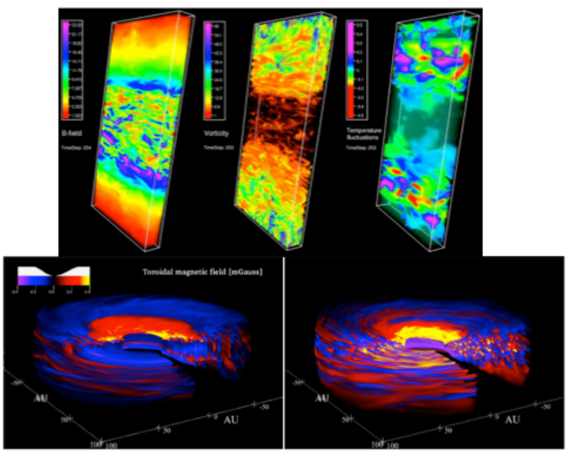
Explosion mechanisms for supernovae, stellar evolution, radiation transport, nucleosynthesis, neutrino transport [explosions of supernovae (left: Janka et al. (MPA, Garching), right: Röpke et al. (HITS, Heidelberg); Vertex,Vertex-Prometheus, Leafs]

A. Crida, W. Kley



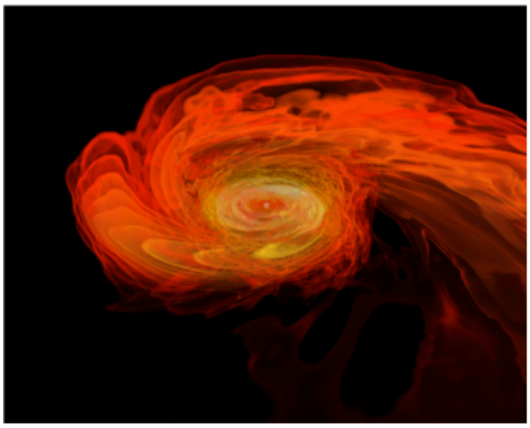
A. Johansen, H.Klahr, T. Henning

M Flaig

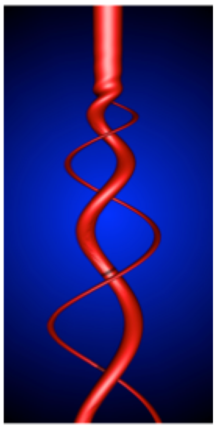


M. Flock

Planet formation, proto-planetary disks, magnetized accretion disks, 3D radiation transport, stellar and planetary atmospheres, and planetesimals [simulations of planetesimal formation (top: Kley, Crida & Flaig et al., Tübingen University, bottom: Johansen, Klahr, Henning et al., MPIA, Heidelberg); used codes: Pluto, Fargo, Nirvana, Pencil, Phoenix]



L. Rezzolla



B. Brügmann

Computational relativistic astrophysics, numerical relativity, mergers of neutron stars and black holes (above pictures), models for gamma-ray bursts, compact binaries and gravitational wave emission, relativistic shocks [simulations of black hole mergers (left: Rezolla et al., ITP, Frankfurt; right: Brügmann et al. TPI, Jena); used codes Cactus, Whisky, BAM]

5. Upcoming challenges in the coming decade

Computational astrophysics will face unprecedented challenges in the next decade. The wave of high-resolution data from modern observing facilities will require simulations at a significantly higher level of physical complexity and increasing predictive power for a meaningful physical interpretation. In particular the inclusion of additional key physical processes will require significantly higher spatial and temporal resolution, and so the computational demand will increase by factors of 10 to 1000.

The computation of the impact of stellar radiation (radiation transfer) on galaxy formation is one example for such an important physical process. Stellar radiation is one of the major energy sources in the Universe but simulating its effect in high-resolution galaxy formation simulations is too computationally demanding at present. Accurate simulations of this process are a major challenge for the next decade and will require optimized algorithmic implementations and supercomputers with at least a factor of ten higher capacity. Another example is the simulation of stellar evolution and explosion. The complex interplay of a multitude of physical processes on various spatial and temporal scales is conventionally tackled by simplifying assumption or by exploitation of symmetries to reduce the dimensionality of the problem. This introduced tunable parameters into the models reducing their predictive power. There is increasing tension with modern high-quality observational data. A new generation of stellar evolution and explosion models attempts to overcome this problem by employing highly resolved multidimensional dynamical simulations. These require new numerical techniques and a substantial increase in the power of available computational hardware.

Further progress will not be possible without the efficient use of upcoming and envisioned supercomputing facilities, partly equipped with special-purpose hardware, in the upper peta-scale and exa-scale scale regime. Such computers would for example make ab-initio calculations, in full general relativity, of the central engine of long and short gamma-ray bursts possible, or allow for Milky-Way formation simulation covering the large scale assembly as well as the formation of star in the interstellar medium on 10^6 times smaller scales. The codes for these groundbreaking simulations will have to access hundreds of thousand compute cores at a high level of concurrency. However, already present day high-performance codes have become extremely complex (many tens of thousands of lines of code) with long development cycles and highly specialized technical requirements for parallel computation, memory access and communication. Most major codes treating complicated multi-scale physics problems only show good parallel scaling up to ~ 1000 cores. The minority of codes can efficiently handle 10.000 CPUs or more and this is mostly for idealized problems. This situation will have to improve significantly as the fastest supercomputers today have several hundred thousand cores an a million cores will be reached in the next decade. The sustained development, appropriate validation and maintenance of parallel codes is of major importance for scientific impact, but these tasks have become too specialized and technical for typical research projects in theoretical astrophysics. The requirements often go beyond the abilities of German physics students in particular as next generation supercomputers will have a large variety of complex architectures (e.g. heterogeneous platforms with GPU, Xeon Phi, ARM). Therefore, fewer but larger groups with sustained and dedicated support for software development are needed to maintain concurrent technical (software) and scientific excellence. In case of insufficient funding for flexible and innovative software development the supercomputing facilities cannot be exploited to full capacity and the German community will fall back compared to e.g. other European, North American, Chinese, or Japanese institutions.

To maintain its high international visibility and impact, and in order to strengthen the key competence and innovation power of German computational astrophysics, a novel funding scheme for developing astrophysical simulation software is required, either through sustained individual grants or via special programs. We make two suggestions in this direction: *(a)* the funding of a virtual nation-wide competence center to support the efficient development of well-used community codes in the respective groups in concordance with the existing HPC centers which support the efficient installation of the codes on their respective hardware (see Fig. 1). *(b)* The combination of large computational grants (with several tens to hundred million CPU hours) at German tier-0 facilities with support for human resources (e.g. Ph.D. or postdoc positions) to exploit the simulation results and with hardware support to store and manage data (see Fig. 2), in analogy to large observing grants in the U.S and Germany (e.g. with HST or Chandra).

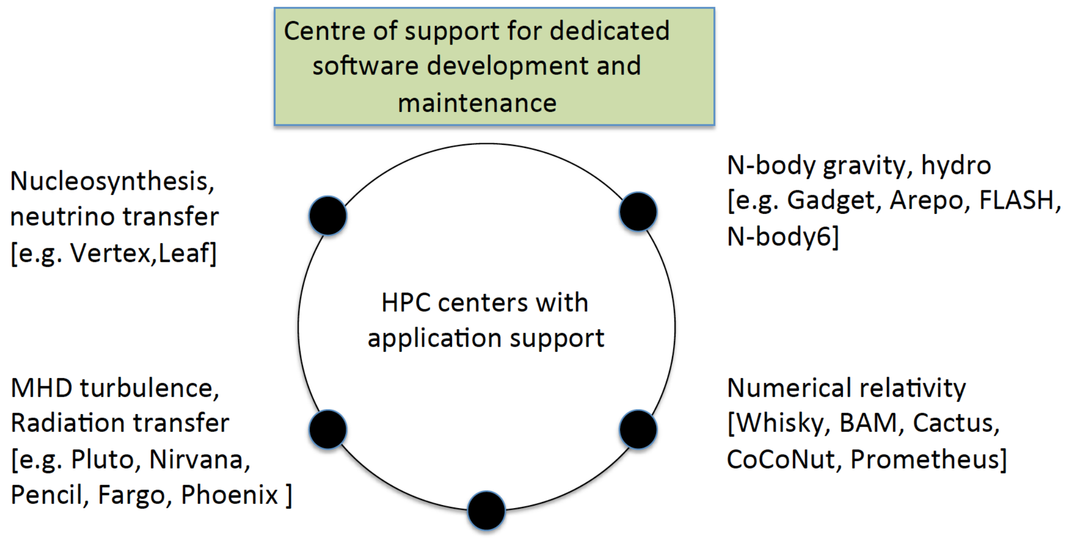


Fig. 1: Framework for a virtual nation-wide competence center to support the efficient development of well-used community codes in collaboration with high-performance computing (HPC) centers.

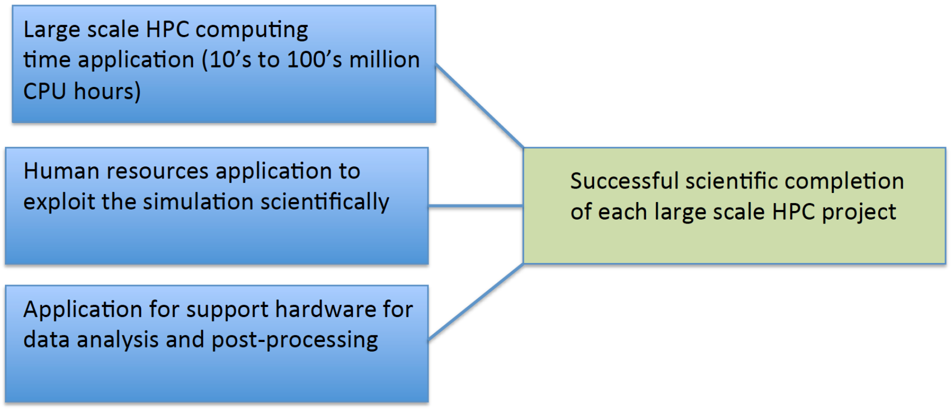


Fig. 2: A possible funding scheme, combining large computational grants (several tens to hundred million CPU hours) with human resources (e.g. Ph.D. and/or postdoc positions) to exploit the simulation results and with hardware support to store and manage data.

In particular at universities, it will be essential to keep software and programming knowledge in the research groups for an extended period of time. Ideally, this includes dedicated 'akademische Mittelbau' positions or at least some means for sustained funding. Also, a modern tenure track system would allow for more flexibility, for the formation of new innovative groups, and for successful completion of long term high-performance computing projects. For innovative future developments the training of software skills for students should be improved: every physics student should have to learn how to program. The universities are aware of the problem and are actively working on improving the situation. These efforts require further support, in combination with special measures for gender balance.

Not only the simulations themselves are computationally challenging but also data analysis and post-processing require intermediate-scale compute clusters with large memory. However, due to high acquisition and maintenance costs for university departments these are often not available even if the scientific excellence is. Improved computational 'Grundaustattung' is required to improve this situation.

6. Summary and Conclusion

Thanks to excellent computing facilities and strong research groups, high-performance computations have become a primary tool for astrophysical research in Germany, with key contributions to our current scientific understanding of astronomy and astrophysics. German computational astrophysicists have become leading international players in a wide range of areas. With about 25% - 30% usage of German supercomputing time computational astrophysics is an example for high-performance computing and technical excellence driven by fundamental science. It will require increased funding both for software and hardware – similar to observational projects – to face future scientific and technical challenges, to maintain its high international impact, and to use current and future facilities to full capacity (i.e. exa-scale computing). Parallel simulation codes have the same purpose and should be treated and funded similar to observational instruments for telescopes.

The excellent international position of German computational astrophysics, its key competence, and innovation power needs to be consolidated and readied to cope with the challenges ahead. Code development for astrophysical high-performance computing applications should be acknowledged as an independent field and a major contribution to fundamental research.

We propose two possible funding lines: *(a)* The establishment of a virtual nation-wide competence center to support the efficient development of well-used community codes in concordance with the existing HPC centers. *(b)* The combination of large computational grants at German tier-0 facilities with support for human resources (e.g. Ph.D. or postdoc positions) to exploit the simulation results together with hardware support to store and manage data and scientific results.