Detailed project description: Astrophysical turbulence and dynamo action

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1 Overview

The microphysics of non-thermal plasmas can only be captured by kinetic simulations. This requires evolving the location and momentum of electrons and ions (or positrons, for pair plasmas) separately as individual (computational) particles, instead of describing the system as a macroscopic fluid. This kind of simulation are known as kinetic plasma simulations. As an new effort at Nordita, we have developed a novel high-performance computing framework to enable such simulations, called RUNKO. Within this framework, we perform simulations of astrophysical turbulence and shocks to investigate the microphysics of particle acceleration, a physical phenomenon where kinetic plasma processes accelerate charged particles up to ultra-relativistic velocities.

Another astrophysics activity at Nordita focuses on the calculation of the stochastic gravitational wave (GW) background. This activity will now primarily be pursued by a new PhD student at Nordita (Yutong He, supervised by Axel Brandenburg). For those calculations we use the PENCIL CODE. The strengths of the resulting GW field at the present time is calculated for a range of GW sources associated with turbulent stresses in the energy-momentum tensor. This activity is supported by a VR grant on "Stochastic Gravitational Wave Background from the Early Turbulent Universe" 2019-04234, January 2020 – December 2022, 4.00 MSEK. The allocation must also partially support the activity of the rest of the Nordita group. Another activity concerns global accretion disk simulations by Patryk Pjanka, a new Nordita fellow who did his PhD with Jim Stone at Princeton University.

2 Resource usage

Our kinetic simulations are performed with the RUNKO framework. The code is open source and is publicly available from GitHub¹. On Dardel our typical kinetic turbulence production runs with RUNKO are 5120^2 mesh points and 3×10^9 particles on 1024 cores. A typical run requires 30,000 time steps. With a standard particle push time of 3μ s/particle/processor, this translates to about 1 day of wall clock time at a cost of 30,000 CPU hours per run. For 3D runs we require about a minimum of 1024^3 mesh points. This is a factor of 40 increase in the cost. With 8192 processors and 30,000 time steps, this translates to about 5 days of wall clock time and 1,000,000 CPU hours per production run. Reconnection runs (both in 2D and in 3D) are of similar cost.

A typical 2D shock simulation has 4096×128 mesh points, 1.7×10^9 particles and requires about 50,000 time steps. On 4096 cores, this amounts to about one day of wall clock time for a cost of ~100,000 CPU hours.

We will also run simulations with the PENCIL CODE², which is hosted by Github³. This is an opensource code developed by Brandenburg, his current and former coworkers, some of whom are part of this project, as well as others that have been invited to join the effort. The performance of this code has been discussed at several international conferences; see, e.g., http://www.nordita.org/~brandenb/ talks/misc/PencilCode09.ppt. The code has been optimized over the years and is still being improved

¹https://github.com/natj/runko

²http://www.nordita.org/software/pencil-code (The Pencil Code Collaboration, 2020)

³https://github.com/pencil-code

in terms of performance and new features are also being added. All of the 33,297 revisions since 2001 are publicly available through our repository. We have adapted and optimized this code for spherical polar coordinate system (Mitra et al., 2009). This addition to the code is used in several of the problems discussed here. The code runs well on all the different platforms.

On Dardel, we run production runs with up to 2304^3 mesh points on 9216 cores. A typical run requires at least 500,000 time steps, but it can sometimes be much more, depending on circumstances. With $4.2 \times 10^{-4} \mu$ s per meshpoint and per timestep on Beskow. Dardel will be faster, so we anticipate that the time will be less than 4 days of wall clock time at a cost of 600,000 CPU hours, while with $3.5 \times 10^{-3} \mu$ s per meshpoint and per timestep, this means less than 3 days of wall clock time at a cost of 30,000 CPU hours per run.

To address properly the critical question of the dependence on the magnetic Reynolds number we have to use high resolution runs. As we move from 288^3 and 576^3 to 2304^3 mesh points (and correspondingly higher magnetic Reynolds numbers), we see the emergence of small-scale dynamo action at all depth. This does not yet affect the 576^3 runs, but for the 2304^3 run, small-scale dynamo action becomes critical. The last of these runs is for a deeper domain, so as to include more safely the deep parts where it is important to reach values of \overline{B}/B_{eq} below 0.01, but this appears not to be possible due to small-scale dynamo action.

To confirm our ideas and to understand the effects of small-scale dynamo action, we plan to perform about 2 big runs per month on Dardel, which requires at least 1,000,000 CPU hours, and about 4 intermediate ones, which requires 150,000 CPU hours on each of them. To shed light on some of the observational features of accretion disks, particularly those related to interactions between the inflow stream and the accretion disk, we must run high-resolution global simulations with radiation. This is a new activity, where each run takes about 300,000 CPU hours. We plan to run three of those. Our total time requirement is therefore 2,500,000 CPU hours on Dardel and Tetralith combined.

Computationally, all machines are comparable, but there can be unexpected future changes or outages on some machines that hamper scientific progress. Important is also the waiting time in the queue and occasional opportunities when jobs start immediately. Most of our activity will reside on Dardel. However, to maximize our scientific productivity, and not to be affected too much by outages and long waiting times, we also apply for time on Tetralith.

Regarding scaling tests, we have previously determined strong scaling of PENCIL code on Triolith for three mesh sizes. The time per time step and mesh point is given for different processor numbers and layouts. Generally, it is advantageous to keep the number of processors in the x direction small. The code is well adapted to modern computing platforms.

3 Data management plan

Computer-generated data need to be stored for later analysis and for restarting new simulations. Those are kept on temporary storage. In all cases, simulation data could be reproduced, if needed, based on the input files that, in turn, are maintained using CVS, the Concurrent Versioning System, and are published at the end of each project; see the references with DOI numbers for 15 examples of data sets published on Zenodo. Also the PENCIL CODE has DOI numbers 10.5281/zenodo.2315093 and 3961647. The Pencil Code Collaboration consists of 38 coauthors on a publication to be published in the Journal of Open Source Software.

Data Format and Content We maintain records of our progress using laboratory notebooks. The notebooks document the development of new ideas and hypotheses, the records of their tests and execution, the results of data analysis and simulation, and the final results of the research. Notebooks could contain drawings, calculations, text, plots, and images. Laboratory notebooks will be legible and reasonably organized. Many ideas may be mentioned and the reasons for choices amongst alternatives will be articulated. Each laboratory notebook entry will normally be marked with the date, and sufficiently detailed and clear account of the hypotheses tried and the decisions made. Every single computer run will be done in a separate directory that is being maintained under CVS, SVN (subversion), and git (GitHub). The same applies to all secondary analysis tools that are being used for all the plots and table outputs.

The computer code itself (the PENCIL CODE) is being maintained by GitHub (http://github.com/pencilcode), allowing every older version to be retrieved both by the researcher and members of the public.

Results of the research will be made available in digital form using formatted or unformatted data, as well as idl save files. Images will be saved in standard image formats. The main research products will be available online in digital form. Manuscripts will appear in PDF format, and will contain text, calculations, drawings, plots, and images. The targeted journals for the results of this research project, such as, The Astrophysical Journal, Phys. Rev. Letters, Phys. Rev. D and E, and Physics of Plasmas, all provide a downloadable PDF copy of the manuscript on the web. In addition, the PIs and co-PIs will link to these journal publications from their respective research websites.

Data Access and Sharing All participants in the project will publish the results of their work. Papers will primarily be published in peer-reviewed journals and/or conference proceedings. The results may also appear in books. Primary data and other supporting materials created or simulated in the course of the work will be shared with other researchers upon reasonable request and within a reasonable time of the request. In many cases, documented data sets will also be made available on the website https://www.nordita.org/~brandenb/projects/.

Data Archiving and Preservation of Access Products of the research will be made available immediately. Preprints of manuscripts submitted to peer-review journals will be available online through the arXiv e-print service prior to publication. After the actual publication in journals, papers will be available online from the respective journal websites and linked to by the PI's research website. All data generated as a result of this project will be backed up daily to protect from loss of data from hardware failures, fire, theft, and other unforeseen events.

4 Scientific challenges

Microphysics of plasmas around black holes and neutron stars. The physics of energy dissipation and nonthermal emission in relativistic magnetized outflows powered by compact objects is still enshrouded with mystery.

By means of massively parallel particle-in-cell simulations within the RUNKO framework, we study how shocks and turbulence, notorious dissipation agents, can produce populations of nonthermal particles.

Kinetic turbulence has been our first application of the framework. Our large 2D simulations during 2019-2020 have enabled us to study the magnetohydrodynamical turbulence from a completely new angle, with a self-consistent fully-kinetic approach. At the moment there are only two other groups with a capability to perform such massive supercomputer simulations. This puts us in a unique position to start exploring this new regime of turbulence even further. Our completed simulations have already revealed a new energy dissipation mechanism for the turbulent plasmas in the form of localized non-thermal particle production in so-called current sheets. This pioneering computational work will help us in formulating a more self-consistent theory of relativistic turbulence from first principles, currently under construction. Our next effort in this field is to start focusing on high-fidelity 3D simulations. This will help us confirm the validity of our previous 2D simulation results and will open up a whole new window into studying the dynamics of the different structures seen in the simulations.

Another particle energization mechanism, that has gained a lot of focus as a promising alternative to turbulence, is relativistic magnetic reconnection. In this microphysical plasma phenomena, the magnetic field changes its topology and the magnetic field lines undergo a microphysical reconnection (Lyubarsky, 2005). The subsequent evolution of the system appears even more intriguing: the configuration is unstable for the plasmoid tearing instability where blobs of plasma are captured by the surrounding and reconnecting magnetic fields and are being accelerated by the dragging motion of the evolving field. Understanding the late-time evolution and coupling of plasma and radiation in reconnection is of paramount importance to astrophysics, because it is thought to power many of nature's most powerful phenomena such as black hole accretion disks and jets. It is also physically interesting to study the coupling of radiation and plasma, made possible by the radiation module in RUNKO. Coupling radiative processes to the plasma under reconnection would mark the first self-consistent study of radiative relativistic reconnection. Other potential cosmic accelerators that have been receiving a lot of attention in the community are shocks. In 2020, we performed simulations of relativistic magnetized shocks interacting with upstream density perturbations and observed promising particle acceleration. As a natural extension of this work, we want to consider next, upstream perturbations with a magnetic component.

Ultimately, we want to conduct for the first time self-consistent simulations of shocks interacting with developed turbulence. Technically, it amounts to combine together our independently tried and tested shock setups and turbulence setups.

Inflationary magnetogenesis and gravitational wave production. In two recent papers with Ramkishor Sharma, a new Nordita postdoctoral researcher, we have performed new simulations of inflationary magnetogenesis and gravitational wave production (Brandenburg, & Sharma, 2021; Brandenburg, He, & Sharma, 2021). In those models, we solved the equations for electromagnetic waves during the post-inflationary phase (the reheating phase), and switched to magnetohydrodynamics at the beginning of the radiation-dominated phase. In future models, we will include equations describing the evolution of scalar potentials in cosmology. This will lead to more realistic models. All models are three-dimensional and typical resolutions are of the order of 1024^3 to 2048^3 mesh points.

Gravitational wave polarization. We study the influence of helical magnetic fields on the production of gravitational waves. Gravitational waves provide an as yet unexplored window into the earliest moments of the Big Bang, not obscured by the last scattering surface given by the hitherto studied cosmic microwave background. The production of gravitational radiation from cosmological turbulence was calculated analytically by Kosowsky et al. (2002) and Gogoberidze et al. (2007). Helical magnetic fields produce non-vanishing cross-polarization in the gravitational wave spectrum (Kahniashvili et al., 2005; Caprini & Durrer, 2006), which would be observable with LISA (Binétruy et al., 2012). Hindmarsh et al. (2017) have recently presented detailed numerical models of gravitational waves from phase transition nucleation bubbles produced during the electroweak phase transition (Kamionkowski et al., 1994; Nicolis, 2004). Our new work involves the calculation of gravitational waves using the PENCIL CODE, where a gravitational wave solver has already been successfully implemented.

Chiral MHD. The chiral magnetic effect leads to a current along a magnetic field if the number of left- and right-handed Fermions is unequal. This effect has received significant attention in just the last few years. We are now able for the first time to perform a comprehensive study of the chiral magnetic effect in real turbulence. Earlier theoretical studies applied to neutron stars and the early Universe did not result in realistic estimates for the turbulence. Thus, the use of simulations is absolutely critical to making significant progress. Our recent work on the early Universe has brought us a significant step forward. We will now focus on neutron stars, which may have several important advantages. First, only one sign of chirality will be produced. Second, the timescales are short, giving us ample time for the subsequent inverse cascade to yield large length scales. Together with the helicity produced from rotation and stratification, the end result may produce a realistic model of observed pulsars.

Effect of convection on magnetized disk accretion and global models of accretion disks. We use radiation magnetohydrodynamic (R-MHD) simulations in a shearing box to study the energy conversion from Keplerian rotation to turbulent magnetic energy by the combined magneto-rotational and dynamo instabilities to heat and radiation near the disk surfaces. We start with a non-uniform, mostly toroidal magnetic field near the midplane of the disk. This field develops into a turbulent field through the magneto-rotational instability which in turn re-amplifies the magnetic field through the dynamo instability (Brandenburg et al., 1995). Most of the earlier simulations have ignored radiative cooling, which is however important when trying to understand global stability of the disk (local dissipation should increase with increased local surface density in the disk). We therefore include radiation transport including the H⁻ opacity as well as partial hydrogen ionization, both of which lead to convection near the surfaces. We study the resulting feedback on the disk accretion rate and its dependence on the surface density, which has implications on understanding transitions from low to high accretion states in disks.

We will also use R-MHD simulations to investigate the global behavior of accretion disks in semidetached binaries, such as cataclysmic variables (CVs) and low-mass X-ray binaries (LMXBs). Certain features of these systems have been, so far, mostly absent in numerical work. Recently, we have explored one such avenue for improvement, by performing the first stratified MHD simulations of these environments, where we included realistic disk feeding accounting for the gas inflow stream (Pjanka & Stone, 2020). At present, we are implementing realistic radiative cooling in our models, which will further improve physical accuracy and enable us to make direct comparisons with observations.

5 Research group and management

The work in the astrophysics group at Nordita covers a broad range of topics from kinetic simulations over gravitational wave physics and the early universe to solar physics and meteorology. Our research group consists currently of the following people:

Dr Akshay Bhatnagar (external collaborator)

Dr Camilia Demidem (Nordita postdoc)

Mr Yutong He (Nordita PhD student, Stockholm U)

Dr Lars Mattsson (assistant professor)

Dr Dhrubaditya Mitra (assistant professor)

Dr Joonas Nättilä (external collaborator)

Dr Patryk Pjanka (Nordita fellow)

Ramkishor Sharma (Nordita, postdoctoral researcher)

Dr Alexandra Veledina (assistant professor at Nordita, shared with University of Turku)

Dr Hongzhe Zhou (Nordita fellow, jointly with the TDLI Institute at Shanghai)

The monthly usage within the group is monitored and discussed during our weekly group meetings.

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