Detailed project description: MHD turbulence

(Nordita, Stockholm)

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1 Overview

In the astrophysics group at Nordita, we are routinely using the Pencil Code[1], which is hosted by Github[2]. Over the past few years, this code has been extended to be accelerated by GPUs. This part is based on the library and framework of Astaroth[3]. Both codes are open source. The Pencil Code group in Finland has been developing Astaroth on LUMI. The speedup is up to a factor 16 for problems of practical interest.

The Pencil Code is 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. The code has been optimized over the years and is still being improved in terms of performance and new features are also being added. All of the 37,375 revisions since 2001 are publicly available through our repository. We have adapted and optimized this code for spherical polar coordinate system. This addition to the code is used in several of the problems discussed here. The code runs well on all the different platforms.

2 Resource usage

We review here the performance of the GPU-accelerated simulations with the Pencil Code using LUMI. All of the scaling results reported here are based on three-dimensional simulations of decaying hydromagnetic turbulence, just as in the recent paper by Brandenburg et al. (2024). Here, we compare the Pencil Code (PC) on CPUs against the PC with Astaroth embedded (PC-A), where Astaroth integrates the partial differential equations of magnetohydrodynamics while the PC performs all peripheral tasks (diagnostics & I/O). We build with `gfortran/gcc` and `nvcc` using the modules:

```
gcc/12.2.0    craype-accel-amd-gfx90a  PDC/23.12
PrgEnv-gnu/8.5.0  cray-mpich/8.1.27   rocm/5.7.0
```

For the timing results, we routinely output with the PC both the wallclock and normalized times per time step and mesh point.

On LUMI, we performed an analogous comparison:
PC-A, 1 node, 8 GPUs, grid size 380^3,

```
 Wall clock time [hours] =  1.522E-02 (+/-  8.3333E-12)
 Wall clock time/timestep/meshpoint [microsec] = 1.1079179E-03
```

Thus, the normalized time per time step and mesh point is 1.1 nanoseconds.
PC, 1 node, 64 CPUs, grid size 352^3

```
 Wall clock time [hours] =  0.192     (+/-  5.5556E-12)
 Wall clock time/timestep/meshpoint [microsec] = 1.7558866E-02
```

[1] `http://www.nordita.org/software/pencil-code` (The Pencil Code Collaboration, 2021)
[2] `https://github.com/pencil-code`
[3] `https://bitbucket.org/jpekkila/astaroth/`

Thus, the normalized time per time step and mesh point is 18 nanoseconds, so the *speedup is about 16.*

Next, we report weak scaling results:

PC-A, 1 node, 8 GPUs, grid size 512^3,

```
Wall clock time [hours] =  4.535E-02 (+/-  5.5556E-12)
Wall clock time/timestep/meshpoint [microsec] = 1.2150889E-03
```

PC-A, 8 nodes, 64 GPUs, grid size 1024^3,

```
Wall clock time [hours] =  1.261E-02 (+/-  5.5556E-12)
Wall clock time/timestep/meshpoint [microsec] = 4.2233689E-05
```

PC-A, 2048^3, 64 nodes, 512 GPUs

```
Wall clock time [hours] =  1.510E-02 (+/-  5.5556E-12)
Wall clock time/timestep/meshpoint [microsec] = 6.3206880E-06
```

The last two runs show roughly equal wallclock time. The longer time for the smallest grid size remains unclear.

We aim to run with up to 4096^3 mesh points. A typical run requires at least 500,000 time steps, but it can sometimes be much more, depending on circumstances.

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 256^3 and 512^3 to 2048^3 and 4096^3 mesh points (and correspondingly higher magnetic Reynolds numbers), we see the development of better scaling. To confirm our ideas and to understand the effects of what can be interpreted as magnetic reconnection, we plan to perform several runs per month.

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; see Brandenburg(2023), Brandenburg & Protiti(2023), Brandenburg et al. (2022a,b), (2023a,b,c), Carenza et al. (2022), Haugen et al. (2021), He et al. (2021,2022), Kahniashvili et al. (2022), Käpylä et al. (2022), Mizerski, et al.(2023), Roper Pol et al. (2022), Sarin et al.(2023), Sharma & Brandenburg(2022), Zhou et al. (2022). Also the Pencil Code has DOI numbers 10.5281/zenodo.2315093 and 3961647. The Pencil Code Collaboration consists of 37 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/pencil-code), 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

Inverse cascading in non-helical MHD. Today, high resolution numerical turbulence simulations are feasible. They allow for fairly large turbulent inertial ranges, but not all the resources must be spent on a large inertial range. It is also important to allow for enough scale separation toward very long length scales to avoid artifacts from a finite domain size. To help optimizing the computational resources, various groups have employed numerical tools to approach the physically relevant regime: (i) reduce the viscous and diffusive subranges by adopting hyperviscosity and magnetic hyperdiffusivity, and (ii) to make the viscous and magnetic diffusion coefficients time-dependent, or do use, for example, slope-limited diffusion to prevent the code from crashing at early times when the turbulence is extremely vigorous and to allow for the physical viscosity to be as small as possible at late times. All these tools imply small artifacts that we need to examine very carefully. The slope-limited diffusion technique has recently been used in some of our simulations of chiral MHD. To assess the role of artifacts in simulations, we now need to perform more detailed studies by monitoring the evolutionary tracks in a pq diagram for different combinations of such numerical tools. We will therefore perform divers surveys to extract physically meaningful results from artifacts. This part will mostly be carried out with GPU-acceleration. However, some of the calculations with radiation transport will use CPUs for now.

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. This part will mostly be carried out with GPU-acceleration, although we have not yet tested the chiral MHD module with GPUs yet. We expect that this will not cause any problems.

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:

Kyrylo Bondarenko (Nordita fellow)
Dr Oksana Iarygina (Marie Curie fellow)

Mr Gustav Larsson (Master student)
Dr Lars Mattsson (guest researcher)
Dr Dhrubaditya Mitra (assistant professor)
Mr Patrik Tengnér (Master student)

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

References

Brandenburg *Datasets for "Quadratic growth during the COVID-19 pandemic: merging hotspots and reinfections" v2023.01.02.* Zenodo, DOI:10.5281/zenodo.7499431 (2023).

Brandenburg, A., Neronov, A., & Vazza, F., "Resistively controlled primordial magnetic turbulence decay," *Astron. Astrophys.* **687**, A186 (2024).

Brandenburg, & Protiti, N. N. *Datasets for "Electromagnetic conversion into kinetic and thermal energies" v2023.08.01.* Zenodo, DOI:10.5281/zenodo.8203242 (2023).

Brandenburg, A., Rogachevskii, I., & Schober, J. *Datasets for "Dissipative magnetic structures and scales in small-scale dynamos" v2022.9.18.* Zenodo, DOI:10.5281/zenodo.7090887 (2022a).

Brandenburg, A., Zhou, H., & Sharma, R. *Datasets for "Batchelor, Saffman, and Kazantsev spectra in galactic small-scale dynamos" v2022.07.19.* Zenodo, DOI:10.5281/zenodo.6862459 (2022b).

Brandenburg, Clarke, E., Kahniashvili, T., Long, A. J., & Sun, G. *Datasets for "Relic gravitational waves from the chiral plasma instability in the standard cosmological model" v2023.07.17.* Zenodo, DOI:10.5281/zenodo.8157463 (2023).

Brandenburg, Sharma, R., & Vachaspati, T. *Datasets for "Inverse cascading for initial MHD turbulence spectra between Saffman and Batchelor" v2023.07.09.* Zenodo, DOI:10.5281/zenodo.8128611 (2023).

Brandenburg, Kamada, K., Mukaida, K., Schmitz, K., & Schober, J. *Datasets for "Chiral magnetohydrodynamics with zero total chirality" v2023.08.20.* Zenodo, DOI:10.5281/zenodo.8267336 (2023).

Brandenburg, Kamada, K., & Schober, J. *Datasets for "Decay law of magnetic turbulence with helicity balanced by chiral fermions" v2023.02.01.* Zenodo, DOI:10.5281/zenodo.7499431 (2023).

Carenza, P., Sharma, R., Marsh, M. C. D., Brandenburg, A., Müller, E. *Datasets for "Magnetohydrodynamics predicts heavy-tailed distributions of axion-photon conversion" v2022.8.8.* Zenodo, DOI:10.5281/zenodo.6974228 (2022).

He, Y., Roper Pol, A., & Brandenburg, A. *Datasets for "Leading-order nonlinear gravitational waves from reheating magnetogeneses" v2021.09.23.* Zenodo, DOI:10.5281/zenodo.5524454 (2021).

Kahniashvili, T., Clarke, E., Stepp, J., & Brandenburg, A. *Datasets for "Big bang nucleosynthesis limits and relic gravitational waves detection prospects" v2021.11.18.* Zenodo, DOI:10.5281/zenodo.5709176 (2021).

Käpylä, M. J., Rheinhardt, M., & Brandenburg, A. *Datasets for "Fully compressible test-field method and its application to shear dynamos" v2022.03.24.* Zenodo, DOI:10.5281/zenodo.6383190 (2022).

Mizerski, K. A., Yokoi, N., & Brandenburg *Datasets for "Cross-helicity effect on α-type dynamo in non-equilibrium turbulence" v2023.02.28.* Zenodo, DOI:10.5281/zenodo.7683615 (2023).

Pencil Code Collaboration: Brandenburg, A., Johansen, A., Bourdin, P. A., Dobler, W., Lyra, W., Rheinhardt, M., Bingert, S., Haugen, N. E. L., Mee, A., Gent, F., Babkovskaia, N., Yang, C.-C., Heinemann, T., Dintrans, B., Mitra, D., Candelaresi, S., Warnecke, J., Käpylä, P. J., Schreiber, A., Chatterjee, P., Käpylä, M. J., Li, X.-Y., Krüger, J., Aarnes, J. R., Sarson, G. R., Oishi, J. S., Schober, J., Plasson, R., Sandin, C., Karchniwy, E., Rodrigues, L. F. S., Hubbard, A., Guerrero, G., Snodin, A., Losada, I. R., Pekkilä, J., & Qian, C., "The Pencil Code, a modular MPI code for partial differential equations and particles: multipurpose and multiuser-maintained," *J. Open Source Softw.* **6**, 2807 (2021).

Roper Pol, A., Mandal, S., Brandenburg, A., & Kahniashvili, T. *Datasets for "Polarization of gravitational waves from helical MHD turbulent sources" v2021.09.24.* Zenodo, DOI:10.5281/zenodo.5525504 (2021).

Sarin, N., Brandenburg, & Haskell, B. *Supplemental Material to "Confronting the neutron star population with inverse cascades" v2023.06.27.* Zenodo, DOI:10.5281/zenodo.8088084 (2023).

Sharma, R., & Brandenburg, A. *Supplemental Material and Datasets for "Low frequency tail of gravitational wave spectra from hydromagnetic turbulence" v2022.08.22.* Zenodo, DOI:10.5281/zenodo.7014823 (2022).

Zhou, H., Sharma, R., & Brandenburg, A. *Datasets for "Scaling of the Hosking integral in decaying magnetically-dominated turbulence" v2022.06.14.* Zenodo, DOI:10.5281/zenodo.7112885 (2022).