The Pencil Code Newsletter

Issue 2021/3

December 7, 2021, Revision: 1.23

Contents

1 PCUM22 at IIA in Bangalore

The Pencil Code User Meeting (PCUM22) is currently being organized by *Piyali Chatterjee* and planned to be held sometime in May-June 2022 with the Indian Institute of Astrophysics (IIA), Bangalore, India as the hosting Institute. The IIA is the leading Institute for Optical Astronomy in India. They are also the nodal Indian Institute for the upcoming thirty meter telescope, the 2m solar telescope (NLST on Pangong Lake, Ladhakh), the VELC coronagraph on board satellite ADITYA-L1 and the existing X-ray space telescope, AstroSat. They operate the Kodaikanal Solar Observatory, where the Evershed effect was discovered in 1909 and this observatory also hosts a century long publicly available archive of sunspot and Ca II images in digitized format. While the IIA would have loved to welcome all of you to India, unfortunately, we will have to hold the meeting virtually due to the current pandemic and related travel restrictions. The actual dates will be decided upon by the Pencil Code community by a poll soon.

Figure 1: Stockholm on December 7, 2021.

2 Recent scaling results

In Stockholm (see Figure 1), we have a new machine called Dardel. Strong scaling tests have been performed for five mesh sizes; see Figure 2. The time per time step and mesh point is given for different processor numbers and layouts. Generally, as Jörn Warnecke pointed out earlier, it is advantageous to minimize the processor surface area, and to keep the number of processors in the x direction small.

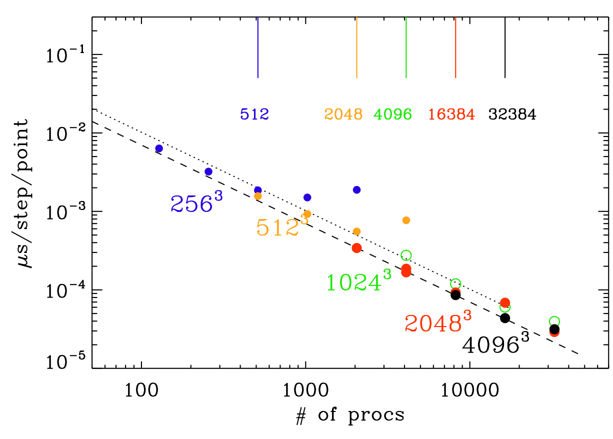

Figure 2: Strong scaling on Dardel. The dotted and dashed lines corresponds to 1.02μs/proc/step/point and 0.70μs/proc/step/point, respectively.

Performancewise, Cray with O2 optimization is equivalent to gnu with O3. While gnu-O3 is able to handle memory or whatever compiler problems much better, it is otherwise not better than Cray-O2, and often some 10–20% slows, but this is within the measurement accuracy. More details can be found on https://github.com/pencil-code/pencil-code/tree/master/doc/timings.

3 Pencil Code office hours

We are always looking forward to hearing new ideas and experiences people make with the code. You may just pop in for the next office hours, which are usually on the second Friday of the month at 14:30 CEST. The next one is this Friday, December 10. For the list of upcoming (and past) dates, see https://www.nordita.org/~brandenb/pencil-code/office_hours/. These events provide great opportunities for brainstorming with others about code-related issues, and also to show some new developments to others. The new zoom address is https://stockholmuniversity.zoom.us/j/69160607217. See you then.

4 Science & code developments

4.1 Graphite rod combustion in hot air

Ewa Karchniwy has extended the overset grid method to work with chemistry. With this she has been able to perform detailed studies of how a graphite rod combusts in hot air. Her work is presented in a new paper, which just appeared in Combustion & Flame (Karchniwy et al., 2022, see below; https://doi.org/10.1016/j.combustflame.2021.111880). Since two very different time scales were relevant in this study (the acoustic time scale and the time to reach steady state, since the original Mach number was very low) – leading to very long run times, she had to make some modifications to mitigate this. One of the very interesting things she did in this paper was therefore to show how to consistently modify the speed of sound for a simulation with chemistry without affecting the results on the flame speed.

4.2 Subtleties with several specials

During the Pencil Code User Meeting 2020, Matthias reported about the possibility of using two (or more) *special* modules at the same time. During some happy coding session, all of a sudden it said "`FATAL ERROR: initialize_mult_special: library src/special.so could not be opened.`" What do you think this is?

Turns out that when several special modules are used, certain compile-time error notifications are suppressed. In this case, a "`use Sub, only: dot_mn`" was forgotten. This normally leads to a clear compile-time error, but not here! This is because such error messages are suppressed when several special modules are used.

So, to avoid such trouble, make sure that special modules also work in isolation. Then you get a clear error message and everything is obvious.

4.3 Trouble with pc_read_var

In idl, there is often the problem that newly implemented variables can't be read in correctly, because this hasn't been prepared yet. A simple way out is to use `pc_read_var_raw,/trimall,obj=var`. This is not a new routine, but it may be new to some of us.

4.4 Spherical slices in star-in-a-box

A new slice type "r-slice" has been implemented, which delivers quantities on spherical surfaces embedded in a Cartesian grid. Think of *star-in-a-box* setups for the most suggestive application. r-slices are activated by setting `r_rslice`, `nth_rslice` and `nph_rslice` to non-zero values. `r_rslice` is the radius of the surface (centered at the origin of the coordinate system) while `nth_rslice`, `nph_rslice` are the latitudinal and longitudinal numbers of grid points on it (latitude and longitude refer to the z axis). At high `nth_rslice`, a few parallels near the axis might be too tiny and are hence suppressed. Collect the processor-wise data as usual through `read_videofiles` or `read_all_videofiles` and read by `pc_read_video`. HDF5 support is in preparation, volunteers welcome for adapting the Python routines.

The committed version would yet show some discontinuities at processor boundaries. These are connected with a feature of the code design, which causes that `f-array` variables on slices have a one-timestep delay relative to derived quantities. A fix has been tested, but not yet committed as it requires four-eyes approval.

4.5 Major design change needed

Performing one substep of the time integration in the Pencil Code comprises the following essential steps, valid for all modules (diagnostics disregarded here):

(i) update the ghost zones = set the boundary conditions and communicate inner ghost zones

(ii) form the right hand sides

(iii) advance the integrated variables (`f-array`).

Sometimes, action is needed before and after communication, for which each physics module provides the `*before_boundary` and `*after_boundary` hooks, which are called before and after (i). However, for optimum performance (i) actually only *initiates* the communication while it is finalized only at some point during (iii). Thus, if an "after-communication" action were to modify the `f-array`, those inner zones of a process which are already "buffered-away" to feed the ghost zones of the neighboring processes would not learn about it and the status of the `f-array` would turn inconsistent. This is really happening with the present state of the code, e.g. in the case of average removal. Hence, the first change has to be to move all such action to the "before-boundary" hooks, which so far has only been accomplished for magnetics. Yet, other trouble arises then: As setting of BCs and communication is encapsulated in one and the same subroutine, an action which is supposed to modify also the ghost zones at the domain boundaries would happen too early. An example is the formation of the quantity $\boldsymbol{U} \cdot \boldsymbol{A}$, needed for the advective gauge 2. To form it properly on those ghost zones, the boundary conditions would have to be set beforehand. Thus, the correct order for the most general case has to be

(i) set the boundary conditions at the domain boundaries (as far as no communication is needed)

(ii) perform "before-communication" actions

(iii) initiate communication

(iv) perform "after-communication" actions
(no modifications of f-array, though)

(v) form the right hand sides
(and finalize communication)

(vi) advance the integrated variables.

Such a modification requires greatest care as it concerns the "core engine" of the code, and should not be executed by a single person. So we need ideas how to organize the change in a reliable way, which also divides labor.

4.6 README.md

We remind the reader of README.md; see `https://github.com/pencil-code/pencil-code/blob/master/README.md`. It is a convenient browsable entry to other web pages related to the Pencil Code. You can find and edit it directly on the Pencil Code source code page. Please help to make sure it is up-to-date.

5 Papers since August 2021

Since the last newsletter of August 25, 7 new papers have appeared on the arXiv, and 13 others, some of which were just preprints and have now been published. We list both here, 20 altogether. Four of them have to do with particles or dust and three of them are about gravitational waves. A browsable ADS list of all Pencil Code papers can be found on: `https://ui.adsabs.harvard.edu/user/libraries/iGR7N57OSy6AlhDMQRTe_A`. If something is missing in those entries, you can also include it yourself in: `https://github.com/pencil-code/pencil-code/blob/master/doc/citations/ref.bib`, or otherwise just email brandenb@nordita.org.

References

Becerra, L., Reisenegger, A., Alejandro Valdivia, J. and Gusakov, M.E., Evolution of random initial magnetic fields in stably stratified and barotropic stars. , 2021, arXiv:2111.10673.

Bhatnagar, A., Pandey, V., Perlekar, P. and Mitra, D., Rate of formation of caustics in heavy particles advected by turbulence. , 2021, arXiv:2110.02568.

Brandenburg, A., Clarke, E., He, Y. and Kahniashvili, T., Can we observe the QCD phase transition-generated gravitational waves through pulsar timing arrays?. *Phys. Rev. D*, 2021a, **104**, 043513.

Brandenburg, A. and Das, U., Turbulent radiative diffusion and turbulent Newtonian cooling. *Phys. Fluids*, 2021, **33**, 095125.

Brandenburg, A., He, Y. and Sharma, R., Simulations of Helical Inflationary Magnetogenesis and Gravitational Waves. *Astrophys. J.*, 2021b, **922**, 192.

Brandenburg, A. and Sharma, R., Simulating Relic Gravitational Waves from Inflationary Magnetogenesis. *Astrophys. J.*, 2021, **920**, 26.

Candelaresi, S. and Del Sordo, F., Stability of plasmas through magnetic helicity. *arXiv e-prints*, 2021, arXiv:2112.01193.

He, Y., Roper Pol, A. and Brandenburg, A., Leading-order nonlinear gravitational waves from reheating magnetogeneses. , 2021, arXiv:2110.14456.

Hyder, A., Lyra, W., Chanover, N., Morales-Juberías, R. and Jackiewicz, J., Vortex Dynamics at the Jovian Pole; in *AAS/Division for Planetary Sciences Meeting Abstracts*, Vol. 53 of *AAS/Division for Planetary Sciences Meeting Abstracts*, Oct., 2021, p. 409.04.

Kahniashvili, T., Clarke, E., Stepp, J. and Brandenburg, A., Big Bang Nucleosynthesis Limits and Relic Gravitational Waves Detection Prospects. , 2021, arXiv:2111.09541.

Käpylä, P.J., Prandtl number dependence of stellar convection: Flow statistics and convective energy transport. *Astron. Astrophys.*, 2021, **655**, A78.

Karchniwy, E., Haugen, N.E.L. and Klimanek, A., A numerical study on the combustion of a resolved carbon particle. *Comb. Flame*, 2022, **238**, 111880.

Kirchschlager, F., Mattsson, L. and Gent, F.A., Supernova induced processing of interstellar dust: impact of ISM gas density and gas turbulence. *Month. Not. Roy. Astron. Soc.*, 2021, p. 32183234.

Mattsson, L. and Hedvall, R., Acceleration and clustering of cosmic dust in a gravoturbulent gas – I. Numerical simulation of the nearly Jeans-unstable case. , 2021, arXiv:2111.01289.

Mtchedlidze, S., Domínguez-Fernández, P., Du, X., Brandenburg, A., Kahniashvili, T., O'Sullivan, S., Schmidt, W. and Brüggen, M., Evolution of primordial magnetic fields during large-scale structure formation. , 2021, arXiv:2109.13520.

Prabhu, A.P., Singh, N.K., Käpylä, M.J. and Lagg, A., Inferring magnetic helicity spectrum in spherical domains: Method and example applications. *Astron. Astrophys.*, 2021, **654**, A3.

Schaffer, N., Johansen, A. and Lambrechts, M., Streaming instability of multiple particle species. II. Numerical convergence with increasing particle number. *Astron. Astrophys.*, 2021, **653**, A14.

Warnecke, J., Rheinhardt, M., Viviani, M., Gent, F.A., Tuomisto, S. and Käpylä, M.J., Investigating Global Convective Dynamos with Mean-field Models: Full Spectrum of Turbulent Effects Required. *Astrophys. J. Lett.*, 2021, **919**, L13.

Yang, C.C. and Zhu, Z., Streaming instability with multiple dust species - II. Turbulence and dust-gas dynamics at non-linear saturation. *Month. Not. Roy. Astron. Soc.*, 2021, **508**, 5538–5553.

Zhou, H. and Blackman, E.G., On the shear-current effect: toward understanding why theories and simulations have mutually and separately conflicted. *Month. Not. Roy. Astron. Soc.*, 2021, **507**, 5732–5746.

This Pencil Code Newsletter was edited by Axel Brandenburg `<brandenb@nordita.org>`, Nordita, KTH Royal Institute of Technology and Stockholm University, SE-10691 Stockholm, Sweden; and Matthias Rheinhardt `<matthias.rheinhardt@aalto.fi>`, Department of Computer Science, Aalto University, PO Box 15400, FI-00076 Aalto, Finland. See `http://www.nordita.org/~brandenb/pencil-code/newsletter` for the online version as well as back issues.