The Pencil Code Newsletter

Issue 2020/2

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1 The 2020 PC User Meeting

This year's Pencil Code (PC) User Meeting of July 27–31 concluded with extremely positive impressions, in particular in terms of the science accomplished with the code in the last year and the joint coding developments during the meeting.

The meeting, which was hosted by Simon Candelaresi of Glasgow University, brought together 47 participants (`http://indico.fysik.su.se/event/6870/registrations/participants`) from nine time zones. Unlike earlier physical User Meetings with online participation, where the quality of microphone and loudspeaker in the lecture room made the experience sometimes painful, this time the participation conditions were uniform and of high quality.

During the social gathering on the last evening (Figure 1), interest in more frequent, but shorter gatherings during the year was expressed, perhaps as monthly "office hours" of some form. This could also be an opportunity to brainstorm about some outstanding changes, and show others how to work with the code.

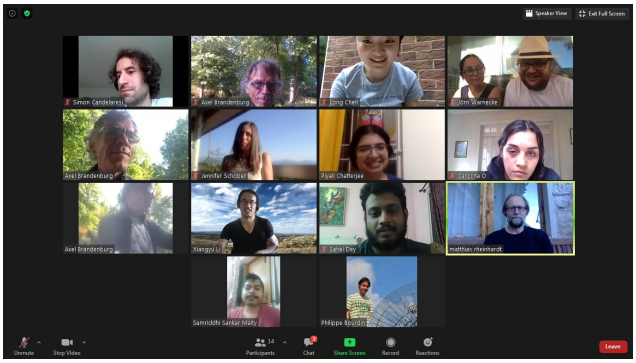

Figure 1: Snapshot from the virtual social gathering.

Science highlights. Particularly impressive simulations were presented by Sahel Dey and his supervisor Piyali Chatterjee on the first successful simulations of spicule formation in the solar atmosphere.

Code developments. The implementation of slope-limited diffusion (SLD) by Jörn and Piyali has now reached some degree of maturity: detailed high-resolution comparisons were presented which showed the individual effects of SLD for density and entropy, momentum, vector potential, and an additional SLD on the current density. Matthias presented the status of the implementation of MPI communication with foreign codes from the Pencil Code. The primary application right now is to run the spherical test-field method on anelastic dynamo simulations performed with other codes. Another important session was that on GPUs, where Miikka Väisälä, Johannes Pekkilä, Maarit Käpylä, and Matthias Rheinhardt reported on the current status. The Astaroth code `https://bitbucket.org/jpekkila/astaroth/` is now running the MHD dynamo problem with helical and nonhelical forcing in production mode at unprecedented speed: single-node speedup of GPU vs. CPU ≈ 35. A paper on large- and small-scale dynamo solutions is submitted to ApJ. Interfacing of Astaroth with Pencil Code is underway (see below).

AAS software citation policy. The Astrophysical Journal (ApJ), and some others, are published by the American Astronomical Society (AAS). August (Gus) Muench, the AAS data analyst, is becoming a familiar face to all of us who write about their numerical results in ApJ. A particularly exciting piece of the information he gave was about JOSS, the Journal for Open Source Software (`http://joss.theoj.org`).

The idea came up to publish a short refereed article on the PENCIL CODE by the *Pencil Code Collaboration* (something that is still to be defined). Another less obvious aspect is that GitHub is not considered a platform providing long-term code preservation unlike, e.g., Software Heritage; see `https://hal.archives-ouvertes.fr/hal-01590958` for a discussion on the long-term vulnerability of research platforms such as GitHub, Bitbucket, SourceForge, etc. See the presentation by Gus for details on the AAS software policy (`https://indico.fysik.su.se/event/6870/contributions/10999/attachments/4543/5277/muench-pencilcodeusersmeeting2020.pdf`).

Figure 2: The new PENCIL CODE t-shirt.

Coding during the meeting. A PC User Meeting wouldn't be satisfactory if there was not enough time to do some new coding during the meeting. It requires the combination of the right people being together at the right time and in the right place. This time, such activity happened in dedicated breakout rooms. During the five days of the meeting, we had 115 check-ins by ten people (`https://github.com/pencil-code/pencil-code/commits/master`), so, on average, we had 23 check-ins per day, or about 12 per person.

As a result, we can now output planar averages (xy, yz, and xz) not only at the instants of time-series output, but also in fixed simulation time intervals by setting `d1davg` (analogously to `d2davg`). This work, which was not urgent, but a welcome convenience to some, was obviously fully mechanical, but fun when done together with somebody.

Additional examples include the possibility to specify the mesh extent in units of π and also the x parallelization of the gravitational wave solver. The decisive realization was that, unlike `fourier_transform`, which returns the result in a swapped state ($xyz \to yxz \to zxy$), `fft_xyz_parallel` returns the unswapped state.

Other items. It was originally planned to have a separate DOI for the manual, because it was regarded as a substitute for a "code paper", which never materialized. Instead, following a suggestion by Jörn, we now made it part of the Zenodo publication of the code (`https://zenodo.org/search?page=1&size=20&q=pencil%20code`).

Slides of the presentations. The slides of many of the presentations can be found on the meeting page `https://indico.fysik.su.se/event/6870/timetable/` (on the timetable page); for example that by Gus Muench is on `https://indico.fysik.su.se/event/6870/contributions/10999/attachments/4543/5277/muench-pencilcodeusersmeeting2020.pdf`.

PC t-shirt. The PC t-shirt (Figure 2) was worn by many participants during the PC User Meeting; see also the group picture in Figure 3.

Figure 3: Group photo of the PC User Meeting.

2 New samples

There are constantly new samples. Only a fraction of them are used for the auto-test. Others are used to alert people of the existence of certain setups and to test new developments across platforms. Below two such examples, of which the second is in response to the commonly asked question whether anything is planned regarding GPUs.

A chiral MHD sample. A new 2-D test for a dynamo, based on the (quantum-mechanical) effect of fermion chirality, is now available under `https://github.com/pencil-code/pencil-code/tree/master/samples/2d-tests/chiral_dynamo`. It illustrates how to use the chiral MHD special module.

The GPU test. Did you say GPU? Yes, if you look at `https://github.com/pencil-code/pencil-code/tree/master/samples/gputest` you see that the `Makefile.local` was already checked in on 2017-04-05 by Matthias. This sample is still under construction and not operational at the moment. When finished, one has not to do more in a PC setup than to set `GPU = gpu_astaroth` – formally – but creating the proper environment requires more action (pulling code from a second repository, localizing the NVIDIA CUDA compiler, or loading a respective set of modules etc.) Then in the code `lgpu = .true.`, which means that, instead of having `call rhs_cpu(f,df,p,...` you'll have `call rhs_gpu(f,itsub,early_finalize)`, that is, instead of the Runge-Kutta/finite-difference MHD solver of PC, the one of the Astaroth code `https://bitbucket.org/jpekkila/astaroth/` is invoked. Both solvers are mathematically equivalent, but the latter runs as a GPU kernel. Get in touch with Matthias if you want more explanations.

Coupling with other codes? Another sample is `https://github.com/pencil-code/pencil-code/tree/master/samples/Pencil-MagIC` but it's not immediately clear what's magic about it. MagIC refers to `https://github.com/magic-sph/magic` which is just another (anelastic, spectral) MHD code. The idea is that the Pencil Code talks simply with an alien code, for which MagIC is just one example. Again, just check with Matthias what the story is. But once it works, one can run the whole test-field suite of the Pencil Code on data of another code.

3 JOSS paper

As discussed at the last PC User Meeting, a short publication for the Journal of Open Source Software (JOSS) has been prepared to define the Pencil Code Collaboration; see `https://joss.theoj.org/about`. An email about this was sent to `http://groups.google.com/g/pencil-code-discuss/members`. Back then, we recalled that "As a rule of thumb, JOSS' minimum allowable contribution should represent not less than three months of work for an individual." Looking at `https://github.com/pencil-code/pencil-code/graphs/contributors` we have 34 people having contributed more than 34 commits. This is only a very rough measure of the effort on the code. In fact, as Figure 4 shows, the effort in terms of additions and modifications of lines in the repository can vary substantially. Also, according the JOSS' rules, "active project direction and other forms of non-code contributions" are taken into account; see `https://joss.readthedocs.io/en/latest/submitting.html#authorship`.

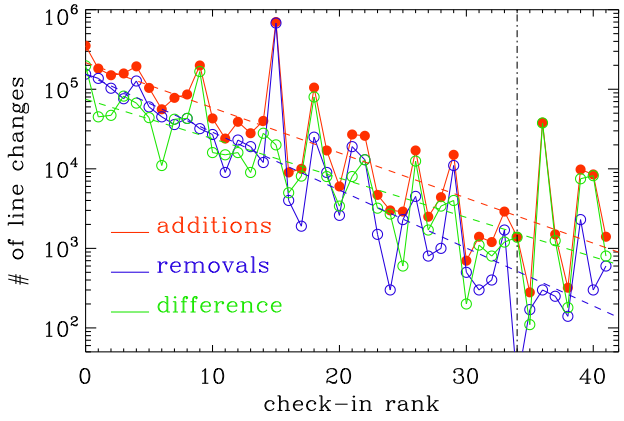

Figure 4: Check-in statistics.

Figure 4 shows that the cutoff line at check-in rank 34 corresponds to a difference between line additions and removals of a little below two thousand. We have therefore encouraged a number of other committers with a large number of line changes to contribute to the JOSS paper as well. The idea is that this paper be quoted every time the GitHub link of PC is mentioned in a paper.

4 Merge branch 'master'

As Philippe pointed out to us, the line changes reported by GitHub include also incidents resulting from what is known as *Merge branch 'master' of https://github.com/pencil-code/pencil-code.* This explains some of the spikes seen in Figure 4. Such merge incidents occur when git users merge upstream into their tracking branch; see page 7 of Wolfgang's "Git Best Practises" (`http://pencil-code.nordita.org/doc/git-best-practises.pdf`) of May 2, 2016, which should be avoided. This problem never occurs when using the svn bridge instead.

5 A fairness issue

The GNU GPL enables free use of the Pencil Code in the versions provided by GitHub. Developers very often commit extensions to the code almost immediately, so as to be able

- to work from different sites or computers,
- to ease work with fellow developers, and
- to test and run on different platforms.

Thus, the situation can occur that users of the code who are not in any way connected with these developers start to use those extensions for production and publication on the scientific topic that the extensions were designed for, while the developers have not yet finished to do so. This could be felt as a "theft" of a scientific topic and the possible loss of priority connected with it could be considered particularly unfair. During the last PC User Meeting, a proposal with recommendations for users was discussed to reduce the risk of such unfairness. Those recommendations, however, cannot be rendered mandatory (conflict with license).

Under the section "License agreement and giving credit" of the PC manual, it says "As a courtesy to the people involved in developing particularly important parts of the program (use `svn annotate src/*.f90` to find out who did what!) we suggest to give appropriate reference to one or several of the following (or other appropriate) papers (listed here in temporal order) ..." we have now added the following text: *Be aware of the fact that certain extensions to the code may still be under intense development or so recent that no paper can be quoted yet. Again, if your work directly profits from such extensions, as a courtesy to their developers, we strongly suggest to contact them, and ask whether there is anything else that can be quoted instead. Acknowledgments or even co-authorship can also be considered.* Our intention is to open herewith the floor for discussion and invite Letters to the Editor for the next newsletter.

6 Letters to the editor

Xiang-Yu Li sent his regards along with Figure 5 from his recent paper (Li and Mattsson, 2020), where we see the accretion of dust grains in supersonic interstellar turbulence. Using solenoidally forced turbulence, they show that in supersonic turbulence, decoupling of gas and dust becomes important and that this leads to an even further accelerated grain growth.

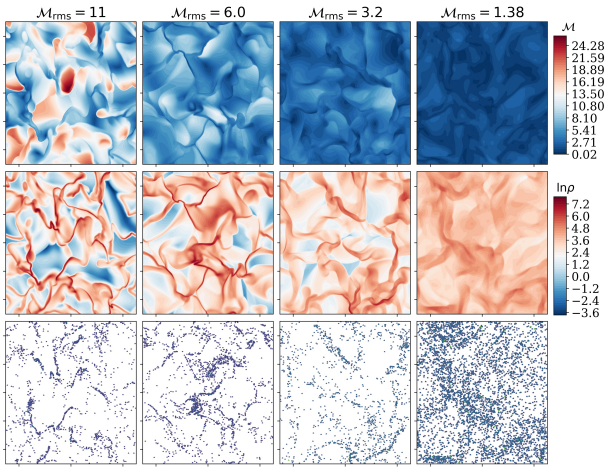

Figure 5: Accretion of dust grains in supersonic interstellar turbulence (Li and Mattsson, 2020). Cross-section of local Mach number, $\mathcal{M}(\boldsymbol{x}, t)$. Bottom row: particle distribution.

7 Changes of defaults

The Pencil Code comes with a lot of default settings. Many of the input parameters are set to what was of interest when a particular module was developed. Likewise, many logicals (switches) are set to whatever a particular person considered useful at that time and what is imposed by the constraint of backward compatibility. Changing this all of a sudden could make others quite upset. To raise awareness of changes that are considered justified, we use the opportunity to highlight changes of defaults in the Newsletter.

`lwrite_last_powersnap=.false.` It used to be `.true.`, which caused the last spectral snapshot to be written at the end of a run, even though the time does not follow the regular interval, set by `dspec`. (At the time, it was thought too precious to skip this information at the end of a long run.) It does, however, cause "glitches" in an otherwise regular record of a long run that has been restarted several times. It is therefore now no longer the default.

8 Three-year postdoc position

A 3-year postdoc position is available at the Laboratory of Astrophysics (LASTRO) of EPFL (Switzerland) in the group of Jennifer Schober. The position is part of a SNF PRIMA project and is within the broad

topics of astrophysical magnetohydrodynamics and radio astronomy. Details on the position and the application process can be found at: `https://jobregister.aas.org/ad/457c88b3`. The deadline is September 30, 2020.

9 Papers since July

Since the last newsletter of July 17, some new papers have appeared on the arXiv, and others that were just preprints, have now been published. We list both.

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This Pencil Code Newsletter was edited by Axel Brandenburg `<brandenb@nordita.org>`, Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, 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.