The Pencil Code Newsletter

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Contents

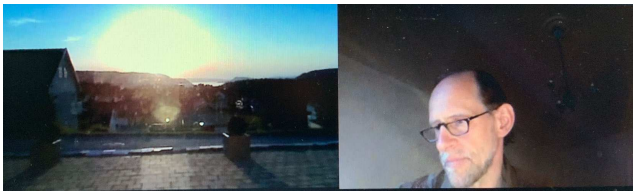

Figure 1: Axel's screenshot at the end of the PCSC meeting showing the view from Nils' window (Trondheim, Norway) and Matthias on the right on skype.

1 Preamble

During the June 2020 meeting of the Pencil Code Steering Committee (PCSC) it was decided that the PCSC issues a regular newsletter about three times a year to update and remind the user community of important results and developments. The minutes and other material of the PCSC can be found on `http://www.nordita.org/~brandenb/pc/PCSC`. Even near the end of the skype meeting almost at 10 pm, the Sun was still high in the sky in Trondheim (Figure 1).

The range of content is still to be decided upon, but what has been mentioned includes recent developments on the code, the conclusions on recent discussions in `http://groups.google.com/g/pencil-code-discuss` and recent publications that have used or mentioned the Pencil Code.

2 Pencil Code User Meeting

We encourage all users to follow and chip in on the presentations at the upcoming Pencil Code User Meeting (PCUM) in Glasgow during 27–31 July 2020. If you forget the link, you can just say `pc_news` to get the link, which is `http://indico.fysik.su.se/event/6870/`; see Figure 2.

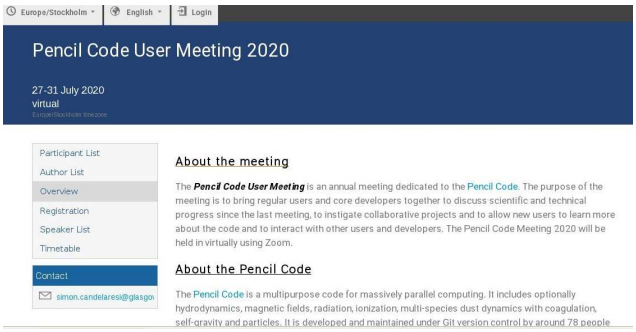

Figure 2: Web page where you can register for the meeting. Please register, even if you want to participate only in a few sessions.

3 Ongoing code developments

Python & HDF5. Simon Candelaresi, Fred Gent, and others have now replaced all Python routines with rewritten versions, following a series of improvements. A major one was the object-oriented approach which led to the transformation of simple functions into more powerful objects. Now all reading routines return an object with the data and some meta data. There have been improvements in the coding style, and a lot of additional comments have been added. The documentation has been greatly extended with every routine having now a full description. IO routines are much more efficient now, with, e.g., the slice reading routine showing a speed-up of 50 for large slice files (2GB+). There have been various additions, such as simulation objects, `rvid_box` plots and particle routines. Lastly,

all routines are Python 3 compatible.

Looking forward, they have implemented a powerful simulation object, which is under development to permit cloning and manipulating existing simulations, to launch arrays of simulations across ranges of parameters, and to assist data analysis of multiple simulations. As larger data sets become more common and feasible, the HDF5 format becomes essential both for computing and post-processing. So, data reading options include HDF5 or Fortran binary format, but also options which take advantage of the alternate low memory `hdf5` object for reading data, and `mpi4py` to operate parallel data analysis of large data sets.

Since the syntax differs, backward compatibility is lost. Therefore, the old Python routines are kept in `python/pencil_old`. and can be imported via: `import pencil_old as pco`.

Shallow water. You may have wondered about recent check-ins about shallow water. Wlad Lyra clarified: "A student of mine (Ali Hyder) is using it to model the polar atmosphere of Jupiter. We added a sample that reproduces the speed of gravity waves." For more info, contact Wlad or Ali, and maybe they'll present something at the upcoming PCUM.

Code profiling. As part of a PRACE project, Jörn Warnecke and colleagues were asked to profile the Pencil Code. It turned out that the considered run (global convective dynamo in a shell) spends too much time in the functions MPI_BARRIER and MPI_ALLREDUCE. Solutions:

- In general, the tasks of a run can be automatically distributed across nodes in a way that slows down communication. To avoid this, set `-m plane=`⟨*number of cores per node*⟩ in the (`sbatch`) job submission script. Best results can be expected if this is a multiple of `nprocx`.
- Global operations like averages for conserving mass and angular momentum slow down a run noticeably when performed in every substep. By the new parameter `it_rmv` in the `run_pars` of `run.in` their frequency can now be controlled: The default `it_rmv=0` means "as usual" while for `it_rmv=`n averages are only taken once every nth time step. `it_rmv=5` turned out to be enough to remove the bottleneck of the averages.

Both tricks together made a total speedup of two. More information and discussion on this is scheduled for the PCUM.

Python within IDL. If you are interested in using Python programs within IDL programs, you can do this through the IDL-to-Python bridge (for IDL version 8.6 or newer and Python 3.5 or newer), you may find inspiration from Christer's `pc_d2_dimension.pro` in `idl/modules/particles/d2_dimension/`, which you can call with `pc_d2_dimension, pvars, /allpython`. However, IDL needs to be launched from an environment where Python invokes a version that is supported by the used version of IDL. `Christer Sandin <christersandin@yahoo.se>` knows the details.

HDF5. The HDF5 format is now in production for more than a year. If anybody notices any bugs or anything weird, please give feedback to Philippe Bourdin `<Philippe.Bourdin@oeaw.ac.at>`. One change is already envisaged: to enable the use of the `persistent` variables as global datasets, so that changing the number of processors (and data distribution) becomes possible. Transition to HDF5 is facilitated by the possibility to choose different schemes for data in- and output: If one wants to restart from distributed Fortran binary data, but to write all output in HDF5 format, set

```
IO = io_hdf5
IO_IN = io_dist
```

and recompile. Further restarts will ignore `IO_IN` even without recompilation (by the lock file `IO_LOCK`). The IO schemes can be freely combined, but "returning from HDF5" is yet experimental. When using this feature, copying data for restart can be replaced by linking: use `pc_copyvar` with `-s` (much faster for big models).

4 Manual update

Incidently, please spend some time reviewing and improving the manual. As discussed at the last PCSC, we plan to assign a DOI number to it during the next PCUM, and those who have contributed should be listed as authors.

5 Contribute to the newsletter

Just send an email to `Axel Brandenburg <brandenb@nordita.org>` or `Matthias Rheinhardt <matthias.rheinhardt@aalto.fi>`. We might edit the material to make it suitable and will let you proofread what we have done with it. The next newsletter will be published about a month after the PCUM.

6 Not on pencil-code-discuss?

There are currently 141 members on pencil-code-discuss,[1] but not even all the developers appear on this list. They would not know what they miss, so if you see somebody missing, please tell them. Normally, everybody would sign up oneself.

7 Top-ten commits: Jan–Jun

The code is soon 20 year old, and still there is a lot of development going on, for the benefit of everybody in the community. On GitHub, you can explore yourself[2] and slide with your pointer a time window where you want to see the developments; see Figure 3 for the entries between January and June 2020. For the entire data record, there are currently 34 contributors who have done at least 34 commits, so the h index of the Pencil Code is – in this sense – 34.

It has happened before, that contributors dropped out of the list because of some mistake by GitHub, but they were able to correct this. If you notice issues with your entry on GitHub, please email them.

8 Scientific usage: updates

The bibtex file. As many of you know, there is a document where we collect all the papers that make use of the Pencil Code.[3] The papers and the corresponding bibtex entries are found with ADS full text search. Unfortunately, ADS does not include papers in *Combustion and Flame*, and some other journals, and sometimes the Pencil Code is used, but not mentioned explicitly. If you find such cases, please email us the bibtex entry, or just add it yourself to `pencil-code/doc/citations/ref.bib`.

Papers during January–June. The bibtex file is checked in on GitHub[4] and used to assemble citations not only by year, but also by topic. The list of papers is now so long that most of the new entries remain easily unnoticed. For convenience, the papers from January to June 2020, so far 37, are assembled in the references at end. The number of papers is unusually high, but explainable by the fact that the special issue in GAFD appeared in this time frame; see also Brandenburg *et al.* (2020a) for the editorial.

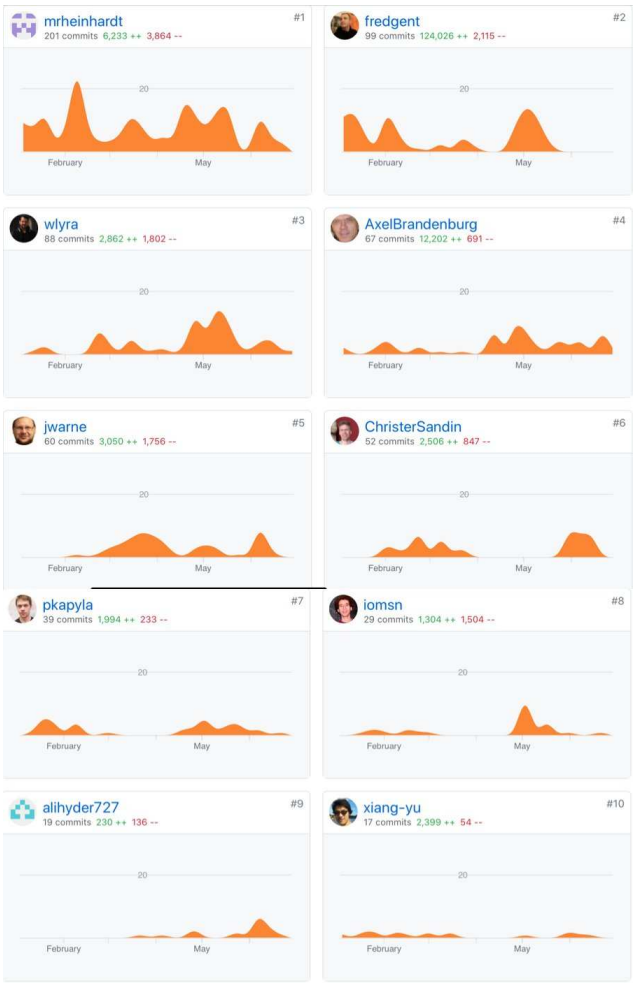

Figure 3: Top-ten commits since January

9 DOIs for simulation data

Scientists who are supported by the Swedish Research Council are required to make their data publicly accessible.[5] For the time being, a workable solution for Pencil Code users is to give DOI numbers to the run directories separately for each paper. There are already several examples;[6] see Figure 4. Even the Pencil Code itself has one; `DOI.org/10.5281/zenodo.2315093` gives a tarball of version v2018.12.16, but also a reference to the life github site. (A code DOI was requested by

[1] http://groups.google.com/g/pencil-code-discuss/members
[2] http://github.com/pencil-code/pencil-code/graphs/contributors
[3] http://www.nordita.org/~brandenb/pencil-code/PCSC/citations.pdf
[4] http://github.com/pencil-code/pencil-code/tree/master/doc/citations
[5] http://www.vr.se/english/mandates/open-science/open-access-to-research-data.html
[6] search for "Pencil Code" on http://zenodo.org
DOI.org/10.5281/zenodo.3897954, DOI.org/10.5281/zenodo.3886562, DOI.org/10.5281/zenodo.3841900, DOI.org/10.5281/zenodo.3692072, DOI.org/10.5281/zenodo.3534739, DOI.org/10.5281/zenodo.3526056.

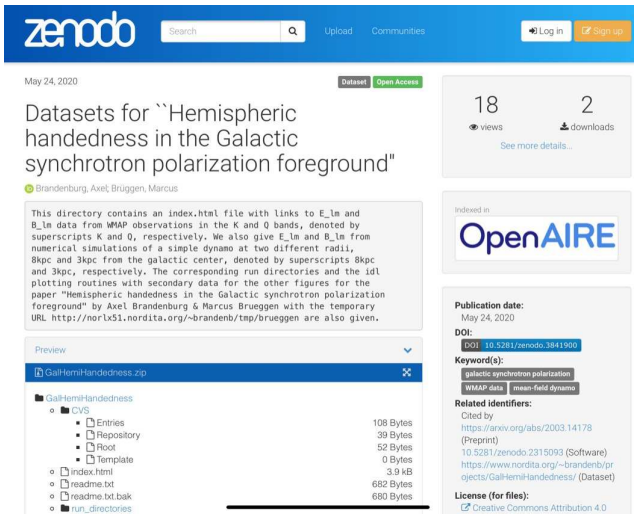

Figure 4: Zenodo page showing data sets with DOI number for `DOI.org/10.5281/zenodo.3841900`.

Atmospheric Chemistry & Physics.[7])

If you have data for a paper in ApJ or any other AAS journal, you may be contacted by `August Muench <august.muench@aas.org>`. You will also have the opportunity to hear and talk to him on Monday of the PCUM.

10 An MHD splinter meeting

Maarit Käpylä informed us about the splinter meeting (`:http://ag2020.astronomische-gesellschaft.de/view_splinter.php?session=Magnetic;`) on "Cosmic magnetic fields" that is being organized as part of the virtual annual meeting of the German Astronomical Society during September 21-25, 2020. The deadline for abstracts is *July 31, 2020*.

The goal of this splinter meeting is to review the current studies of the generation and the consequences of cosmic magnetic fields. The aim is to bring together experts in observation, theory and modelling of cosmic magnetic fields at various scales.

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[7] `http://ui.adsabs.harvard.edu/abs/2019ACP....19..639L`

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