The Pencil Code Newsletter

Issue 2022/3

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Contents

1 Code developments

1.1 New Fourier output devices

Hongzhe Zhou (now at the Tsung-Dao Lee Institute in Shanghai) wrote us about a new subroutine `power_fft3d_vec` that is now available in `power_spectrum.f90`. It outputs real and imaginary parts of the components of the Fourier transform of a vector field. The following input parameters in `&power_spectrum_run_pars` can be taken:

- `tout_min` and `tout_max` to limit the time range of the output.
- `kout_max`: Only the modes with $-$`kout_max` $\leq k_{x,y,z} \leq$ `kout_max` will be taken.

Because it is implemented in `power_spectrum.f90`, the output frequency is determined by `dspec`.

To use the subroutine, the switches in `&run_pars` of the form `var_sp` can be turned on, where `var` = `uu`, `oo`, `bb`, `jj`, `ee`, and `sp` = `fft3d`, `xkyz`, `kx0z`, `k00z`. The variables have their usual meanings in the code. The `sp` part further specifies which modes of the vector field f_i we want:

- `fft3d`: Outputs $\tilde{f}_i(\boldsymbol{k})$ with $-$`kout_max` $\leq k_{x,y,z} \leq$ `kout_max`.
- `xkyz`: Outputs $\tilde{f}_i(x, k_y, k_z)$, i.e., the x direction is not Fourier-transformed, and the centermost 2`kout_max`+1 y–z planes will be taken. This might be useful when the x direction is inhomogeneous, e.g., in a shearing box.
- `kx0z`: Outputs $\tilde{f}_i(k_x, k_y = 0, k_z)$, i.e., the $k_y = 0$ slice in the Fourier space.
- `k00z`: Outputs $\tilde{f}_i(k_x = k_y = 0, k_z)$.

The output data files have names `fft3dvec_sp_var_{x,y,z}_{re,im}.dat`, meaning the real or imaginary part of the x, y, or z component. Hence for each switch `var_sp`, there will be 6 output files. For each of them, the data structure is

t_1

$f(i_1, j_1, k_1), f(i_2, j_1, k_1), \cdots,$
$f(i_1, j_2, k_1), f(i_2, j_2, k_1), \cdots,$
$f(i_1, j_1, k_2), f(i_2, j_1, k_2), \cdots$

t_2

$\ldots$

Therefore for each snapshot, there will be (2`kout_max`+1)^3 field values if `sp` = `fft3d`, `xkyz`, or (2`kout_max`+1)^2 field values if `sp` = `kx0z`, or 2`kout_max` + 1 field values if `sp` = `k00z`. For Mathematica users, these files can be read by the `read3DFFT` or `read2DFFT` function.

1.2 Spectra always too late by dt

The output time for spectra was always too late by dt, so therefore, as an option (not the default), we add dt to the current time, so as to output at the correct time. This is being invoked by putting `lspec_at_tplusdt=T` in `run_pars`. At some point, this should be made the default.

1.3 "True binning" for shell-integrated spectra

When forming shell-integrated (say, power) spectra, integer-valued components of the wavevector $\boldsymbol{k}$ result in general in non-integer moduli k. Integration over shells was so far performed such that integer bins of

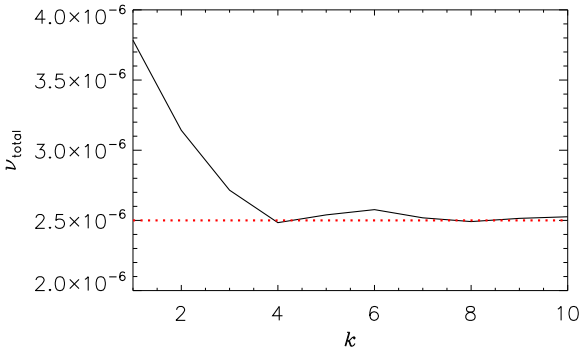

Figure 1: Total = explicit + numerical diffusivity derived from the k dependent decay rate with rounded binning. Red dotted: explicit value 2.5×10^{-6}.

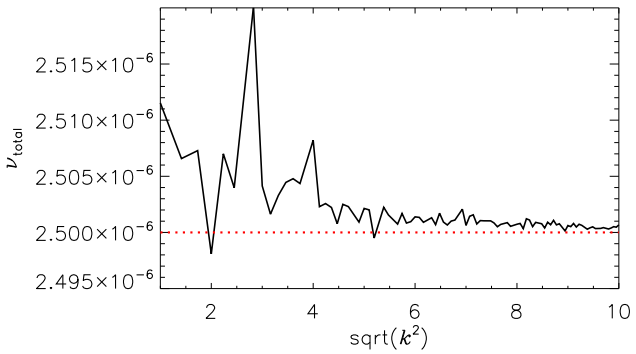

Figure 2: As Fig. 1, but with true binning. The scatter at low k is because of limited integration time.

k were formed to collect the power contributions, requiring (most of) the k's to be rounded. As a consequence, particularly for small k, contributions belonging to rather different scales were summed up. This became obvious when simulating the free decay of a fluid in a periodic box where all waves with the same k have to decay with the rate νk^2. However, with integer k binning, contributions with, say $k^2 = 1$ and $k^2 = 2$ are put into the same bin, the amplitude of which does therefore not at all decay as expected, see Fig. 1. To obtain proper decay rates, suited, e.g. to assess numerical viscosity, "true binning" was introduced by forming bins of k^2, hence avoiding roundoff errors (activate by `ltrue_binning=T` in `power_spectrum_run_pars`). See the strikingly different values for the deduced total (explicit+numerical) viscosity in Fig. 2. Of course the number of bins increases roughly quadratically, and for large grids, outputting all the corresponding amplitudes may turn prohibitive. That's why, an upper limit for k^2 may be chosen (`max_k2`). The k^2 values and their number are output into the `power*.dat` files, from where they are read by the IDL routine `power.pro` and available via keyword parameter `qk`. Volunteers for PYTHON etc. welcome. So far, the new scheme is only available for quantities output by routine `power`, that is, `u, r2u, r3u, o, b, a, ud`.

1.4 Pencils across special modules

With multiple special modules, it can occur that one of them provides specific pencils, which are used by others. The providing module, however, can possibly also be left out of the setup. While at runtime, employing respective switches, a try to use of the now undefined pencils will be prevented, compilation requires nevertheless that they are always *declared*. One could simply include `! PENCILS PROVIDED` meta-statements in the modules, which potentially employ these pencils but this would be misleading when reading the code. That's why we have now also the `! PENCILS EXPECTED` meta-statement for use in the headers of such modules. With respect to the generated code, there is no difference between the two meta-statements except that the occurrence of multiple `! PENCILS PROVIDED` for the same pencil issues a warning, but that of multiple `! PENCILS EXPECTED` does not as the latter case bears no risks. Likewise, occurrence of one `! PENCILS PROVIDED` along with (one or more) `! PENCILS EXPECTED` for the same pencil doesn't issue a warning either as it is in general meaningful.

1.5 MPI with huge buffers

With huge grids, the size of MPI communication buffers can exceed the maximum length representable by 4-Byte integers. This problem would first occur in `io_collect.f90` and `io_collect_xy.f90`. To avoid it, new routines `mpi[send|recv]_real_arr_huge` have been implemented in `mpicomm.f90`, which employ a newly declared MPI datatype having just the maximum possible size. For extreme-scale models, the issue could even become relevant for the communication buffers employed in ghost zone updating. Then the send/recv calls in `initiate_isendrcv_bdry` and `finalize_isendrcv_bdry` of `mpicomm.f90` had to be adjusted accordingly.

2 Operational aspects

2.1 Watch `src/revision.txt`

Wolfgang just fixed the writing of `src/revision.txt` at the end of the compilation. This seems to work well and this file is now also written with the updated `bin/cvsci_run`.

2.2 Linking order

The CRAY compiler (version 14.0.2) turned out to produce worrisome warnings during the link stage. To avoid these, the order of the object files in the linker commands (see `Makefile.src` macros' `$(technical)`, `$(physics)` and `$(technical_nompi)` definition and use) has been carefully adjusted. Please do not change it. New objects can always be added at the end of those lists as long as they are not providing public data (which should anyway be avoided).

2.3 HDF5 on Dardel

Lars Mattsson reported the following to us regarding the use of Pencil on Dardel, a supercomputer in Stockholm:

A central issue appears to be that static linking is not supported on Dardel but `h5pfc` uses static linking by default. Hence, to build the code, launch `pc_build -f compilers/Cray LDFLAGS+=-shlib` to override static linking, until the issue is fixed by the Dardel/HPE staff. In addition, the compression library `zlib` is not by default available when building with HDF5 (say with `module load cray-hdf5-parallel/1.12.0.7`), thus breaking the build. Yet, it is available on Dardel as a module to be loaded by:

```
module load PDC/21.11
module load zlib/1.2.11 .
```

Even with these modifications, we couldn't yet start and run due to some MPI-related issue. Eventually we found out that there has to be the 'shebang' `#!/bin/bash -l` at the top of the batch script. The important thing here is the flag `-l`, which appears to be needed to get the environment set properly. As Linux systems are normally setup such that it shouldn't matter, we asked the Dardel staff to look into this.

3 Postdoc advertisement

Some of you may be looking for jobs. Many of the astrophysics group at Nordita are using the Pencil Code. Now there is a new call for postdocs at Nordita; see `https://academicjobsonline.org/ajo/jobs/22743`. The deadline is Nov 15. The ranking is done by Nordita's Research Subfield Committee; `https://www.nordita.org/aboutus/organization/research_subfield_committees/`. Scientific excellence and independence are important criteria.

4 Scientific program deadline

One of Nordita's specialities are *scientific programs*. These are one-month long meetings where scientists from around the world come together to work in an inspiring atmosphere on aspects of common interest. Everybody can apply for organizing a program; see `https://www.nordita.org/organizers/proposal/` The ranking of proposals is done by Nordita's program committee `https://www.nordita.org/aboutus/organization/program_committee/` and the final decision is taken by Nordita's Board. The deadline for proposal applications is Nov 15.

5 Galactic magnetic program

Nordita will be hosting a highly relevant program titled "Towards a Comprehensive Model of the Galactic Magnetic Field", during 3–28 April 2023, organized by Jennifer West, Tess Jaffe, Anvar Shukurov, Torsten Ensslin, Jörg Härandel, Francois Boulanger, Fred Gent, and Marijke Haverkorn. For pre-registration; see `https://docs.google.com/forms/d/e/1FAIpQLScMM-X_bu2UwXWIjJLhdesifflbLVeKZV83cdEGZOBGTqW8IQ/viewform`.

6 Papers since June 2022

As usual, we look here at new papers that make use of the Pencil Code. Since the last newsletter of June 15, 11 new papers have appeared on the arXiv, and 10 others, some of which were just preprints and have now been published. We list both here, 21 altogether. A browsable ADS list of all Pencil Code papers can be found on: `https://ui.adsabs.harvard.edu/user/libraries/iGR7N570Sy6AlhDMQRTe_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. A compiled version of this file is available as https://github.com/pencil-code/website/blob/master/doc/citations.pdf, where we also list a total of now 102 code comparison papers in the last section "Code comparison & reference". Those are not included in our list below, nor among the now total number of 630 research papers that use the Pencil Code.

References

Baehr, H., Zhu, Z. and Yang, C.C., Direct Formation of Planetary Embryos in Self-gravitating Disks. *Astrophys. J.*, 2022, **933**, 100.

Becerra, L., Reisenegger, A., Valdivia, J.A. and Gusakov, M., Stability of axially symmetric magnetic fields in stars. *Month. Not. Roy. Astron. Soc.*, 2022, **517**, 560–568.

Brandenburg, A., Rogachevskii, I. and Schober, J., Dissipative magnetic structures and scales in small-scale dynamos. *Month. Not. Roy. Astron. Soc., submitted*, 2022a, arXiv:2209.08717.

Brandenburg, A., Quadratic growth during the COVID-19 pandemic: merging hotspots and reinfections. *J. Phys. A: Math. Theor., submitted*, 2022, arXiv:2206.15459.

Brandenburg, A., Zhou, H. and Sharma, R., Batchelor, Saffman, and Kazantsev spectra in galactic small-scale dynamos. *Month. Not. Roy. Astron. Soc., submitted*, 2022b, arXiv:2207.09414.

Carenza, P., Sharma, R., Marsh, M.C.D., Brandenburg, A. and Müller, E., Magnetohydrodynamics predicts heavy-tailed distributions of axion-photon conversion. *arXiv e-prints*, 2022, arXiv:2208.04333.

Gent, F.A., Mac Low, M.M., Korpi-Lagg, M.J. and Singh, N.K., The small-scale dynamo in a multiphase supernova-driven medium. *arXiv e-prints*, 2022, arXiv:2210.04460.

Hyder, A., Lyra, W., Chanover, N., Morales-Juberías, R. and Jackiewicz, J., Exploring Jupiter's Polar Deformation Lengths with High-resolution Shallow Water Modeling. *Planet. Sci. J.*, 2022, **3**, 166.

Käpylä, M.J., Rheinhardt, M. and Brandenburg, A., Compressible Test-field Method and Its Application to Shear Dynamos. *Astrophys. J.*, 2022, **932**, 8.

Käpylä, P.J., Transition from anti-solar to solar-like differential rotation: Dependence on Prandtl number. *arXiv e-prints*, 2022, arXiv:2207.00302.

Käpylä, P.J. and Singh, N.K., Turbulent Prandtl number from isotropically forced turbulence. *J. Fluid Mech., in press*, 2022, arXiv:2207.10335.

Li, X.Y., Mehlig, B., Svensson, G., Brandenburg, A. and Haugen, N.E.L., Collision Fluctuations of Lucky Droplets with Superdroplets. *J. Atmosph. Scie.*, 2022, **79**, 1821–1835.

Lipatnikov, A.N. and Sabelnikov, V.A., Flame folding and conditioned concentration profiles in moderately intense turbulence. *Phys. Fluids*, 2022, **34**, 065119.

Masada, Y. and Sano, T., Rotational Dependence of Large-scale Dynamo in Strongly-stratified Convection: What Causes It?. *Astrophys. J., submitted*, 2022, arXiv:2206.06566.

Mtchedlidze, S., Domínguez-Fernández, P., Du, X., Schmidt, W., Brandenburg, A., Niemeyer, J. and Kahniashvili, T., Inflationary and phase-transitional primordial magnetic fields in galaxy clusters. *Astrophys. J., submitted*, 2022, arXiv:2210.10183.

Navarrete, F.H., Käpylä, P.J., Schleicher, D.R.G., Ortiz, C.A. and Banerjee, R., Origin of eclipsing time variations: Contributions of different modes of the dynamo-generated magnetic field. *Astron. Astrophys.*, 2022, **663**, A90.

Ortiz-Rodríguez, C.A., Schleicher, D.R.G., Käpylä, P.J. and Navarrete, F.H., Simulations of fully convective M dwarfs: dynamo action with varying magnetic Prandtl numbers. *Bol. Asoc. Argentina Astron. La Plata Argentina*, 2022, **63**, 62–64.

Sengupta, D. and Umurhan, O.M., Turbulence in particle laden midplane layers of planet forming disks. *Astrophys. J., in press*, 2022, arXiv:2209.11205.

Stejko, A.M., Kosovichev, A.G., Featherstone, N.A., Guerrero, G., Hindman, B.W., Matilsky, L.I. and Warnecke, J., Constraining Global Solar Models through Helioseismic Analysis. *Astrophys. J.*, 2022, **934**, 161.

Tschernitz, J. and Bourdin, P.A., Influence of the kinematic viscosity on solar convection simulations; in *44th COSPAR Scientific Assembly. Held 16-24 July*, Vol. 44, Jul., 2022, p. 2553.

Zhou, H., Sharma, R. and Brandenburg, A., Scaling of the Hosking integral in decaying magnetically-dominated turbulence. *J. Plasma Phys.*, 2022, arXiv:2206.07513.

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