The Journal of Open Source Software

The Pencil Code, a modular MPI code for partial differential equations and particles: multipurpose and multiuser-maintained

The Pencil Code Collaboration[1], Axel Brandenburg[1, 2, 3], Anders Johansen[4], Philippe A. Bourdin[5, 6], Wolfgang Dobler[7], Wladimir Lyra[8], Matthias Rheinhardt[9], Sven Bingert[10], Nils Erland L. Haugen[11, 12, 1], Antony Mee[13], Frederick Gent[9, 14], Natalia Babkovskaia[15], Chao-Chin Yang[16], Tobias Heinemann[17], Boris Dintrans[18], Dhrubaditya Mitra[1], Simon Candelaresi[19], Jörn Warnecke[20], Petri J. Käpylä[21], Andreas Schreiber[15], Piyali Chatterjee[22], Maarit J. Käpylä[9, 20], Xiang-Yu Li[1], Jonas Krüger[11, 12], Jørgen R. Aarnes[12], Graeme R. Sarson[14], Jeffrey S. Oishi[23], Jennifer Schober[24], Raphaël Plasson[25], Christer Sandin[1], Ewa Karchniwy[12, 26], Luiz Felipe S. Rodrigues[14, 27], Alexander Hubbard[28], Gustavo Guerrero[29], Andrew Snodin[14], Illa R. Losada[1], Johannes Pekkilä[9], and Chengeng Qian[30]

1 Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden **2** Department of Astronomy, Stockholm University, Sweden **3** McWilliams Center for Cosmology & Department of Physics, Carnegie Mellon University, PA, USA **4** GLOBE Institute, University of Copenhagen, Denmark **5** Space Research Institute, Graz, Austria **6** Institute of Physics, University of Graz, Graz, Austria **7** Bruker, Potsdam, Germany **8** New Mexico State University, Department of Astronomy, Las Cruces, NM, USA **9** Astroinformatics, Department of Computer Science, Aalto University, Finland **10** Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen, Germany **11** SINTEF Energy Research, Trondheim, Norway **12** Norwegian University of Science and Technology, Norway **13** Bank of America Merrill Lynch, London, UK **14** School of Mathematics, Statistics and Physics, Newcastle University, UK **15** No current affiliation **16** University of Nevada, Las Vegas, USA **17** Niels Bohr International Academy, Denmark **18** CINES, Montpellier, France **19** School of Mathematics and Statistics, University of Glasgow, UK **20** Max Planck Institute for Solar System Research, Germany **21** Institute for Astrophysics, University of Göttinge, Germany **22** Indian Institute of Astrophysics, Bengaluru, India **23** Department of Physics & Astronomy, Bates College, ME, USA **24** Laboratoire d'Astrophysique, EPFL, Sauverny, Switzerland **25** Avignon Université, France **26** Institute of Thermal Technology, Silesian University of Technology, Poland **27** Radboud University, Netherlands **28** Department of Astrophysics, American Museum of Natural History, NY, USA **29** Physics Department, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil **30** State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, China

DOI: 10.21105/joss.02807

Software

- Review
- Repository
- Archive

Editor: Arfon Smith

Reviewers:

- @zingale
- @rtfisher

Submitted: 17 September 2020
Published: 21 February 2021

License
Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License (CC BY 4.0).

Summary

The Pencil Code is a highly modular physics-oriented simulation code that can be adapted to a wide range of applications. It is primarily designed to solve partial differential equations (PDEs) of compressible hydrodynamics and has lots of add-ons ranging from astrophysical magnetohydrodynamics (MHD) (A. Brandenburg & Dobler, 2010) to meteorological cloud microphysics (Li et al., 2017) and engineering applications in combustion (Babkovskaia et al., 2011). Nevertheless, the framework is general and can also be applied to situations not related to hydrodynamics or even PDEs, for example when just the message passing interface or input/output strategies of the code are to be used. The code can also evolve Lagrangian (inertial and noninertial) particles, their coagulation and condensation, as well as their interaction with the fluid. A related module has also been adapted to perform ray tracing

and to solve the eikonal equation.

The code is being used for Cartesian, cylindrical, and spherical geometries, but further extensions are possible. One can choose between different time stepping schemes and different spatial derivative operators. High-order first and second derivatives are used to deal with weakly compressible turbulent flows. There are also different diffusion operators to allow for both direct numerical simulations (DNS) and various types of large-eddy simulations (LES).

High-level functionality

An idea about the range of available modules can be obtained by inspecting the examples under pencil-code/samples/. Those are low resolution versions related to applications published in the literature. Some of the run directories of actual production runs are published through Zenodo. Below a list of method papers that describe the various applications and tests:

- Coagulation and condensation in turbulence (Johansen et al., 2008; Li et al., 2017),
- Radiative transfer (Barekat & Brandenburg, 2014; A. Brandenburg & Das, 2020; Heinemann et al., 2006),
- Chiral magnetic effect in relativistic plasmas (Schober et al., 2018),
- Primordial gravitational waves (Roper Pol et al., 2020),
- Modeling homochirality at the origin of life (Axel Brandenburg, 2019; A. Brandenburg & Multamäki, 2004),
- Modeling of patterned photochemical systems (Emond et al., 2012),
- Gaseous combustion and detonation (Babkovskaia et al., 2011; Krüger et al., 2017; Zhang et al., 2020),
- Burning particles, resolved or unresolved (Qian et al., 2020),
- Flows around immersed solid objects (Aarnes et al., 2019, 2020; N. E. L. Haugen & Kragset, 2010),
- Test-field method for turbulent MHD transport (A. Brandenburg et al., 2010; Rheinhardt & Brandenburg, 2010; Warnecke et al., 2018),
- Mean-field MHD (Jabbari et al., 2013; Kemel et al., 2013),
- Spherical shell dynamos and convection (P. J. Käpylä et al., 2020; Mitra et al., 2009),
- Boris correction for coronal physics (Chatterjee, 2020),
- Thermal instability and mixing (C.-C. Yang & Krumholz, 2012),
- Implicit solver for temperature (Gastine & Dintrans, 2008),
- Dust-gas dynamics with mutual drag interaction (C.-C. Yang & Johansen, 2016; Youdin & Johansen, 2007),
- Boundary conditions for the solar atmosphere and HDF5 format (Philippe-A. Bourdin, 2020).

Statement of need and purpose of software

The code is an easily adaptable tool for solving both standard MHD equations as well as others, such as the test-field equations. Significant amounts of runtime diagnostics as well as Python and IDL libraries for post-processing are available.

Among the currently 83 developers with check-in permission, there are currently 18 owners who can give others check-in permission. Of the developers, 35 have done more than 35 commits. Users have access to the latest development version and can ask to join the circle of developers by contacting one of the owners.

Every revision on GitHub is verified on 9 tests on travis-ci.com. The current version is also automatically being tested on 59 hourly tests and on 79 daily tests. Continuous progress on the code is driven by the research of individual developers.

Further developments and interactions between developers and users are being promoted through annual user meetings since 2004 and a newsletters since 2020. Since 2016, a steering committee of five elected owners reviews the progress and can take decisions of general concern to the Pencil Code community.

Ongoing research using the Pencil Code

Current research includes topics from stellar physics, interstellar and intercluster medium, the early universe, as well as from meteorology and engineering: small-scale dynamos and reconnection; primordial magnetic fields and decaying turbulence; gravitational waves from turbulent sources; planet formation and inertial particles; accretion discs and shear flows; coronal heating and coronal mass ejections; helical dynamos, helical turbulence, and catastrophic quenching; helioseismology; strongly stratified MHD turbulence and negative effective magnetic pressure instability; convection in Cartesian domains; global convection and dynamo simulations; turbulent transport and test-field methods; hydrodynamic and MHD instabilities and turbulence; chiral MHD; turbulent gaseous and solid combustion, particle clustering and deposition on solid walls, front propagation, radiation & ionization. As of July 2020, 564 papers have been published that acknowledge use of the Pencil Code (A. Brandenburg, 2020).

Key references

The Pencil Code is unique in two ways: the high level of flexibility and modularity, and the way it is organized (open source, distributed ownership, openness of development version).

Other software addressing related needs include: Athena, CO5BOLD, ENZO, MuRAM, NIRVANA, Stagger, ZEUS, Snoopy, and several other LES codes. There are also several other engineering DNS codes such as Sandia-3-Dimensional (S3D), a high-order compressible code, optimized for combustion, which is not open source, however. Another example is SpECTRE, a task-based discontinuous Galerkin code for relativistic astrophysics (Kidder et al., 2017). In addition, there are frameworks like Dedalus or Cactus, which allow one to program the equations in symbolic form.

Some recent research areas that made use of the Pencil Code, as evidenced by the aforementioned document listing all those papers (A. Brandenburg, 2020), include:

- Flows around immersed solid objects (N. E. L. Haugen & Kragset, 2010),
- Particle clustering in supersonic and subsonic turbulence (Karchniwy et al., 2019; Mattsson et al., 2019),
- Cloud microphysics (Li et al., 2017),
- Planet and planetesimal formation (Johansen et al., 2007; Lyra et al., 2009; Oishi et al., 2007),
- Global simulations of debris disks (Lyra & Kuchner, 2013),
- Stratified shearing box simulations, also with dust (Oishi & Mac Low, 2011; Schreiber & Klahr, 2018; C.-C. Yang et al., 2018),
- Supernova-driven turbulence (Gent et al., 2013),
- Solar dynamo and sunspots (A. Brandenburg, 2005; Heinemann et al., 2007),
- Solar corona above active regions (Bingert & Peter, 2011; P.-A. Bourdin et al., 2013; Chatterjee et al., 2016),
- Fully convective star in a box (Dobler et al., 2006),
- Dynamo wave in spherical shell convection (P. J. Käpylä et al., 2012; Warnecke et al., 2014),
- Convection with Kramers opacity law (P. J. Käpylä et al., 2020; Petri J. Käpylä et al., 2017; P. J. Käpylä, 2019),
- MHD turbulence and cascades (N. E. Haugen et al., 2004),
- Turbulent diffusivity quenching with test fields (A. Brandenburg et al., 2008; Karak et al., 2014).

Acknowledgements

We acknowledge contributions from all submitters and their supporting funding agencies. In particular, we mention the ERC Advanced Grant on Astrophysical Dynamos (No 227952), the Swedish Research Council, grants 2012-5797, 2013-03992, 2017-03865, and 2019-04234, the National Science Foundation under the grant AAG-1615100, the FRINATEK grant 231444 under the Research Council of Norway, SeRC, the grant "Bottlenecks for particle growth in turbulent aerosols" from the Knut and Alice Wallenberg Foundation, Dnr. KAW 2014.0048, the ReSoLVE Centre of Excellence (grant number 307411), the research project 'Gaspro,' financed by the Research Council of Norway (267916), the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Project UniSDyn, grant agreement n:o 818665), and the Deutsche Forschungsgemeinschaft (DFG) Heisenberg programme grant KA 4825/2-1.

References

Aarnes, J. R., Haugen, N. E. L., & Andersson, H. I. (2019). High-order overset grid method for detecting particle impaction on a cylinder in a cross flow. *Int. J. Comput. Fluid Dynam.*, *33*, 43–58. https://doi.org/10.1080/10618562.2019.1593385

Aarnes, J. R., Jin, T., Mao, C., Haugen, N. E. L., Luo, K., & Andersson, H. I. (2020). Treatment of solid objects in the Pencil Code using an immersed boundary method and overset grids. *Geophys. Astrophys. Fluid Dynam.*, *114*, 35–57. https://doi.org/10.1080/03091929.2018.1492720

Babkovskaia, N., Haugen, N. E. L., & Brandenburg, A. (2011). A high-order public domain code for direct numerical simulations of turbulent combustion. *J. Comp. Phys.*, *230*, 1–12. https://doi.org/10.1016/j.jcp.2010.08.028

Barekat, A., & Brandenburg, A. (2014). Near-polytropic stellar simulations with a radiative surface. *571*, A68. https://doi.org/10.1051/0004-6361/201322461

Bingert, S., & Peter, H. (2011). Intermittent heating in the solar corona employing a 3D MHD model. *530*, A112. https://doi.org/10.1051/0004-6361/201016019

Bourdin, Philippe-A. (2020). Driving solar coronal MHD simulations on high-performance computers. *Geophys. Astrophys. Fluid Dynam.*, *114*, 235–260. https://doi.org/10.1080/03091929.2019.1643849

Bourdin, P.-A., Bingert, S., & Peter, H. (2013). Observationally driven 3D magnetohydrodynamics model of the solar corona above an active region. *555*, A123. https://doi.org/10.1051/0004-6361/201321185

Brandenburg, A. (2005). The case for a distributed solar dynamo shaped by near-surface shear. *625*, 539–547. https://doi.org/10.1086/429584

Brandenburg, Axel. (2019). The limited roles of autocatalysis and enantiomeric cross-inhibition in achieving homochirality in dilute systems. *Origins of Life and Evolution of the Biosphere*, *49*, 49–60. https://doi.org/10.1007/s11084-019-09579-4

Brandenburg, A. (2020). *Scientific usage of the Pencil Code*. http://doi.org/10.5281/zenodo.3466444

Brandenburg, A., Chatterjee, P., Del Sordo, F., Hubbard, A., Käpylä, P. J., & Rheinhardt, M. (2010). Turbulent transport in hydromagnetic flows. *Phys. Scripta Vol. T*, *142*, 014028. https://doi.org/10.1088/0031-8949/2010/T142/014028

Brandenburg, A., & Das, U. (2020). The time step constraint in radiation hydrodynamics. *Geophys. Astrophys. Fluid Dynam.*, *114*, 162–195. https://doi.org/10.1080/03091929.

2019.1676894

Brandenburg, A., & Dobler, W. (2010). *Pencil Code: Finite-difference Code for Compressible Hydrodynamic Flows*. https://doi.org/10.5281/zenodo.2315093

Brandenburg, A., & Multamäki, T. (2004). How long can left and right handed life forms coexist? *Int. J. Astrobiology*, *3*, 209–219. https://doi.org/10.1017/S1473550404001983

Brandenburg, A., Rädler, K.-H., Rheinhardt, M., & Käpylä, P. J. (2008). Magnetic diffusivity tensor and dynamo effects in rotating and shearing turbulence. *676*, 740–751. https://doi.org/10.1086/527373

Chatterjee, P. (2020). Testing Alfvén wave propagation in a "realistic" set-up of the solar atmosphere. *Geophys. Astrophys. Fluid Dynam.*, *114*, 213–234. https://doi.org/10.1080/03091929.2019.1672676

Chatterjee, P., Hansteen, V., & Carlsson, M. (2016). Modeling repeatedly flaring δ sunspots. *116*, 101101. https://doi.org/10.1103/PhysRevLett.116.101101

Dobler, W., Stix, M., & Brandenburg, A. (2006). Magnetic field generation in fully convective rotating spheres. *638*, 336–347. https://doi.org/10.1086/498634

Emond, M., Le Saux, T., Allemand, J.-F., Pelupessy, P., Plasson, R., & Jullien, L. (2012). Energy propagation through a protometabolism leading to the local emergence of singular stationary concentration profiles. *Chem. Eur. J.*, *18*(45), 14375–14383. https://doi.org/10.1002/chem.201201974

Gastine, T., & Dintrans, B. (2008). Direct numerical simulations of the κ-mechanism. I. Radial modes in the purely radiative case. *484*, 29–42. https://doi.org/10.1051/0004-6361:20078936

Gent, F. A., Shukurov, A., Fletcher, A., Sarson, G. R., & Mantere, M. J. (2013). The supernova-regulated ISM - I. The multiphase structure. *432*, 1396–1423. https://doi.org/10.1093/mnras/stt560

Haugen, N. E., Brandenburg, A., & Dobler, W. (2004). Simulations of nonhelical hydromagnetic turbulence. *70*, 016308. https://doi.org/10.1103/PhysRevE.70.016308

Haugen, N. E. L., & Kragset, S. (2010). Particle impaction on a cylinder in a crossflow as function of stokes and reynolds numbers. *Journal of Fluid Mechanics*, *661*, 239–261. https://doi.org/10.1017/S0022112010002946

Heinemann, T., Dobler, W., Nordlund, Å., & Brandenburg, A. (2006). Radiative transfer in decomposed domains. *448*, 731–737. https://doi.org/10.1051/0004-6361:20053120

Heinemann, T., Nordlund, Å., Scharmer, G. B., & Spruit, H. C. (2007). MHD simulations of penumbra fine structure. *669*, 1390–1394. https://doi.org/10.1086/520827

Jabbari, S., Brandenburg, A., Kleeorin, N., Mitra, D., & Rogachevskii, I. (2013). Surface flux concentrations in a spherical α^2 dynamo. *556*, A106. https://doi.org/10.1051/0004-6361/201321353

Johansen, A., Brauer, F., Dullemond, C., Klahr, H., & Henning, T. (2008). A coagulation-fragmentation model for the turbulent growth and destruction of preplanetesimals. *486*, 597–611. https://doi.org/10.1051/0004-6361:20079232

Johansen, A., Oishi, J. S., Mac Low, M.-M., Klahr, H., Henning, T., & Youdin, A. (2007). Rapid planetesimal formation in turbulent circumstellar disks. *448*, 1022–1025. https://doi.org/10.1038/nature06086

Karak, B. B., Rheinhardt, M., Brandenburg, A., Käpylä, P. J., & Käpylä, M. J. (2014). Quenching and anisotropy of hydromagnetic turbulent transport. *795*, 16. https://doi.org/10.1088/0004-637X/795/1/16

Karchniwy, E., Klimanek, A., & Haugen, N. E. L. (2019). The effect of turbulence on mass transfer rates between inertial particles and fluid for polydisperse particle size distributions. *J. Fluid Mech.*, *874*, 1147–1168. https://doi.org/10.1017/jfm.2019.493

Käpylä, P. J. (2019). Overshooting in simulations of compressible convection. *631*, A122. https://doi.org/10.1051/0004-6361/201834921

Käpylä, P. J., Gent, F. A., Olspert, N., Käpylä, M. J., & Brandenburg, A. (2020). Sensitivity to luminosity, centrifugal force, and boundary conditions in spherical shell convection. *Geophys. Astrophys. Fluid Dynam.*, *114*, 8–34. https://doi.org/10.1080/03091929.2019.1571586

Käpylä, P. J., Mantere, M. J., & Brandenburg, A. (2012). Cyclic magnetic activity due to turbulent convection in spherical wedge geometry. *755*, L22. https://doi.org/10.1088/2041-8205/755/1/L22

Käpylä, Petri J., Rheinhardt, M., Brandenburg, A., Arlt, R., Käpylä, M. J., Lagg, A., Olspert, N., & Warnecke, J. (2017). Extended subadiabatic layer in simulations of overshooting convection. *845*, L23. https://doi.org/10.3847/2041-8213/aa83ab

Kemel, K., Brandenburg, A., Kleeorin, N., Mitra, D., & Rogachevskii, I. (2013). Active region formation through the negative effective magnetic pressure instability. *287*, 293–313. https://doi.org/10.1007/s11207-012-0031-8

Kidder, L. E., Field, S. E., Foucart, F., Schnetter, E., Teukolsky, S. A., Bohn, A., Deppe, N., Diener, P., Hébert, F., Lippuner, J., & al., et. (2017). SpECTRE: A task-based discontinuous galerkin code for relativistic astrophysics. *Journal of Computational Physics*, *335*, 84–114. https://doi.org/10.1016/j.jcp.2016.12.059

Krüger, J., Haugen, N. E. L., & Løvås, T. (2017). Correlation effects between turbulence and the conversion rate of pulverized char particles. *Combustion and Flame*, *185*, 160–172. https://doi.org/10.1016/j.combustflame.2017.07.008

Li, X.-Y., Brandenburg, A., Haugen, N. E. L., & Svensson, G. (2017). Eulerian and Lagrangian approaches to multidimensional condensation and collection. *J. Adv. Model. Earth Systems*, *9*, 1116–1137. https://doi.org/10.1002/2017MS000930

Lyra, W., Johansen, A., Zsom, A., Klahr, H., & Piskunov, N. (2009). Planet formation bursts at the borders of the dead zone in 2D numerical simulations of circumstellar disks. *497*, 869–888. https://doi.org/10.1051/0004-6361/200811265

Lyra, W., & Kuchner, M. (2013). Formation of sharp eccentric rings in debris disks with gas but without planets. *499*, 184–187. https://doi.org/10.1038/nature12281

Mattsson, L., Bhatnagar, A., Gent, F. A., & Villarroel, B. (2019). Clustering and dynamic decoupling of dust grains in turbulent molecular clouds. *483*, 5623–5641. https://doi.org/10.1093/mnras/sty3369

Mitra, D., Tavakol, R., Brandenburg, A., & Moss, D. (2009). Turbulent dynamos in spherical shell segments of varying geometrical extent. *697*, 923–933. https://doi.org/10.1088/0004-637X/697/1/923

Oishi, J. S., & Mac Low, M.-M. (2011). Magnetorotational turbulence transports angular momentum in stratified disks with low magnetic Prandtl number but magnetic Reynolds number above a critical value. *740*, 18. https://doi.org/10.1088/0004-637X/740/1/18

Oishi, J. S., Mac Low, M.-M., & Menou, K. (2007). Turbulent torques on protoplanets in a dead zone. *670*, 805–819. https://doi.org/10.1086/521781

Qian, C., Wang, C., Liu, J., Brand enburg, A., Haugen, N. E. L., & Liberman, M. A. (2020). Convergence properties of detonation simulations. *Geophys. Astrophys. Fluid Dynam.*, *114*, 58–76. https://doi.org/10.1080/03091929.2019.1668382

Rheinhardt, M., & Brandenburg, A. (2010). Test-field method for mean-field coefficients with MHD background. *520*, A28. https://doi.org/10.1051/0004-6361/201014700

Roper Pol, A., Brandenburg, A., Kahniashvili, T., Kosowsky, A., & Mandal, S. (2020). The timestep constraint in solving the gravitational wave equations sourced by hydromagnetic turbulence. *Geophys. Astrophys. Fluid Dynam.*, *114*, 130–161. https://doi.org/10.1080/03091929.2019.1653460

Schober, J., Rogachevskii, I., Brandenburg, A., Boyarsky, A., Fröhlich, J., Ruchayskiy, O., & Kleeorin, N. (2018). Laminar and turbulent dynamos in chiral magnetohydrodynamics. II. simulations. *858*, 124. https://doi.org/10.3847/1538-4357/aaba75

Schreiber, A., & Klahr, H. (2018). Azimuthal and vertical streaming instability at high dust-to-gas ratios and on the scales of planetesimal formation. *861*, 47. https://doi.org/10.3847/1538-4357/aac3d4

Warnecke, J., Käpylä, P. J., Käpylä, M. J., & Brandenburg, A. (2014). On the cause of solar-like equatorward migration in global convective dynamo simulations. *796*, L12. https://doi.org/10.1088/2041-8205/796/1/L12

Warnecke, J., Rheinhardt, M., Tuomisto, S., Käpylä, P. J., Käpylä, M. J., & Brandenburg, A. (2018). Turbulent transport coefficients in spherical wedge dynamo simulations of solar-like stars. *609*, A51. https://doi.org/10.1051/0004-6361/201628136

Yang, C.-C., & Johansen, A. (2016). Integration of particle-gas systems with stiff mutual drag interaction. *224*, 39. https://doi.org/10.3847/0067-0049/224/2/39

Yang, C.-C., & Krumholz, M. (2012). Thermal-instability-driven turbulent mixing in galactic disks. I. Effective mixing of metals. *758*, 48. https://doi.org/10.1088/0004-637X/758/1/48

Yang, C.-C., Mac Low, M.-M., & Johansen, A. (2018). Diffusion and concentration of solids in the dead zone of a protoplanetary disk. *868*, 27. https://doi.org/10.3847/1538-4357/aae7d4

Youdin, A., & Johansen, A. (2007). Protoplanetary Disk Turbulence Driven by the Streaming Instability: Linear Evolution and Numerical Methods. *662*, 613–626. https://doi.org/10.1086/516729

Zhang, H., Luo, K., Haugen, N. E. L., Mao, C., & Fan, J. (2020). Drag force for a burning particle. *Comb. Flame*, *217*, 188–199. https://doi.org/10.1016/j.combustflame.2020.02.016