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

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

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, Brandenburg, Haugen, & Svensson, 2017) and engineering applications in combustion (Babkovskaia, Haugen, & Brandenburg, 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, Brauer, Dullemond, Klahr, & Henning, 2008; Li et al., 2017),
- Radiative transfer (Barekat & Brandenburg, 2014; A. Brandenburg & Das, 2020; Heinemann, Dobler, Nordlund, & Brandenburg, 2006),
- Chiral magnetic effect in relativistic plasmas (Schober et al., 2018),
- Primordial gravitational waves (Roper Pol, Brandenburg, Kahniashvili, Kosowsky, & Mandal, 2020),
- Modeling homochirality at the origin of life (Brandenburg, 2019; Brandenburg & Multamäki, 2004),
- Modeling of patterned photochemical systems (Emond et al., 2012),
- Gaseous combustion and detonation (Babkovskaia et al., 2011; Krüger, Haugen, & Løvås, 2017; Zhang, Luo, Haugen, Mao, & Fan, 2020),
- Burning particles, resolved or unresolved (Qian et al., 2020),
- Flows around immersed solid objects (Aarnes, Haugen, & Andersson, 2019; Aarnes et al., 2020; 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, Brandenburg, Kleeorin, Mitra, & Rogachevskii, 2013; Kemel, Brandenburg, Kleeorin, Mitra, & Rogachevskii, 2013),
- Spherical shell dynamos and convection (Käpylä, Gent, Olspert, Käpylä, & Brandenburg, 2020; Mitra, Tavakol, Brandenburg, & Moss, 2009),
- Boris correction for coronal physics (Chatterjee, 2020),
- Thermal instability and mixing (Yang & Krumholz, 2012),
- Implicit solver for temperature (Gastine & Dintrans, 2008),
- Dust-gas dynamics with mutual drag interaction (Yang & Johansen, 2016; Youdin & Johansen, 2007).

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, 34 have done more than 34

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, 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. 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 (Haugen & Kragset, 2010),
- Particle clustering in supersonic and subsonic turbulence (Karchniwy, Klimanek, & Haugen, 2019; Mattsson, Bhatnagar, Gent, & Villarroel, 2019),
- Cloud microphysics (Li et al., 2017),
- Planet and planetesimal formation (Johansen et al., 2007; Lyra, Johansen, Zsom, Klahr, & Piskunov, 2009; Oishi, Mac Low, & Menou, 2007),
- Global simulations of debris disks (Lyra & Kuchner, 2013),
- Stratified shearing box simulations, also with dust (Oishi & Mac Low, 2011; Schreiber & Klahr, 2018; Yang, Mac Low, & Johansen, 2018),
- Supernova-driven turbulence (Gent, Shukurov, Fletcher, Sarson, & Mantere, 2013),
- Solar dynamo and sunspots (Brandenburg, 2005; Heinemann, Nordlund, Scharmer, & Spruit, 2007),
- Solar corona above active regions (Bingert & Peter, 2011; Bourdin, Bingert, & Peter, 2013; Chatterjee, Hansteen, & Carlsson, 2016),

- Fully convective star in a box (Dobler, Stix, & Brandenburg, 2006),
- Dynamo wave in spherical shell convection (Käpylä, Mantere, & Brandenburg, 2012; Warnecke, Käpylä, Käpylä, & Brandenburg, 2014),
- Convection with Kramers opacity law (Käpylä, 2019; Käpylä et al., 2020, 2017),
- MHD turbulence and cascades (Haugen, Brandenburg, & Dobler, 2004),
- Turbulent diffusivity quenching with test fields (Brandenburg, Rädler, Rheinhardt, & Käpylä, 2008; Karak, Rheinhardt, Brandenburg, Käpylä, & Käpylä, 2014).

Acknowledgements

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. doi: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. doi: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. doi:10.1016/j.jcp.2010.08.028

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

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

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

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

Brandenburg, A. (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. doi:10.1007/s11084-019-09579-4

Brandenburg, A. (2020). Scientific usage of the Pencil Code. Retrieved July 16, 2020, from 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. doi: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. doi:10.1080/03091929.2019.1676894

Brandenburg, A., & Dobler, W. (2010). Pencil Code: Finite-difference Code for Compressible Hydrodynamic Flows. doi: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. doi: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. doi: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. doi:10.1080/03091929.2019.1672676

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

Dobler, W., Stix, M., & Brandenburg, A. (2006). Magnetic field generation in fully convective rotating spheres, *638*, 336–347. doi: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. doi: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. doi: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. doi:10.1093/mnras/stt560

Haugen, N. E., Brandenburg, A., & Dobler, W. (2004). Simulations of nonhelical hydromagnetic turbulence, *70*, 016308. doi: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. doi:10.1017/S0022112010002946

Heinemann, T., Dobler, W., Nordlund, Å., & Brandenburg, A. (2006). Radiative transfer in decomposed domains, *448*, 731–737. doi: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. doi: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. doi: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. doi: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. doi: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. doi: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. doi:10.1017/jfm.2019.493

Käpylä, P. J. (2019). Overshooting in simulations of compressible convection, *631*, A122. doi: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. doi: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. doi:10.1088/2041-8205/755/1/L22

Käpylä, P. J., Rheinhardt, M., Brandenburg, A., Arlt, R., Käpylä, M. J., Lagg, A., Olspert, N., et al. (2017). Extended subadiabatic layer in simulations of overshooting convection, *845*, L23. doi: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. doi:10.1007/s11207-012-0031-8

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. doi: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. doi: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. doi: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. doi: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. doi: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. doi: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. doi: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. doi: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. doi:10.1080/03091929.2019.1668382

Rheinhardt, M., & Brandenburg, A. (2010). Test-field method for mean-field coefficients with MHD background, *520*, A28. doi: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. doi: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. doi: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. doi: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. doi: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. doi:10.1051/0004-6361/201628136

Yang, C.-C., & Johansen, A. (2016). Integration of particle-gas systems with stiff mutual drag interaction, *224*, 39. doi: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. doi: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. doi: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. doi: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. doi:10.1016/j.combustflame.2020.02.016