

Coral: a parallel spectral solver for fluid dynamics and partial differential equations

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Summary

Coral is a fast, flexible, and efficient time-stepper for solving a large class of partial differential equations, at the core of which are the Navier-Stokes equations that govern fluid motions. Written in Fortran and employing the MPI standard for parallelization, the scalability of Coral allows the code to leverage the resources of high-performance computing infrastructures (up to hundreds of thousands of core, see Li & Laizet (2010)), while running efficiently on laptops and workstations. Equations are entered by the user in the form of a plain text file following a simple and legible syntax. No coding proficiency in Fortran is required. This flexibility makes Coral suitable for both students and researchers with no coding experience.

Statement of need

Natural and industrial flows exist in numerous different flavours, including homogeneous incompressible flows, shear flow, stably or unstably stratified flows, rotating flows, and flows of an electrically conducting fluid. These flows, however, have in common that they can be modelled by sets of (quadratic) advection-diffusion equations for the velocity, and possibly for the density, the temperature, the salinity, the magnetic field, etc. Hard-coding the sets of equations corresponding to each of these flow configurations is complex, time-consuming, and error-prone. These difficulties impede the development of new models. While Coral was initially motivated by the study of Convection in Rapidly rotating Layers, its scope has broadened and now encompasses solving homogeneous guadratic partial differential equations in a plane-layer geometry, i.e., a 3D domain with periodic boundary conditions along the two horizontal directions x and y. Internally, Coral expands the variables along Fourier basis (horizontal directions) and Chebyshev polynomials (vertical direction). Transforms from physical to spectral space and domain decomposition are handled by the 2decomp&fft library (Li &Laizet, 2010). The quasi-inverse technique permits employing an arbitrarily large numbers of Chebyshev polynomials, resulting in the ability to resolve thin boundary layers characteristic of turbulent flows without suffering from loss of accuracy. Early versions of Coral have been used for studies concerning the turbulent motion of convective flows in presence of internal heat sources and sinks (Miquel et al., 2019, 2020).

Validation and examples

Coral has been validated on a variety of test cases (gathered in etc/benchmarks) found in the literature: Rayleigh-Bénard convection (Chandrasekhar, 1961), rotating convection (Julien et al., 1996), and convective dynamos (Cooper et al., 2020; Stellmach & Hansen, 2004). Those

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Software

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accuracy benchmarks, bound to grow in number, also constitute a library of examples for defining PDEs in Coral.

State of the field

Among the existing flexible spectral solvers for marching in time PDEs in Cartesian geometries, alternatives to Coral include Dedalus (Burns et al., 2020), spectralDNS (Mortensen, 2018), FluidDyn (Augier et al., 2019), and FluidSim (Mohanan et al., 2019). For more complex geometries, options include nek5000 (Fisher, n.d.), Nektar++ (Moxey et al., 2020), Freefem++ (Hecht, 2012), and Fenics (Alnæs et al., 2015).

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References

- Alnæs, M. S., Blechta, J., Hake, J., Johansson, A., Kehlet, B., Logg, A., Richardson, C., Ring, J., Rognes, M. E., & Wells, G. N. (2015). The FEniCS project version 1.5. Archive of Numerical Software, 3(100).
- Augier, P., Mohanan, A. V., & Bonamy, C. (2019). FluidDyn: A Python open-source framework for research and teaching in fluid dynamics by simulations, experiments and data processing. *Journal of Open Research Software*, 7. https://doi.org/10.5334/jors.237
- Burns, K. J., Vasil, G. M., Oishi, J. S., Lecoanet, D., & Brown, B. P. (2020). Dedalus: A flexible framework for numerical simulations with spectral methods. *Phys. Rev. Research*, 2, 023068. https://doi.org/10.1103/PhysRevResearch.2.023068
- Chandrasekhar, S. (1961). *Hydrodynamic and hydromagnetic stability*. Clarendon Press: Oxford University Press.
- Cooper, R. G., Bushby, P. J., & Guervilly, C. (2020). Subcritical dynamos in rapidly rotating planar convection. *Phys. Rev. Fluids*, 5, 113702. https://doi.org/10.1103/ PhysRevFluids.5.113702
- Fisher, L., P. F. (n.d.). http://nek5000.mcs.anl.gov
- Hecht, F. (2012). New development in FreeFem++. J. Numer. Math., 20(3-4), 251–265. https://doi.org/10.1515/jnum-2012-0013
- Julien, K., Legg, S., McWilliams, J., & Werne, J. (1996). Rapidly rotating turbulent Rayleigh-Bénard convection. J. Fluid Mech., 322, 243–273. https://doi.org/10.1017/ S0022112096002789
- Li, N., & Laizet, S. (2010). 2DECOMP&FFT a highly scalable 2D decomposition library and FFT interface. In *Cray user group 2010 conference*. Edinburgh. http://www.2decomp. org/pdf/17B-CUG2010-paper-Ning_Li.pdf



- Miquel, B., Bouillaut, V., Aumaître, S., & Gallet, B. (2020). On the role of the Prandtl number in convection driven by heat sources and sinks. J. Fluid Mech., 900, R1. https: //doi.org/10.1017/jfm.2020.485
- Miquel, B., Lepot, S., Bouillaut, V., & Gallet, B. (2019). Convection driven by internal heat sources and sinks: Heat transport beyond the mixing-length or "ultimate" scaling regime. *Phys. Rev. Fluids*, 4, 121501. https://doi.org/10.1103/physrevfluids.4.121501
- Mohanan, A. V., Bonamy, C., Linares, M. C., & Augier, P. (2019). FluidSim: Modular, object-oriented Python package for high-performance CFD simulations. *Journal of Open Research Software*, 7. https://doi.org/10.5334/jors.239
- Mortensen, M. (2018). Shenfun: High performance spectral Galerkin computing platform. *Journal of Open Source Software*, 3(31), 1071. https://doi.org/10.21105/joss.01071
- Moxey, D., Cantwell, C. D., Bao, Y., Cassinelli, A., Castiglioni, G., Chun, S., Juda, E., Kazemi, E., Lackhove, K., Marcon, J., Mengaldo, G., Serson, D., Turner, M., Xu, H., Peiró, J., Kirby, R. M., & Sherwin, S. J. (2020). Nektar++: Enhancing the capability and application of high-fidelity spectral/hp element methods. *Computer Physics Communications*, 249, 107110. https://doi.org/10.1016/j.cpc.2019.107110
- Stellmach, S., & Hansen, U. (2004). Cartesian convection driven dynamos at low Ekman number. Phys. Rev. E, 70, 056312. https://doi.org/10.1103/PhysRevE.70.056312