Software Impacts 1 (2019) 100002

Contents lists available at ScienceDirect

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Original software publication

Eulerian–Lagrangian fluid dynamics platform: The `ch4-project`

Enrico Calzavarini

Unité de Mécanique de Lille, EA 7512 (UML), Univ. Lille, F-59000 Lille, France

ARTICLE INFO

Keywords:
Computational fluid dynamics
Turbulence
Thermal convection
Particle transport

ABSTRACT

`Ch4-project` is a developing computational fluid dynamics code that is used for the investigation of a range of different turbulent flows – periodic or bounded, thermally driven, with phase change interfaces – and a variety of Lagrangian phenomena, such as particles' transport, mixing and clustering. After an introduction on the genesis of this project and its position on the wide landscape of computational fluid dynamics, its current structure and features are briefly presented. An overview of its achievements on topics as varied as global scaling in non-ideal high-Rayleigh number convection, acceleration statistics of bubbles in developed turbulence, time-series analysis from propelled probes in a fluid environment along with ongoing studies are provided.

Code metadata

Current code version	Not used
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2019-1
Legal Code License	GNU GPLv3
Code versioning system used	git
Software code languages, tools, and services used	C, python
Compilation requirements, operating environments & dependencies	mpi, hdf5 libraries
If available Link to developer documentation/manual	https://github.com/ecalzavarini/ch4-project/wiki
Support email for questions	enrico.calzavarini@polytech-lille.fr

1. In silico fluid dynamics

Fluid dynamics research deals with phenomena for which the dynamical evolution equations are often well known while their particular solutions are not. This is due to either the huge number of degrees of freedom characterizing flow phenomena and/or the inherent non-linearities of their dynamics, which cause also sensitivity to initial conditions, chaotic and turbulent behaviours [1]. The discipline has been shaken-up by the advent of computers, which allowed for the first time to compute approximate solutions of the known dynamical equations by means of different types of discretization techniques [2]. Nowadays the numerical simulations in fluid dynamics often (but not always) achieve the prominence of *numerical experiments*, a status that puts them on the same epistemological level of real world experiments.

Many Computational Fluid Dynamics (CFD) [3] codes and software are currently available for the study of fluid related phenomena, ranging from commercial ones which are widely used in the industry, to community or open codes. Although a standardization in CFD tools is also going on in the academia, this community relies on less standardized tools. The reasons for this are inherent to scientific research: on one hand the optimization and development of new method is an active area of study, on the other hand scholars require to have full control on the employed algorithms, a matter that is tightly related to the reproducibility of research (see e.g. [4] for a discussion).

The code named `ch4-project` belongs to the class of computer programs tailored for fluid dynamics research in academia. It has been developed since late 2012 as a platform to study the phenomenology of turbulent flow both from the Eulerian and Lagrangian perspectives, and having as users mostly graduate students or junior researchers. A CFD research code of such type needs to have a key feature: it must have a design that is sufficiently flexible to accommodate for changes which were not necessarily planned at the beginning of the code development. A dream for principal investigators in this field is to not have to deal with different (and soon mutually incompatible) code versions for each project and junior researcher in his/her own group. In this respect an

E-mail address: enrico.calzavarini@polytech-lille.fr.
URL: https://www.ecalzavarini.info.

https://doi.org/10.1016/j.simpa.2019.100002
Received 11 May 2019; Received in revised form 22 May 2019; Accepted 29 May 2019

object-oriented modular code structure would be the ideal one, but this makes the code less prone to modifications by the less experienced users. The choice made here is to rely on a systematic use of *C* language preprocessing directives and on a hierarchical naming convention in order to configure the desired simulation setting in a module-like fashion at compiling time. We adopt the Message Passing Interface (MPI) for parallelization tasks and the Hierarchical Data Format (HDF5) library for the handling of massively parallel input/output, both now standard in the CFD environment.

2. Code structure and features

The backbone of the Eulerian part of the code is a Lattice Boltzmann (LB) equations solver which is employed to simulate the weakly-compressible Navier–Stokes equation. The LB algorithm is based on the standard stream-and-collide implementation with single relaxation time collision operator on a uniform cartesian grid [5]. However, a finite volume formulation of the algorithm (allowing for grid-refinement [6]) and a two-relaxation-time collision operator [7] can be optionally activated. The default velocity lattice topologies are of 9 microscopic distributions (dubbed populations in the LB jargon) in two-dimensional systems, 19 in three-dimensional ones, but alternatives are supported. Additionally, the advection–diffusion dynamics of up to two scalar fields can be switched on. By default the first scalar is assumed to be a temperature field while the second is a passive-scalar concentration, but this setting can easily be modified. The scalar fields are also evolved through a LB algorithm, following the so called multi-population approach [7]. The most common type of boundary conditions, no-slip or free-slip for the velocity field and Dirichlet or Neumann for scalars, can be enabled on all plane boundaries along cartesian directions. Fluid forcing and source term for scalars allow for the simulation of turbulence in statistically homogeneous and isotropic conditions, for laminar or turbulent channel flow and for thermally driven flows in the Oberbeck–Boussinesq approximation. An enthalpy based algorithm for the simulation of melting or solidification phase-change dynamics is also implemented [8]. Such features can be enabled at compiling time by the definition of preprocessor flags.

The Lagrangian part of the code evolves point-like particles with dynamics described by ordinary differential equations. Particles are coupled in a one-way fashion to the flow field, meaning that they do not have a feedback on the velocity, fluid density or scalar concentration fields. The simplest dynamical equation is the one of a Lagrangian fluid tracer, which is implemented by means of linear interpolations in two-/three-dimensions of the fluid velocity field at particle position and by a second-order Adams–Bashforth time-stepping. The inertial particle dynamic is accounted for by means of an implementation of the Maxey–Riley–Gatignol equation [9,10]. More specifically we account for the Stokes drag force with/without Shiller–Naumann correction [11], added mass force, buoyancy, and the Auton's expression of lift force [12]. The history force and Faxén terms are not presently implemented. Several internal degrees of freedom can be added to the particles, for instance the one accounting for their spatial orientation, whose evolution is simulated by the Jeffery equation [13], or others related to the scalar values at the particle position. Additionally one can activate the so-called propelling terms on particles in order to simulate motile particles such as the ones used for elementary modelling of micro-organisms [14,15]. The Lagrangian part of the code has a sufficiently modular structure, comprising (i) field interpolations, (ii) evaluation of hydrodynamic forces (iii) temporal integration, to allow for future changes and additions in the particles equation of motion. One remarkable feature of the Lagrangian algorithm is the capability to simulate simultaneously different types of particles. This allows to explore large particle parameter spaces in a single simulation experiment (see e.g. [16]).

The `ch4-project` code produces outputs of two types: (i) runtime computed averaged quantities (ii) fields and particles raw data. The first set, in ASCII format, is useful for monitoring and diagnosing possible problems as the simulation proceeds. They include both instantaneous and cumulative in time spatial averages at prescribed rates, and spatially global (over all the simulation domain) and local averages along the cartesian directions. The second set, can be saved on disk at an independent adjustable rate. They are in *HDF5* format which can be interpreted and visualized with the presently most common scientific software. Fig. 1 displays a gallery of visualizations obtained from the output data for a variety of simulated systems. Additionally, a set of post-processing routines in *Python* language is provided. These script tools perform standard tasks such as changing the spatial resolution of a flow configuration, extracting single particle trajectories from the database, or performing custom statistical analysis in turbulence (temporal correlations, structure functions, pair-distribution-functions, etc.).

Finally, on the parallelization strategy adopted: the `ch4-project` employs a decomposition of the spatial simulation domain on a regular two-/three-dimensional cartesian grid. The LB algorithm naturally allows for a domain decomposition on a grid (rather than on slabs or pencils) because differently from the majority of others CFD methods it involves only exchanges of data located at the boundaries of the subdomains and does not need long-range communications. The computation of the evolution of each particle is also performed with the same domain decomposition. However, an all-to-all MPI communication is present in the code to share the particles which are leaving/entering the subdomains, between parallel processes at each time-step. This is less efficient than exchanging particles just across the boundaries of neighbouring subdomains. This choice allows to make particles disappear/die at a boundary and being regenerated in any other locations of the domain (a feature that can be useful in applications). The computational overhead of the Lagrangian part of the code grows approximately linearly with the number of particles and depends sensibly on the number of field interpolations and operations entailed by the particles evolution equation.

3. Impact overview

The `ch4-project` code was initially designed for the investigation of turbulent thermal convection. Its first application was a simulation of the Rayleigh–Bénard system in two and three dimensions with lateral periodic boundaries. This study dealt with a comparison in terms of accuracy and computational costs of the standard stream-and-collide LB scheme with an original variant based on a finite volume discretization, which allowed to accommodate cartesian grids with resolution refinement at the walls [6]. Despite the interest of the latter approach, it was shown that at comparable or even smaller computational cost the standard algorithm was less affected by numerical instabilities. However, this first LB finite volume scheme proof-of-concept in a developed turbulent flow setting has stimulated further improvements by other researchers [17].

The code was later employed in a collaborative project, involving both simulations and experiments, aimed at characterizing the variation of the global heat transfer across a Rayleigh–Bénard cubic cell with lateral no-slip adiabatic walls, under the effect of an imposed inclination angle. The study addressed the unexplored case of a highly viscous fluid (with respect to thermal diffusivity) and at the same time high turbulent flow state. Conditions which are of relevance e.g. in volcanic magma chambers (the Rayleigh and Prandtl numbers were respectively $\sim 10^9$, ~ 500). The numerical results matched well with experiments. They allowed to show the surprisingly little sensitivity of the global heat transfer to the drastic reduction of turbulent intensity which occurs for large inclination angles [18].

In the frame of a research project motivated by geophysical applications – the problem of ice melt pond growth in the Arctic – the `ch4-project` code was employed to study the dynamic of solid-to-liquid melting driven by turbulent thermal convection. In such a

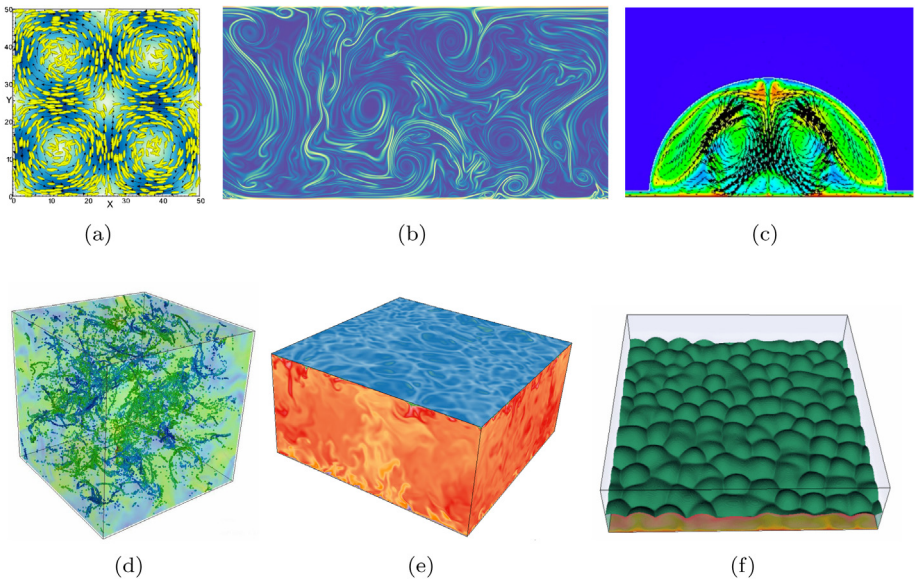

Fig. 1. A gallery of visualizations from different simulations in two (top row) and three (bottom row) dimensions: (a) anisotropic rod-like particles in a laminar steady cellular flow; (b) thermal energy dissipation rate in a turbulent two-dimensional Rayleigh–Bénard system at Rayleigh (Ra) number 10^9; (c) convective flow in a semicircular cavity undergoing melting phase-change; (d) instantaneous distribution of dissipative-scale bubbles in homogeneous and isotropic tri-periodic turbulent flow at Taylor–Reynolds number $O(100)$; (e) temperature field in the three-dimensional Rayleigh–Bénard system at $Ra = 10^{10}$ with wall-grid refinement; (f) solid–fluid interface in convective melting with $O(1)$ Stefan number.

condition the flow is non-stationary, of variable turbulent intensity and enclosed by an irregular end evolving bounding geometry. It was numerically demonstrated that despite the complexity of the flow the melt rate can still be well approximated by the heat-flux scaling laws developed for the standard Rayleigh–Bénard system [8].

The dispersion of bubbles and material spherical particles of small inertia in homogeneous and isotropic turbulence has been the focus of another collaborative research. In this case the trajectories of a large amount ($\sim 10^6$) of small inertial particles were tracked into a developed turbulent flow in a cubic three-periodic domain. The study focused on the measurements of the fluctuations of accelerations of bubbles and small material particles denser than the fluid. The simulations allowed to interpret earlier experimental measurements on the dispersion of sub-millimetric bubbles in a turbulent channel flow. The study characterized the statistical properties of acceleration and showed that even micro-bubbles/particles cannot be considered unbiased fluid tracer proxies [16].

Another work motivated by marine sciences application tackled the study of signals recorded by propelled probes that drift in and are advected by a developed turbulent flow. The goal was to understand which biases are introduced in the measurements of concentrations of scalar quantities (e.g. of biogeochemicals or pollutants) at increasing the probe propulsion speed. To this end a series of simulations of the advection and diffusion of a passive scalar field in a three-periodic turbulent box together with the tracking of point-like inertialess probes were performed. The study allowed to characterize the statistical features of mixed Lagrangian–Eulerian measurements and to understand the conditions for the recovery of the so-called frozen-flow state [19].

The code is currently used for the investigation of the dynamics of anisotropic particles in turbulent flows. Beside the widespread industrial and environmental applications related to the fluid advection of particles of irregular shape, this topic has been proven useful also in understanding the small scale properties of turbulent flows [20]. The particle mean rotation rate is in fact determined by the Lagrangian statistics of spatial fluid velocity gradient. This relatively recent line of research, which began in the context of idealized homogeneous and isotropic turbulence [21], needs to be extended to more realistic flow conditions. In this context, the `ch4-project` is a suitable tool and it is currently employed to explore the orientational evolution of anisotropic particles in thermally driven flows. A further ongoing project addresses the settling processes of tiny spherical crystals in thermal convective turbulence in the conditions which are relevant to the geophysical problem of fractional crystallization in planetary magma oceans [22].

In conclusion, the `ch4-project` is a free, well validated fluid dynamics numerical platform which has been proven effective in producing original research in the fields of turbulence, thermally driven flows and on the great variety of associated Lagrangian transport problems.

Declaration of competing interest

None declared.

Acknowledgements

This project has been supported by the Innocold consortium, Dunkerque, France; by the French National Agency for Research (ANR), grant (SEAS: ANR-13-JS09-0010); by Centre National de la Recherche Scientifique (CNRS) program Défi INFINITI 2018. I wish to acknowledge my former students K. Shrestha and B. Rabbanipour Esfahani who contributed to the development and testing of the code.

References

[1] T. Bohr, M.H. Jensen, G. Paladin, A. Vulpiani, Dynamical Systems Approach to Turbulence, second ed., Cambridge University Press, 2005.

[2] P. Lynch, The origins of computer weather prediction and climate modeling, J. Comput. Phys. 227 (7) (2008) 3431–3444, http://dx.doi.org/10.1016/j.jcp.2007.02.034.

[3] J.H. Ferziger, M. Peric, Computational Methods for Fluid Dynamics, third ed., Springer, 2001.

[4] O. Mesnard, L.A. Barba, Reproducible and replicable computational fluid dynamics: It's harder than you think, Comput. Sci. Eng. 19 (4) (2017) 44–55.

[5] S. Succi, The Lattice Boltzmann Equation: For Complex States of Flowing Matter, first ed., Oxford University Press, 2018.

[6] K. Shrestha, G. Mompean, E. Calzavarini, Finite-volume versus streaming-based lattice Boltzmann algorithm for fluid-dynamics simulations: A one-to-one accuracy and performance study, Phys. Rev. E 93 (2016) 023306, http://dx.doi.org/10.1103/PhysRevE.93.023306.

[7] T. Krüer, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva, E. Viggen, The Lattice Boltzmann Method - Principles and Practice, first ed., Springer, 2016.

[8] B. Rabbanipour Esfahani, S.C. Hirata, S. Berti, E. Calzavarini, Basal melting driven by turbulent thermal convection, Phys. Rev. Fluids 3 (2018) 053501, http://dx.doi.org/10.1103/PhysRevFluids.3.053501.

[9] M.R. Maxey, J.J. Riley, Equation of motion for a small rigid sphere in a nonuniform flow, Phys. Fluids 26 (4) (1983) 883–889, http://dx.doi.org/10.1063/1.864230.

[10] R. Gatignol, The Faxén formulae for a rigid particle in an unsteady non-uniform Stokes flow, J. Méc. Théor. Appl. 1 (2) (1983) 143–160.

[11] E. Calzavarini, R. Volk, E. Leveque, J.-F. Pinton, F. Toschi, Impact of trailing wake drag on the statistical properties and dynamics of finite-sized particle in turbulence, Physica D 241 (3) (2012) 237–244 (Special Issue on Small Scale Turbulence), http://dx.doi.org/10.1016/j.physd.2011.06.004.

[12] T. Auton, The lift force on a spherical body in a rotational flow, J. Fluid Mech. 183 (1987) 199–218, http://dx.doi.org/10.1017/S002211208700260X.

[13] G.B. Jeffery, The motion of ellipsoidal particles immersed in a viscous fluid, Proc. R. Soc. A 102 (715) (1922) 161–179, http://dx.doi.org/10.1098/rspa.1922.0078.

[14] T.J. Pedley, J.O. Kessler, Hydrodynamic phenomena in suspensions of swimming microorganisms, Annu. Rev. Fluid Mech. 24 (1) (1992) 313–358, http://dx.doi.org/10.1146/annurev.fl.24.010192.001525.

[15] H. Ardeshiri, I. Benkeddad, F.G. Schmitt, S. Souissi, F. Toschi, E. Calzavarini, Lagrangian model of copepod dynamics: Clustering by escape jumps in turbulence, Phys. Rev. E 93 (2016) 043117, http://dx.doi.org/10.1103/PhysRevE.93.043117.

[16] V. Mathai, E. Calzavarini, J. Brons, C. Sun, D. Lohse, Microbubbles and microparticles are not faithful tracers of turbulent acceleration, Phys. Rev. Lett. 117 (2016) 024501, http://dx.doi.org/10.1103/PhysRevLett.117.024501.

[17] J.T. Horstmann, T.L. Garrec, D.-C. Mincu, E. Lévêque, Hybrid simulation combining two space–time discretization of the discrete-velocity Boltzmann equation, J. Comput. Phys. 349 (2017) 399–414, http://dx.doi.org/10.1016/j.jcp.2017.08.029.

[18] L. Jiang, C. Sun, E. Calzavarini, Robustness of heat transfer in confined inclined convection at high Prandtl number, Phys. Rev. E 99 (2019) 013108, http://dx.doi.org/10.1103/PhysRevE.99.013108.

[19] E. Calzavarini, Y.X. Huang, F.G. Schmitt, L.P. Wang, Propelled microprobes in turbulence, Phys. Rev. Fluids 3 (2018) 054604, http://dx.doi.org/10.1103/PhysRevFluids.3.054604.

[20] G.A. Voth, A. Soldati, Anisotropic particles in turbulence, Ann. Rev. Fluid Mech. 49 (1) (2017) 249–276, http://dx.doi.org/10.1146/annurev-fluid-010816-060135.

[21] S. Parsa, E. Calzavarini, F. Toschi, G.A. Voth, Rotation rate of rods in turbulent fluid flow, Phys. Rev. Lett. 109 (2012) 134501, http://dx.doi.org/10.1103/PhysRevLett.109.134501.

[22] V. Patocka, E. Calzavarini, N. Tosi, Settling of crystals with variable density and size in turbulent convection, Geophys. Res. Abst. 21 (2019) EGU2019–5752, https://meetingorganizer.copernicus.org/EGU2019/EGU2019-5752.pdf.