Computer Physics Communications 320 (2026) 109956

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

New Version Announcement

MHIT36: Extension to wall-bounded turbulence and scalar transport equation

Alessio Roccon [a,b]

[a] Polytechnic Department of Engineering and Architecture, University of Udine, Udine, 33100, Italy
[b] Institute of Fluid Mechanics and Heat Transfer, TU-Wien, Vienna, 1060, Austria

ARTICLE INFO

The review of this paper was arranged by Prof. J Ballantyne

Keywords:
Phase-field method
Direct numerical simulation
Finite difference
GPU-computing
Domain decomposition

ABSTRACT

We present an extended version of MHIT36 [1], a GPU-tailored solver for interface-resolved simulations of multiphase turbulence. The framework couples direct numerical simulation (DNS) of the Navier–Stokes equations, which describe the flow field, with a phase-field method to capture interfacial phenomena. In addition, the transport equation for a scalar can also be solved. The governing equations are discretized using a second-order finite difference scheme. The Navier–Stokes equations are time advanced with an explicit fractional-step method, and the resulting pressure Poisson equation is solved using a FFT-based method. The accurate conservative diffuse interface (ACDI) formulation is used to describe the transport of the phase-field variable. Simulations can be performed in two configurations: a triply-periodic cubic domain or a rectangular domain of arbitrary dimensions bounded by two walls. From a computational standpoint, MHIT36 employs a two-dimensional domain decomposition to distribute the workload across MPI tasks. The cuDecomp library [2] is used to perform pencil transpositions and halo updates, while the cuFFT library and OpenACC directives are leveraged to offload the remaining computational kernels to the GPU. MHIT36 is developed using the managed memory feature and it provides a baseline code that is easy to further extend and modify. MHIT36 is released open source under the MIT license.

NEW VERSION PROGRAM SUMMARY

Program Title: MHIT36
CPC Library link to program files: https://doi.org/10.17632/yb2dt99swr.2
Developer's repository link: https://github.com/MultiphaseFlowLab/MHIT36
Licensing provisions: MIT
Programming language: Modern Fortran
Supplementary material: Validation of the new solver for the turbulent channel flow configuration.
Journal reference of previous version: A. Roccon, L. Enzenberger, D. Zaza and A. Soldati, MHIT36: A Phase-Field Code for GPU Simulations of Multiphase Homogeneous Isotropic Turbulence, Comput. Phys. Commun. 316 (2025) 109804, DOI: https://doi.org/10.1016/j.cpc.2025.109804
Does the new version supersede the previous version?: Yes
Reasons for the new version: The original MHIT36 program was developed to solve the governing equations within a triple-periodic domain using a uniform cubic grid along all three periodic directions. The code has now been extended to handle rectangular domains of arbitrary dimensions bounded by fixed or moving walls, enabling the simulation of wall-bounded flows. In this configuration, the grid spacing along the wall-normal direction can be stretched/clustered using an arbitrary distribution function. In addition, MHIT36 now can also solve the transport equation for a passive scalar, enabling the investigation of heat and mass transfer phenomena. Finally, the performance on GPUs has also been optimized to achieve improved computational efficiency.

Summary of revisions:

- To extend the code to wall-bounded flows, no-slip boundary conditions can be applied at the two walls using the halo nodes. The cuDecomp configuration is also updated accordingly. Additionally, the solution method

E-mail address: alessio.roccon@uniud.it

https://doi.org/10.1016/j.cpc.2025.109956
Received 10 November 2025; Accepted 13 November 2025
Available online 25 November 2025

for the Poisson pressure equation is adjusted to account for the inhomogeneous boundary conditions in the wall-normal direction and grid stretching. The Poisson equation is discretized using Fourier transforms in the periodic directions (streamwise and spanwise), while second-order finite differences are used in the wall-normal direction. The resulting system of tridiagonal linear equations is efficiently solved using a Tridiagonal Matrix Algorithm (TDMA).

- To simulate heat and mass transfer phenomena, the transport equation for a passive (or active) scalar is implemented. The feedback on the momentum equation can be modified, and the actual implementation mimics buoyancy effects along the wall-normal direction.
- The validation data of the present version is available in the Supplementary material. The following configurations have been tested: i) single-phase turbulent channel flow ($Re_\tau = 590$) [3]; ii) mixing of a passive scalar in a turbulent channel flow ($Re_\tau = 550$ and $Pr = 1$) [4]; iii) drop-laden turbulent channel flow ($Re_\tau = 180$ and $We = 6.0$) iv) Rayleigh-Bénard convection (from $Ra = 10^6$ up to $Ra = 10^{10}$ and $Pr = 4.3$) [5].
- The performance on GPUs has been significantly improved, achieving a speed-up of approximately 5× compared to the original version. The default configuration of the cuDecomp library now features full autotuning: during initialization, the library automatically selects the optimal domain decomposition and communication backend to ensure the best performance.

Nature of problem: Solving the three-dimensional incompressible Navier–Stokes equations in a triply-periodic box or a channel flow configuration. A phase-field method based on the accurate conservative diffuse interface (ACDI) formulation is used to describe the shape and topological changes of the interface. In addition, a transport equation for a passive (or active) scalar is also implemented.
Solution method: The system of governing equations is advanced in time using an explicit strategy while the governing equations are discretized in space using a second-order finite difference approach. A fractional step is used to solve the Navier–Stokes equations and an FFT-based method is used to solve the resulting Poisson equation for pressure. The parallelization relies on a 2D domain decomposition strategy and all intra- and inter-node communications are handled by the cuDecomp library. The cuFFT library and OpenACC directives are used to entirely offload code execution to GPUs.

CRediT authorship contribution statement

Alessio Roccon: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Validation, Visualization, Writing – original draft.

Data availability

The data presented in this study are openly available in the following Figshare repository: doi.org/10.6084/m9.figshare.28082252.

Declaration of competing interest

The authors declare that they have no conflict of interest.

Acknowledgements

The authors gratefully acknowledge the Austrian Science Fund (FWF) [Modeling And sImulation of emulsiOns (MAIO), 10.55776/PAT9292123], and the Italian Ministry for Research [The fluid dynamics of interfaces: mesoscale models for bubbles, droplets, and membranes and their coupling to large scale flows, PRIN Project No. 2022R9B2MW_PE8]. We acknowledge CINECA for the availability of high-performance computing resources and support (projects HP10BFFQIZ). This work was completed in part at the CINECA Open Hackathon, part of the Open Hackathons program and we would like to thank Matt Bettencourt, Josh Romero, Laura Bellentani and Alessio Piccolo.

Supplementary material

Supplementary material associated with this article can be found in the online version at 10.1016/j.cpc.2025.109956.

References

[1] A. Roccon, L. Enzenberger, D. Zaza, A. Soldati, MHIT36: a phase-field code for GPU simulations of multiphase homogeneous isotropic turbulence, Comput. Phys. Commun 316 (2025) 109804. https://doi.org/10.1016/j.cpc.2025.109804
[2] J. Romero, P. Costa, M. Fatica, Distributed-memory simulations of turbulent flows on modern GPU systems using an adaptive pencil decomposition library, in: Proceedings of the Platform for Advanced Scientific Computing Conference, 2022, pp. 1–11. https://doi.org/10.1145/3539781.3539797
[3] P. Costa, E. Phillips, L. Brandt, M. Fatica, GPU acceleration of CaNS for massively-parallel direct numerical simulations of canonical fluid flows, Comput. Math. Appl. 81 (2021) 502–511. https://doi.org/10.1016/j.camwa.2020.01.002
[4] S. Pirozzoli, D. Modesti, Direct numerical simulation of one-sided forced thermal convection in plane channels, J. Fluid Mech. 957 (2023) 31. https://doi.org/10.1017/jfm.2023.104
[5] C. Xu, C. Zhang, L. Brandt, J. Song, O. Shishkina, Direct numerical simulations of turbulent Rayleigh–Bénard convection with polymer additives, J. Fluid Mech. 1014, A22. https://doi.org/10.1017/jfm.2025.10286