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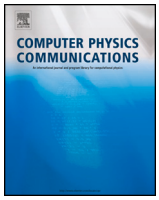

New Version Announcement

DeepFlame 2.0: A new version for fully GPU-native machine learning accelerated reacting flow simulations under low-Mach conditions

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ABSTRACT

This paper presents *DeepFlame* v2.0, a significant computational framework upgrade designed for high-performance combustion simulations on GPU-based heterogeneous architectures. The updated version implements a comprehensive CUDA-accelerated architecture incorporating fundamental combustion modelling components, including: implicit/explicit finite volume method (FVM) discretisation schemes, chemical kinetics integrators, thermophysical property models, and subgrid-scale closures for both fluid dynamics and combustion processes. The redesigned code supports diverse boundary conditions and discretisation schemes for broad applicability across combustion configurations. Key performance optimisations integrate advanced CUDA features including data coalescing techniques, CUDA Graphs for kernel scheduling, and NCCL-based multi-GPU communication. Validation studies employing the fully-implicit low-Mach solver demonstrate two-order-of-magnitude acceleration compared to conventional CPU implementations across canonical test cases, while maintaining numerical accuracy.

NEW VERSION PROGRAM SUMMARY

Program Title: DeepFlame V2.0
CPC Library link to program files: https://doi.org/10.17632/3pg9xmypp3.2
Developer's repository link: https://github.com/deepmodeling/deepflame-dev
Licensing provisions: GPLv3
Programming language: C++, CUDA
Journal reference of previous version: Comput. Phys. Commun. 291 (2023) 108842
Does the new version supersede the previous version?: Yes
Reasons for the new version: The previous version of *DeepFlame* integrated OpenFOAM, Cantera, and PyTorch libraries, enabling the utilisation of CVODE solver, detailed thermo-transport models and deep learning algorithms in simulating reactive flow [1]. Despite these advancements, the software did not support GPU-like heterogeneous accelerators, which have demonstrated game-changing impacts in both machine learning and computational fluid dynamics fields. Consequently, the primary goal for the new version is to achieve fully GPU porting of *DeepFlame* to further enhance its performance.
Summary of revisions: In this new version, we have developed a plug-in library to enable the GPU porting of *DeepFlame* [2,3]. This library integrates all GPU-related operations, primarily including the implicit/explicit finite volume method, chemical source integrator, and detailed thermo-transport models. Common boundary conditions and numerical schemes are implemented within this library, with unimplemented features easily addable through carefully designed APIs. The library also includes turbulence and combustion models to support large eddy simulations and Reynolds-averaged Navier–Stoke approach. Furthermore, this library can be easily adopted by other OpenFOAM-based CFD platforms because its open-source nature.
Nature of problem: Conducting reacting flow simulations carrying detailed transport and chemistry remains highly resource-intensive within current combustion CFD codes. This computational burden primarily arises from: (i) solving high-dimensional Navier–Stokes type partial differential equations (PDEs) for conservative variables; (ii) integrat-

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ing stiff ordinary differential equations (ODEs) for the chemical source terms; and (iii) calculating high-order polynomials for thermophysical properties. Each of these computational patterns contributes to the overall computational cost and has distinct characteristics that require specific acceleration methods.

Solution method: DeepFlame aims to leverage artificial intelligence (AI) and high-performance computing (HPC) technologies to accelerate reactive CFD simulations. Building on the deep learning-empowered simulation methods from the previous version, the current iteration has ported and optimised all computational tasks for high-performance GPU hardware. This enhancement boosts computational performance by orders of magnitude across various combustion scenarios.

CRediT authorship contribution statement

Runze Mao: Investigation, Methodology, Software. **Xinyu Dong:** Software. **Xuan Bai:** Software. **Ziheng Wu:** Validation. **Guanlin Dang:** Software. **Han Li:** Software. **Zhi X. Chen:** Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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