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PeleLMeX: an AMR Low Mach Number Reactive Flow Simulation Code without level sub-cycling

Lucas Esclapez [1], **Marc Day** [1], **John Bell** [2], **Anne Felden** [2], **Candace Gilet**[4], **Ray Grout** [1], **Marc Henry de Frahan** [1], **Emmanuel Motheau** [2], **Andrew Nonaka** [2], **Landon Owen**[3], **Bruce Perry** [1], **Jon Rood** [1], **Nicolas Wimer** [1], **and Weiqun Zhang** [2]

1 High Performance Algorithms and Complex Fluids, National Renewable Energy Laboratory, USA **2** Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory, USA **3** Sandia National Laboratory, USA **4** Independent Researcher, USA

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Summary

PeleLMeX simulates chemically reacting low Mach number flows with block-structured adaptive mesh refinement (AMR). The code is built upon the AMReX (Zhang et al., 2019) library, which provides the underlying data structures and tools to manage and operate on them across massively parallel computing architectures. PeleLMeX algorithmic features are inherited from its predecessor PeleLM (PeleLM Team, 2022) but key improvements allow representation of more complex physical processes. Together with its compressible flow counterpart PeleC (Henry de Frahan et al., 2023), the thermo-chemistry library PelePhysics and the multi-physics library PeleMP, it forms the Pele suite of open-source reactive flow simulation codes.

PeleLMeX uses a finite volume approach to solve the multi-species reacting Navier-Stokes equations in their low Mach number limit (Day & Bell, 2000), where the characteristic fluid velocity is small compared to the speed of sound, and the effect of acoustic wave propagation is unimportant to the overall dynamics of the system. Accordingly, acoustic wave propagation can be mathematically removed from the equations of motion, allowing for a numerical time step based on an advective CFL condition. This low Mach number limit mathematically translates into a constraint on the divergence of the velocity field (Majda & Sethian, 1984). The momentum equation is then solved for using a predictor/corrector method initially developed for incompressible flows (Almgren et al., 1998) and later extended to reactive, variable-density flows (Pember et al., 1998). In the low Mach framework, the thermodynamic pressure is uniform in space but can evolve in time when simulating closed domains with chemical reactions and additional mass injections (Nonaka et al., 2018). PeleLMeX uses an iterative Spectral Deferred Correction (SDC) time advancement scheme (Nonaka et al., 2012, 2018) to ensure a tight coupling of the fast diffusion/reaction and the comparatively slow advection, while iteratively enforcing the low Mach number constraint. Advection terms are treated explicitly using second-order Godunov schemes (AMReX-Hydro Team, 2022), diffusion terms are treated semi-implicitly with a Crank-Nicholson scheme and the often stiffer reaction term is obtained using a fully implicit Backward Differentiation Formula scheme (specifically, the CVODE integrator (Balos et al., 2021) of the Sundials suite (Gardner et al., 2022; Hindmarsh et al., 2005)). The solution of the linear systems arising in the implicit diffusion and velocity projections are handled using AMReX's native geometric multigrid (GMG) solver, but can also be transferred to HYPRE (Falgout & Yang, 2002) if GMG fails. In contrast with PeleLM, PeleLMeX relies on a non-subcycling approach to advance the numerical solution on an AMR hierarchy, where all the levels are advanced together using the same time step, the size of which is prescribed by a CFL condition across all the levels. This distinctive feature drove the development of PeleLMeX as it enables extending the closed chamber algorithm described in

(Nonaka et al., 2018) to an AMR hierarchy and incorporating more complex physical processes such as flame/plasma interactions (Esclapez et al., 2020).

In addition, PeleLMeX uses an Embedded Boundary (EB) approach to represent complex geometries: an arbitrary surface can be intersected with the Cartesian matrix of uniform cells, and the numerical stencils are modified near cells that are cut by the EB. Redistribution schemes (Giuliani et al., 2022) are then used for the explicit advection and diffusion updates in order to alleviate the constraint associated with small cut cells. Through its dependency to the multi-physics library PeleMP, PeleLMeX also inherits the ability to include Lagrangian sprays as well as soot and radiation models.

PeleLMeX is written in C++ and is built upon the AMReX (Zhang et al., 2019) library from which it inherits its parallel paradigm. It uses a MPI+X approach where MPI is used to distribute AMR grid patches across CPU ranks and each grid can be further divided into logical tiles spread across threads using OpenMP for multi-core CPU machines, or spread across GPU threads using CUDA/HIP/SYCL on GPU-accelerated machines.

Statement of Need

Several software tools for reactive flow simulations can found online (often with limited access), including unstructured body-fitted solvers based on OpenFOAM (Hassanaly et al., 2018), the structured solver NGA2 (NGA2 Team, 2023), and the Sierra/Fuego solver (Domino et al., 2003). In contrast with the aforementioned solvers, PeleLMeX is fully publicly available and documented. Its unique features consist in combining an AMR approach with a low Mach number formulation to achieve high performances from a small desktop station to the world's largest supercomputer. Recent code developments focused on enabling massively parallel simulations at scale on high-performance accelerated computer architectures to tackle the challenging requirements of fundamental and applied combustion research, as well as extending the solver modeling capabilities by including Large Eddy Simulation (LES) closure models and support for data-driven combustion models (Perry et al., 2022).

PeleLMeX is intended for students, researchers and engineers interested in understanding complex combustion processes by performing high fidelity simulations. Although it can be used to study laminar flames, its distinctive features make it particularly attractive for studying the fine scale flame/turbulence interactions in combustion applications where AMR is necessary to tackle the large scale separation and the computational resources available on the latest heterogeneous exascale platform can be leveraged. In order to achieve energy, transport and industrial decarbonization, fuel-flexible combustion devices must be designed and deployed to accommodate hydrogen, ammonia and a wide range of biofuels. In this context, PeleLMeX can prove a valuable tool to study alternative fuels combustion characteristics, flame dynamics or pollutant formation mechanisms, both in academic idealized cases (Howarth et al., 2023) as well as in device scale simulations (Appukuttan et al., 2023).

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