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IAMReX: an adaptive framework for the multiphase flow and fluid-particle interaction problems

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Summary

IAMReX is an adaptive C++ solver designed for multiphase flow and fluid-particle interaction problems. It is built in an object-oriented style and capable of high-performance massively parallel computing for complex systems (e.g., gas-fluid interaction, clusters of particles).

The original goal of IAMReX is to extend the capabilities of IAMR codes (Almgren et al., 1998), which only use a density-based solver to capture the diffuse interface of the two-phase flow. IAMReX offers a level set (LS) method and reinitialization techniques for accurately capturing the two-phase interface (Zeng et al., 2022), which increase the robustness of simulations with high Reynolds numbers (Zeng et al., 2023). In IAMR codes, particles are only treated as passive scalars. In IAMReX, however, both passive scalars and fully resolved particle cases are supported. To simulate the resolved particles, IAMReX employs the multidirect forcing immersed boundary method (Li et al., 2024). The associated Lagrangian markers used to resolve fluid-particle interfaces only exist on the finest-level grid, which greatly reduces memory cost. Both the subcycling and non-subcycling time advancement methods are implemented, and these methods help to decouple the time advancement at different levels. Like its predecessor, the IAMR library, IAMReX is also a publicly accessible platform designed specifically for developing massively parallel block-structured adaptive mesh refinement (BSAMR) applications. With the help of the AMReX framework, both IAMR and IAMReX support hybrid parallelization using either pure MPI or MPI & OpenMP for multicore machines (Zhang et al., 2019), and we have ensured that new features introduced in IAMReX do not compromise this cross-platform support.

The IAMReX code has undergone considerable development since 2023 and gained a few new contributors in the past two years. Although the projection-based flow solver is inherited from IAMR, IAMReX has added over 3,000 lines of new code, introduced 10 new test cases, and contributed approximately 60 new commits on GitHub. The key differences between IAMR and IAMReX are summarized in this webpage. The versatility, accuracy, and efficiency of the present IAMReX framework are demonstrated by simulating two-phase flow and fluid-particle interaction problems with various types of kinematic constraints. We carefully designed the document such that users can easily compile and run cases. Input files, profiling scripts, and raw post-processing data are also available for reproducing all results.

Scholarly effort

IAMReX's scholarly effort lies in its transformation from a standard incompressible flow solver into a unified, high-performance, multi-physics framework for complex interfacial and particulate flows. This is achieved through several key contributions. First, IAMReX introduces a modular architecture that supports distinct and advanced physics modules within a single platform. This includes a sharp-interface model for immiscible two-phase flows using an advanced level set method, complete with conservative advection and mass-preserving reinitialization schemes. Simultaneously, it offers a robust framework for particle-resolved fluid-structure interaction (FSI) by implementing a Diffused Immersed Boundary Method (DIBM). Second, a significant effort was dedicated to developing a comprehensive system for particle-resolved simulations. This system features a DIBM implementation for handling the motion of 6-DOF rigid bodies without requiring mesh conformity. It is further enhanced with a particle-particle collision model using spatial hashing for efficient detection and a repulsive potential model for resolution. Last but not least, IAMReX leverages the GPU acceleration capabilities to ensure efficiency for particle-resolved simulations. All major particle operations, including fluid-solid coupling, force spreading, and collision detection, are designed to be GPU-compatible. A key optimization for memory efficiency involves constraining the Lagrangian markers used for the fluid-particle interface to exist only on the finest grid level.

Relation to previous work

IAMReX is built upon the foundations established in three of our previous publications. The implementation of the level set method is adapted from Zeng et al. (Zeng et al., 2022), with a key distinction: IAMReX employs a semi-staggered grid rather than a collocated grid, which strengthens the pressure-velocity coupling during the solution process. Furthermore, the Diffused Immersed Boundary Method is derived from Li et al. (Li et al., 2024); while the original work was limited to CPU-based parallelism and a basic particle collision model, IAMReX has been tested on GPUs for select cases and is designed to accommodate more advanced collision models. Finally, our approach to optimizing computational efficiency through the Adaptive Mesh Refinement (AMR) technique, particularly the selection of simulation parameters, was informed by the guidance provided in Liu et al. (Liu et al., 2025).

Statement of need

IAMReX is suitable for modeling multiphase flow problems and fluid-structure interaction problems. Its level set-based interface capturing technique can be beneficial for researchers studying phenomena such as wind over waves, breaking waves, and simulating the formation and disappearance of bubbles and droplets. Additionally, the immersed boundary method along with the collision models can parallelly resolve large-scale particles and capture their motions. Researchers working on studies of biological particle aggregation, sandstorms, wind erosion of ground surfaces, and seawater erosion of riverbeds are also among the target audience for this software.

State of the field

We made great efforts to simulate more complex multiphase flows at higher resolution using IAMReX. One effort is to combine the AMR technique with the multidirect forcing immersed boundary method to resolve particles only on the finest-level grid. It significantly reduces the grid requirements for particle-resolved simulations compared with commonly used uniform grid solvers Incompact3d, CaNS, and CP3d. Additionally, we utilized a subcycling technique to alleviate the time step constraint on coarser levels. It minimizes the total number of time steps needed for time advancement compared with the non-subcycling technique used in other AMR-related packages, such as IBAMR, Basilisk, and incflo.

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