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Mesh refinement algorithms in an unstructured solver for multiphase flow simulation using discrete particles

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ABSTRACT

This study developed spray-adaptive mesh refinement algorithms with directional sensitivity in an unstructured solver to improve spray simulation for internal combustion engine application. Inadequate spatial resolution is often found to cause inaccuracies in spray simulation using the Lagrangian–Eulerian approach due to the over-estimated diffusion and inappropriate liquid–gas phase coupling. Dynamic mesh refinement algorithms adaptive to fuel sprays and vapor gradients were developed in order to increase the grid resolution in the spray region to improve simulation accuracy. The local refinement introduced the coarse-fine face interface that requires advanced numerical schemes for flux calculation and grid rezoning with moving boundaries. To resolve the issue in flux calculation, this work implemented the refinement/coarsening algorithms into a collocated solver to avoid tedious interpolations in solving the momentum equations. A pressure correction method was applied to address unphysical pressure oscillations due to the collocation of pressure and velocity. An edge-based algorithm was used to evaluate the edge-centered quantities in order to account for the contributions from all the cells around an edge at the coarse-fine interface. A quasi-second-order upwind scheme with strong monotonicity was also modified to accommodate the coarse-fine interface for convective fluxes. To resolve the issue related to grid rezoning, rezoning was applied to the initial baseline mesh only and the new locations of the refined grids were obtained by interpolating the updated baseline mesh. The time step constraints were also re-evaluated to account for the change resulting from mesh refinement. The present refinement algorithm was used in simulating fuel sprays in an engine combustion chamber. It was found that the present approach could produce the same level of results as those using the uniformly fine mesh with substantially reduced computer time. Results also showed that this approach could alleviate the artifacts related to the Lagrangian discrete modeling of spray drops due to insufficient spatial resolution.

1. Introduction

Modeling fuel sprays in internal combustion engines is a challenging task due to the complex physical processes involved. For dilute sprays, a commonly used approach is based on the Lagrangian discrete particle method [1] in which the properties of representative droplet parcels are randomly chosen from empirical or theoretical distribution functions. The continuous gas phase is described using an Eulerian method. Liquid–gas interactions are modeled by the coupling source terms for the exchange of mass, momentum, energy and turbulence. Various sub-models are used to describe the droplet breakup,

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collision, turbulent dispersion, evaporation and wall interaction [2–7]. The accuracy of simulation results not only relies on the fidelity of the models but also on the temporal and spatial resolutions of the governing equations.

Numerous numerical studies have indicated that spray simulation is subject to the influence of the grid resolution and the mesh type [8–15]. The grid dependence can be partially attributed to the inadequate spatial resolution of the coupling between the gas and liquid phases. In the region near the injector exit, the velocity and species density gradients can be strong when a high-velocity spray is injected into a slowly moving gas. Inadequate space resolution in the spray region can result in a much higher relative velocity between the gas and liquid and an over-estimation of diffusion [16]. The higher relative velocity then affects the liquid penetration and vaporization since the relative velocity is used to calculate spray breakup and vaporization. Thus the use of a fine mesh is often required in the region near the injector to improve spray modeling, while the use of a coarser mesh is recommended away from the injector to save computer time.

Grid resolution also inherently affects the performance of various spray sub-models [8–16]. The stochastic collision algorithm [3] adopted in many CFD codes inevitably depends on the grid resolution since the algorithm only allows parcels within the same cell to collide. Collision probability in this algorithm also depends on the grid resolution, since the cell volume is considered in the calculation. In evaporation calculation, fuel vapor is assumed to be uniformly distributed within a computational cell. This treatment can result in over-estimated vapor diffusion (lower vapor density) because the vapor mass fraction in the cell is compared to that at the droplet surface to determine evaporation rate [17]. Furthermore, the statistical convergence of the stochastic discrete approach may not be guaranteed or may progress very slowly, and a better phase coupling is needed [8].

While improving the sub-models to reduce the grid dependence has attracted much attention [12–21], the improvements may still be subject to further validation and tuning of model constants for specific conditions. Another way to obtain more accurate spray simulations is to increase the spatial resolution. However, the volume of the droplets inside a cell should be small enough compared to the cell volume in order to satisfy the dilute spray assumption for the Lagrangian liquid phase description. A uniformly fine mesh is limited not only by the available computer power but also by the flexibility of choosing grid resolution to meet the Lagrangian assumption.

Adaptive mesh refinement (AMR) [21–23] can be utilized to increase the spatial resolution in the spray region to improve the phase coupling and to alleviate the mesh dependence without incurring a significant computational cost. In particular, AMR can provide a greater flexibility in adapting to highly transient spray with adequate spatial resolution that otherwise would not be readily available if a uniformly fine mesh is used. A goal of this study was to develop AMR algorithms to simulate transient engine sprays in the unstructured KIVA-4 code [24], earlier versions of which have been widely used in the engine research community. The original KIVA-4 adopted a staggered approach for solving momentum equations and density-based equations for compressible flows. To simplify the numerical scheme and implementation for using AMR, this paper adopted a collocated approach in which velocity is solved at the cell center for the momentum equations and used for the gas–liquid coupling terms. A pressure correction method proposed by Rhie and Chow [25] was used to address unphysical pressure oscillations due to the collocation of pressure and velocity [26].

The current AMR approach determined data structure and numerical methods based on the features of the KIVA-4 solver. This approach attached new child cells to the existing cells and used a hierarchical structure to establish relationship between the parent cell and its child cells. The refined cells were coarsened to reduce computational cost if a higher grid density was not required. These dynamic procedures were controlled by using an adaptation criterion that incorporated the normalized fuel mass within a computational cell and the gradients of vapor mass fraction.

AMR requires advanced numerical methods to deal with the coarse-fine face interface where cells in different refinement levels meet. The calculation of diffusive fluxes needs to consider all the active cell edges for the edge-centered quantities and consider all the active cell faces for the surface fluxes. Note that a regular hexahedral cell consists of only 12 edges by definition. On the coarse-fine interface, one edge is divided into two edges. Therefore, the total number of edges of a coarse cell at the interface increases as a result of mesh refinement, and all the edges need to be considered in calculating the edge-centered values. On the other hand, the convective fluxes were determined from the second-order upwind scheme that meets strong monotone conditions to prevent under-shoot and over-shoot of the fluxes. Face normal velocities of the refined cells at the interface were utilized to advance the Lagrangian cell volume change in the pressure iteration and in the convective fluxing.

The remainder of this paper is organized as follows. In Section 2, mesh refinement algorithms along with the adaptation criteria are presented. In Section 3, *the numerical methods* dealing with the coarse-fine interface are described, followed by Section 4 in which numerical tests are performed to validate AMR implementation and demonstrate the benefits of spray simulations using AMR. Conclusions are summarized in Section 5.

2. Spray-adaptive mesh refinement algorithms

The current adaptation increases the grid density by splitting a cell into smaller child cells. This method provides flexibilities in the mesh construction and is consistent with the characteristics of the finite volume solver with the arbitrarily unstructured mesh [27]. The adaptation starts with an initial coarse mesh (level 0) and creates new grids with higher levels (level l) continuously as the computation progresses. Meanwhile, the refined grids are coarsened to the lower-level grids if the fine grid is not needed in order to reduce the computational cost.