Coupling of Particle-Based and Grid-Based Methods within Object-Oriented Multi-Physics CFD Framework

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ABSTRACT

The multi-physics solver MϕC[1-4], developed within the CFD Laboratory at the University of Liverpool was designed for hybrid simulations with a coupling of numerical methods for different mathematical models in different parts of the flow domain. A key feature of the framework is the object-oriented design, i.e. the framework constitutes a library of C++ clases on top of which a range of particle-based methods (Molecular-Dynamics, Vortex Particle method) as well as mesh-based methods for the Navier-Stokes equations and the kinetic Boltzmann equations (Shakhov/Rykov-BGK and Ellipsoidal Statistical (ES) models) were built. For coupling the various models and methods, the framework includes a number of coupling methods, including flow-state based and flux-based methods. The design as a library enables a large degree of re-use of software for different methods as well as prototyping of novel coupling approaches. In previous works, the framework was demonstrated for coupled Navier-Stokes/Molecular Dynamics problems involving nano-scale flow of liquids[1-3] as well as coupled Navier-Stokes/kinetic-Boltzmann simulations[4].

The present work focusses on recent developments of the particle-based methods in the framework: the development of molecular dynamics modelling of diatomic gas flows in strong thermodynamic non-equilibrium and the coupling of the molecular-level modelling to mesh-based kinetic models. The rotational motion of diatomic molecules is assumed to be 'fully excited' degrees of freedom, for which a classical MD model can be used, while for the vibrational excitation present in high-temperature conditions, a semi-classical model is typically required.

The paper presents a detailed account of the recently developed particle methods as well as the coupling methods and the implementation in the framework. The unification and re-use of the implementation of different meyhods/models will be described. The partially rarefied gas flow of a diatomic gas through a shock wave and the flow around a spaceplane configuration are considered as applications

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