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DEVELOPMENT OF PARALLEL COMPUTATIONAL FRAMEWORK FOR MULTI-PHYSICS FLOW SIMULATIONS

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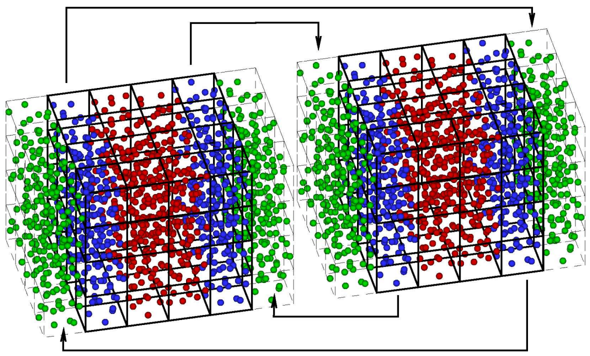
ABSTRACT

The present paper describes the development of a computational framework for simulating multi-physics flow problems, with the emphasis on aerospace applications. At present, the computational fluid dynamics methods which have found their way into routine use within the aerospace industry are mainly methods for solving the Reynolds-averaged Navier-Stokes equations. Although successful in a wide range of applications, a number of limitations arise from this approach. The computational requirements are often excessive for routine, design analysis, applications. At the same time, the flow physics requiring physical modelling at the level of the Navier-Stokes equations are often limited to small regions of the domain. For this type of applications, the computational efficiency can be improved by employing the Navier-Stokes equations only locally, while using governing equations at a lower level of physical detail elsewhere. In other applications, the Navier-Stokes equations may not be adequate in certain regions of the computational domain, e.g. in flows with locally non-continuum flow physics. Locally, one needs to resort to more detailed models. The computational framework under development aims to simulate such multi-physics flow problems with (partially) overlapping sub-domains in which different sets of governing equations are used. The presentation focuses on the development of the coupling methods between the different physical models.

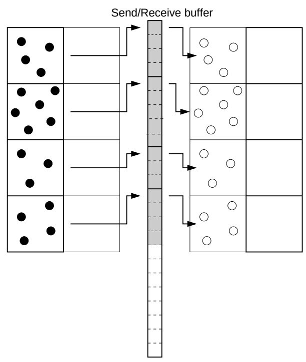
For simulations of flow problems combining regions of continuum flow and rarefied flow regions, the presented work is closely related to the significant volume of recently published work in modelling complex fluids, micro- and nano-fluid flows with hybrid methods combining molecular dynamics and continuum modelling based on the Navier-Stokes equations, e.g. Refs.[1-4]. For rarefied, high-speed gas flows, numerical simulation of the Boltzmann equation forms a more efficient alternative to molecular dynamics simulations. Coupling methods for the Boltzmann and Navier-Stokes equations have have been investigated extensively in the past decade, e.g. Refs.[5-6].

To investigate modelling multi-physics flow problems based on different sets of governing equations in different parts of the computational domain, a prototype computational framework is currently being developed. This framework is built on a generalized domain decomposition approach, i.e. the formulation can handle a wide range of data structures defining a numerical solution on a computational domain decomposed in multiple sub-domains. Independent of the particular details of the solution methods, a layer

of halo-cells is created Independent of the particular details of the solution methods, a layer of halo-cells is created around each sub-domain. The generalized approach is designed to work with particle-based methods (Molecular Dynamics, Lagrangian Vortex Method), hybrid Lagrangian/Eulerian methods (e.g. Vortex-In-Cell) as well as mesh-based methods. The framework is implemented as a C++ template-class library, and includes functions for message-passing and synchronisation based on the MPI library. The particular details of the solution methods are introduced by specialising a set of member functions and overloaded operators of either a particle-method base class or a base class for mesh-based solution methods. Sofar, this framework has been used to implement a prototype Molecular Dynamics solver, a finite-difference method for the incompressible Navier-Stokes equations, as well as, a Navier-Stokes solver based on the Vortex-In-Cell method. In the presentation, two multi-physics examples are investigated in detail. First, the coupling of a molecular dynamics with the Navier-Stokes equations. This coupling has been researched recently by various researchers, and the main aim here is to highlight the implementation of this type of coupling in the current framework. The second example involves the coupling of a mesh-based Navier-Stokes method for compressible flow (i.e. here the model at the higher level of detail) with a a vortex-particle based method as 'wake' model.



(a) MD example



(b) send/receive buffer

Figure 1: Computational framework is built on a generalized domain decomposition approach, which for mesh-based methods forms 'traditional' halo-cells. For particle-based methods, halo cells with 'ghost' particles are formed. (a) MD domain split in two sub-domains, (b) formation of send/receive buffer in parallel implementation.

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