

On steering coupled models.

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Coupled models are set to become increasingly important in all aspects of science and engineering as a means to study complex systems in an integrative manner, particularly in systems biology and materials science. In computational terms, our aim is to embrace, within a single simulation, all necessary length and time scale processes to describe the system of interest. Such coupled, hybrid simulations typically communicate data between the component models of which they are comprised relatively infrequently, and so a Grid is expected to present an ideal architecture on which to run them. Computational steering is a powerful tool for interacting with simulations as they run, allowing the user to alter physical parameters, algorithmic parameters or even to migrate their simulation to another machine on the Grid. Hybrid models present new challenges in these respects. We describe a simple, flexible and extensible architecture for coupled models based on the RealityGrid computational framework and discuss its implementation for the case of a two-component hybrid molecular-continuum fluid dynamics scheme.

Multi-scale modelling of physical systems is often employed to enable an accurate but computationally expensive model to be applied to regions of a system where it is required while a less accurate model can be used elsewhere. This enables far larger systems/longer timescales to be modelled than can be tackled using the accurate model alone.

Within the RealityGrid project (<http://www.realitygrid.org>) and Integrative biology (<http://www.integrativebiology.ac.uk>) we are investigating the use of coupled models in several areas. A process of nano-indentation where a nano-scale tip is pushed into a semiconductor surface and then retracted. The interaction of the tip with the surface must be modelled atomistically using quantum mechanics but this method is too expensive to be applied to the bulk of the surface. Instead, a continuum method is used to model the propagation over the surface of the stresses resulting from the indentation [1]. Another area of application is the study of fluid flow over a molecular surface. Here, the interaction of fluid molecules with the surface is modelled atomistically using classical molecular dynamics while the bulk of the fluid flow is modelled using a continuum method. Integrative biology is also developing an integrated approach to multiscale computational modelling of the heart and cancer tumor.

A multi-scale model may be constructed by coupling together different simulation codes, each specializing in modelling a region of the system on one particular scale. Such a model then consists of a set of two or more codes which are synchronized through the (repeated) exchange of information as they execute. A coupled model could be written as a single executable code, but for flexibility, scalability and ultimately, performance reasons, we consider the case of a coupled model constructed from independent components which are

interfaced to allow them to exchange information. These components are then free to be deployed in such a way as to make the best use of available resources; something that is particularly important in a Grid environment.

Over the course of the RealityGrid project, the introduction of computational steering functionality to existing scientific codes has proved key [2, 3]. The process of “computational steering” refers to the interaction of a scientist with his/her running application. At its simplest, this may consist of monitoring the values of a few key variables to check the progress of the application. More advanced uses may involve the scientist altering variables that control algorithms within the code or altering parameters of the physical problem. Such use enables the scientist to further develop and apply their intuition to the investigation of the system under study. On-line visualization of the system is a powerful aid in this process since it can provide the user with visual feedback on the consequences of their steering activity.

We demonstrate the use of steering coupled models with the RealityGrid library for a two component model coupling MD and hydrodynamics. We are able to change several global and non-global parameters and observe the collective results by monitoring the molecular system via online visualization using the RealityGrid modified version of VMD. We use an AVS/Express-based visualization to monitor the continuum region. The system is set-up with a small MD region surrounded by a large continuum domain. The amplitude and frequency of pressure wave oscillations coming from the continuum hydrodynamics region are freely changed and steered in the molecular region.

Over the past few years, we have been developing a new approach to the modelling and simulation of complex fluid flow for application to a wide range of

problems in soft condensed matter science and engineering. Our approach is based on a multiscale hybrid scheme, in which two or more contiguous sub-domains are dynamically coupled together, the simplest case corresponding to one sub-domain being described by molecular dynamics, the other by continuum fluid dynamics (CFD) [4, 5]. The motivation for this hybrid approach to the description of fluids is that it enables us to tackle problems that are not addressable by any one single technique; such problems include situations in which hydrodynamic effects influence molecular interactions at interfaces, lipid bilayer membranes and within individual macromolecules or assemblies of them. Since the computational overhead of coupling the molecular and continuum regions is very low, we can use this approach to perform coupled simulations using small MD domains which are free of finite size effects, whilst reducing the computational cost compared with fully atomistic simulations. The approach can be used to probe limitations to CFD descriptions which are known to break down in situations where molecular phenomena play a large role, such as the moving contact line between two immiscible fluids and a boundary.

This component-based approach has significant advantages. Not least of these is that each individual component can be developed, tested and used independently as a standalone code. In practise, each component can be run on a different machine and it is easy to extend this scheme to multiple components (three, four, *etc.*) as is required when adding an extra level of description to the physical model (*e.g.* quantum mechanical).

Although several specialised coupling frameworks exist, particularly in the field of atmospheric and ocean modelling, we have chosen to use a very simple solution since our current models contain only two components and do not use any particular features of such frameworks. To enforce synchronisation and permit data exchange, we have constructed a communication “switch” service that implements a store and forward message-passing scheme. The interface to this switch service con-

sists simply of a *put* operation and an blocking *get* operation. It is the use of the latter that enforces inter-component synchronisation. In order to avoid deadlock in such a scheme, each component executes its ‘puts’ before its ‘gets’.

This work signals the beginning, but only the beginning, of a journey into the world of coupled models which can be deployed on a general purpose Grid. It is straightforward to extend the scheme described here to the case of multiple components; within computational materials science and systems biology [6] there is a need to couple levels of description from the quantum mechanical, through classical molecular dynamics and coarse-grained particulate representations to the continuum level described by computational fluid dynamics, finite-element descriptions and so on. Both the EPSRC-funded Integrative Biology e-Science Pilot Project and the BBSRC-funded Integrative Biological Simulation Bioinformatics and e-Science Programme Project have an interest in such multi-level coupled modelling capabilities.

Steering such multicomponent coupled models is not expected to provide any fundamental problems given that the couplings are always between nearest neighbours in the space-time hierarchy of model descriptions. Moreover, we are particularly interested in developing an ability to insert and delete component models on-the-fly when highest or lowest levels of resolution are warranted. Grid deployment is likely to be important for obtaining good load-balancing of such coupled simulations and we expect to be able to use existing and developing RealityGrid middleware to facilitate this. The problem of performance control is particularly interesting for coupled models; we expect to be able to provide this initially via manual migration of individual components between compute resources on a Grid. Ultimately, we hope to include automated performance control within the RealityGrid steering system, but that is another story.

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