

The RealityGrid Web Portal

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Introduction

The scientific aims of the RealityGrid project [1] are the study of complex materials via computation and simulation. Such materials include complex fluids (e.g., multicomponent fluids with colloidal particles or surfactants) and solid interfaces at the microscopic scale. The study of this type of system makes use of a number of powerful computational techniques such as the lattice Boltzmann method and molecular dynamics, and perhaps combinations of these techniques. Allowing the user to monitor and interact with large numerical simulations as they are running can be very useful scientifically. RealityGrid has therefore developed a generic API for application codes to allow such monitoring and steering.

The web browser is a very powerful and almost ubiquitous tool for computer users. In building a client to provide an interface to the application codes via the steering API and architecture, a natural choice is then browser-based. The construction of such an interface is the aim of the RealityGrid Web Portal. This paper will provide an overview of the Web Portal and our current thinking on future developments.

The Web Portal

The RealityGrid portal is based on open source Gridsphere [2] portlet technology. The idea is that a number of portlets, each concerned with a specific task, can be combined and administered within a Gridsphere container to create a bespoke portal. Gridsphere provides common portlets as standard, and these can be extended or added to in the form of new portlets. The portlets are implemented in Java and so are easily developed. Indeed, the overall view of development within the Gridsphere framework has been generally positive.

Portlets have been written which allow resource discovery, application control and parameter monitoring and steering. These portlets form a basis for the RealityGrid portal. The portal interacts with a steering grid service (SGS) started by the application which then allows clients to communicate with the application via HTTP and SOAP as defined by the RealityGrid architecture. Another portlet under development provides an interface to a checkpoint tree via the SGS. This is a linked

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series of simulation output which can form the basis of investigation of parameter space and control of simulation history.

While parameter based steering and control are useful, one significant issue — visualisation — provides more of a challenge to the development of a flexible and general portal interface. A useful interface here requires at least visualisation of snapshots of simulation state, and preferably animation.

Real Problems and Visualisation

A large run of a lattice Boltzmann code might require many hours on a parallel machine to achieve a respectable amount of simulation time. The system might evolve to some steady state, or may continue to evolve, but will almost always evolve slowly in real time. A very powerful way to gain a feel for what the system is doing dynamically is to make an animation of an appropriate physical quantity (some illustrations will be given). Typically this is done after the simulation has finished and may use data from some hundreds of snapshots of the system.

Correspondingly, the question the scientist often wants to ask of a running simulation is: what does my simulation look like so far? Still frames can be of use, but in general will evolve too slowly in real time to provide any useful impression of simulation dynamics. A possible solution, therefore, is to use stored snapshots to provide an animation upon request.

Such a feature would make the web portal a very powerful tool, but clearly presents a number of challenges: where are the snapshots to be stored? how are they to be stitched together to form an animation? is the user allowed to select the details of the animation interactively? how is the animation to be delivered to the portal? Some of these issues can be addressed from the point of view of checkpoints — the SGS will know the location of a series of checkpoints which can be used as sources of data for the snapshots. Possible solutions to the other problems are under investigation.

References

- [1] <http://www.realitygrid.org/>
- [2] <http://www.gridisphere.org/>