Robust Grid-based environment for large scale lattice-Boltzmann simulations

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The use of Grid technologies should enable scientists to efficiently perform research by devising workflows that involve the deployment of computationally intensive simulations on heterogeneous and geographically distributed high performance computing resources [1]. In this paper we describe the RealityGrid infrastructure and outline the problems and progress achieved so far in its deployment, with particular attention to the end-user perspective. To illustrate the advantages of using Grid infrastructure for routine scientific research, we describe the application of the massively parallel and steerable lattice-Boltzmann code (LB3D) to the study of single and two phase flow in porous media.

I. INTRODUCTION

RealityGrid [2] is a four year EPSRC e-Science pilot project intended to bring Grid technology to bear on the field of condensed-matter science, including large-scale computer simulation.

To be able to exploit existing Grid infrastructure and available resources—specifically, the full UK National Grid Service (including its supercomputing resources at HPCx and CSAR) and the US TeraGrid, both of which use the Globus Toolkit [3] version 2 (GT2) middleware—it is important to create a stable and persistent environment that scientists can routinely and reliably use for scientific research.

In this article we will discuss the steps undertaken at the Centre for Computational Science (CCS, University College London), in collaboration with Manchester Computing, to create a self-standing, usable and persistent Grid framework.

As a result of this joint collaboration, the process of getting new users “up-and-running” and doing relevant science on a Grid now requires considerably less effort and time compared to our previous experiences with one-off, and extremely labour intensive, projects such as TeraGyroid [4–6]. We have sought to overcome the limitations of such previous endeavours in terms of their acute lack of usability and persistence.

II. COMPUTATIONAL STEERING AND GRID INFRASTRUCTURE

The concept of steering both simulations and Grid-enabled experiments is of central importance to RealityGrid. Computational steering refers to the process by which a scientist interacts with a running application to make optimal use of the resources [7].

RealityGrid components are instrumented for steering by making calls to a library of routines provided for the purpose [8, 9]. The aim throughout has been to enable existing scientific computer programs (often written in FORTRAN90 and designed for multi-processor supercomputers) to be made steerable with a minimum of effort, minimising the number of changes that an application scientist must make to an existing program. In light of these requirements, the steering library has been implemented in C which allows it to be used with a variety of common scientific languages such as FORTRAN90, C and C++. We have interfaced the RealityGrid steering library with several highly scalable parallel scientific codes, including the lattice-Boltzmann code LB3D and the molecular dynamics code NAMD [10]. For their performance and scalability, both codes reside in the highest performance class at the HPCx (UK) capability computing service.

The steering library allows remote launching, monitoring, steering, visualising, checkpointing, restarting and migrating of simulations between heterogeneous architectures, to optimise the use of the available resources and to open new routes to scientific research, such as dynamic parameter space exploration [11].

To enable the end user to launch an entire simulation pipeline from a unified interface a registry service, implemented using the OGSI::Lite middleware [12] was developed. OGSI::Lite solves the problem of exposing programs as Grid services. It builds on existing implemented standards (such as SOAP for remote messaging) meaning that specialised client software is not required, and leaving to the scientist maximum versatility in the choice of steering client. We are now able to steer and control a running application using PDA-, Web- and Qt-based steering clients. The RealityGrid steering library communicates with the rest of the Grid by exposing itself as
a “Grid Service”. Through the registry service, steering clients are able to find, dynamically attach to, communicate with, and detach from steering services to control a simulation or visualisation process (see Figure 1).

It is important to bring to note that now OGSI::Lite has been superseded by WSRF::Lite. WSRF::Lite is a Perl implementation of the Web Service Resource Framework to create a container for lightweight web-service based hosting environment, and does not require the user to install Globus (or any other Grid middleware) on the client machine even if, as is currently the case, the Grid uses Globus as its middleware. The lightweight-hosting environment will be distributed via the Open Middleware Infrastructure Institute (OMII) in the second half of 2005 [13].

![Architecture for RealityGrid steering within the Open Grid Services Infrastructure (OGSI).](image)

FIG. 1: Architecture for RealityGrid steering within the Open Grid Services Infrastructure (OGSI). The application and client communicate by exchanging messages through intermediate Grid services. The Grid service (GS) provides the public interface through which clients can steer the applications.

The RealityGrid steering architecture was designed in a sufficiently general manner that visualisation services can also be represented by Steering Grid Services (SGS): to establish a connection between the visualisation process and the corresponding simulation, the simulation SGS can be found through the registry, and then interrogated for the information required to open the link.

Running large scale simulations usually implies that large data sets (order of tens of gigabytes) are generated, which have to be efficiently transferred for analysis and job migration across the nodes on the Grid. Also, as a typical requirement for our lattice-Boltzmann applications, it is often useful to monitor the progress of a simulation using visualisation. If large data sets are to be rendered, the output of a simulation has to be streamed to a dedicated visualisation platform with the required capabilities of memory and CPU resources. Using the RealityGrid steering libraries based on the SOAP communication protocol, the data can be transmitted via sockets from the computing resources to a visualisation resource. However, if low bandwidth links are used, the communication can be very slow, effectively preventing the scientist from inspecting the results of the running simulation in real time, and to intervene via steering. Also, the sometimes limited storage capabilities of the computational resources on the Grid may pose the necessity to transfer the data produced to a high capacity archive, as well as for the reason that the scientist may want his/her results organised in one place instead of scattered all over the resources he/she used to run the simulations. RealityGrid exploits the UK National Grid Service (NGS) infrastructure [14], and international large scale computational resources at Pittsburgh Supercomputing Center and on the US TeraGrid [15] (through NSF, PACI and NRAC grants). High bandwidth, low latency connection between the UK and US Grid resources is provided by UKLight circuit-switched networks in the context of the EPSRC/PPARC/MRC funded Exploitation of Switched Lightpaths For E-Science Applications (ESLEA) project. ESLEA aims to exploit the UKLight network for a variety of applications including high energy particle physics, radio astronomy, computational science and e-Health. The project has academic partners in four UK universities, the United States and Europe, and industrial partners in the UK (Cisco and BT).

III. THE UPHILL ROAD TO A ROBUST GRID-BASED ENVIRONMENT: A USER PERSPECTIVE

A major success of RealityGrid was the TeraGyroid project, a true scientific endeavour with the aim of studying defect dynamics in amphiphilic liquid crystals, using Grid-based lattice-Boltzmann simulations [4–6]. RealityGrid’s computational steering, on-line visualisation and job migration between the US TeraGrid and the UK’s supercomputing resources at HPCx and CSAR were able to realise their full potential. A non-trivial effort from UK and US staff was required in order to build a transcontinental Grid. The TeraGyroid project was showcased at Supercomputing 2003 and won the award for “Most Innovative Data-Intensive Application” in the HPC Challenge competition.

When we decided to perform routine scientific research using the Grid infrastructure put together for the TeraGyroid project, we had to recognise the fact that this infrastructure was no longer in place, since many of the links, resources and authorisations, depended on temporary agreements between participating institutions and resource providers. We had then to face the challenge to reinstate those capabilities in a robust and persistent manner. This situation was far from ideal with respect to the ultimate aim of the RealityGrid project, and more generally of any scientific Grid computing [1], which is to allow the average scientist to fully exploit the advantages offered by Grid technologies, without having to deal with heavy technical and administrative problems every time he/she wants to do scientific research. Resources should be available at any time, the Grid infrastructure should be robust and persistent, the middleware should be transparent to the general user, security and authentication issues should not be an impediment to the pursuit of scientific research, and co-allocation of resources for compu-
Computational steering and visualisation of running simulations should be easily and readily available.

In order to avoid the disappointing and all too frequent scenario where the Grid infrastructure has a life limited to a demo session, scientists at the CCS in London, in collaboration with Manchester Computing, worked together over two months to create a usable, robust and persistent computational Grid. Several problems were encountered in the process. Portability issues and different compilers and environment settings made it a lengthy task to deploy our codes on the platforms available within the UK and US supercomputing centres. Security and certification issues arose, such as UK e-Science certificates not being recognised on the US TeraGrid resources. To improve the robustness of the Grid infrastructure we also worked to implement a local registry at the CCS (UCL). While previously we had to rely on a single Manchester registry to store checkpoints trees and Grid Service Handles, with the risk of not being able to use Grid capabilities if the Manchester registry was not accessible, now we can rely on much more flexible and dynamic access to the Grid resources, in which either the UCL or the Manchester containers can be used, depending on their availability and convenience. Thus, for example, if the Manchester node is connected to the TeraGrid via the fast UKLight optical network, it may be more convenient to register a simulation to run on the TeraGrid via the Manchester container in order to improve the communication between the steering and visualisation threads and the running application.

At the EPSRC Annual e-Science meeting 2005 (Edinburgh), we had the opportunity of harnessing the results of our efforts by presenting a demo which exploited the newly reinstated Grid infrastructure capabilities. However, only during the EPSRC meeting itself were we finally able to exploit the high bandwidth (1 GB/s) of UKLight connection between a visualisation resource in Manchester and the US TeraGrid. This allowed us to access real time visualisation of running lattice-Boltzmann simulations of binary fluid flow in porous media. Through steering we could monitor and change “on the fly” the parameters controlling the running applications (such as the output file dumping frequency) and the fluid behaviour, to investigate the dependence of phase separation in the confined geometry of the porous medium and the dynamics of fluid interfaces.

Also, exploiting UKLight, around 0.6 Terabytes of data were transferred in less than a night using gridftp with up to 30 streams opened at the same time between NCSA and a storage facility at UCL in London (see Figure 2). The same transfer would have taken several days on a normal network. The infrastructure used in the EPSRC 2005 meeting is shown in Figure 3.

Unfortunately, once the EPSRC demo was over, the persistence of the UKLight connectivity was, once again, not guaranteed. Many efforts since then were made by the UKLight engineers, staff at Manchester Computing Centre and UCL, to create a persistent link via UKLight within UK resources and between UK and US Grids.

The progress toward a persistent high bandwidth, low latency connectivity network was slowed down by the disruption of a trans-Atlantic cable, by UCL-related security issues in dual-homing the SGI Prism (a visualisation system at UCL) to UKLight as well as to the UCL production network. Also, routes and IP addresses associated with the dual-homing had to be defined and authorisation to use these routes had to be obtained from the United Kingdom Education and Research Networking Association (UKERNA). Even at the time of writing this paper, UKLight connectivity is not yet established to the Prism, although we expect progress toward persistent connectivity fairly soon.

Since steering and visualisation require the computational and visualisation resources to be co-allocated so that the scientist knows when his/her simulations are running, reservation of nodes on the TeraGrid resources and the UK National Grid Services (NGS) was necessary for the demonstrations at the EPSRC meeting. Node reservation is currently possible on the TeraGrid upon prior agreement, but there is no such provision in the NGS. However, the ideal situation would be to provide automated advance reservation and co-allocation procedures.

IV. A SCIENTIFIC PROJECT: SINGLE AND TWO PHASE FLOW IN POROUS MEDIA USING THE LATTICE-BOLTZMANN METHOD

The understanding of multi-phase fluid flow in porous media is one of the long-standing problems of computational fluid dynamics and is of great theoretical and practical interest. Problems such as enhanced recovery of oil, drainage and imbibition in soil, hydrocarbon migration, and ground water flow are but a few of the processes of interest to petroleum engineers, hydrologists and soil scientists. The description of two-phase fluid flow phenomena is far more complicated than single-phase flow, because it involves more complex interactions, such as surface tension and wettability. Recently, the lattice-Boltzmann method (LBM) has been introduced as a new computational tool to investigate multi-phase fluid flow in porous media [16, 17]. The LBM presents many ad-
rock used in LBM simulations should be of the same or-

vantages: it is easy to implement and due to the local
nature of the interactions and the lattice geometry its
algorithm is “embarrassingly” parallel. Moreover, flow
within complex boundaries, like porous media or blood
vessels, is easily treated, and multiphase flow properties
emerge from the simulation, without the need to es-

Several advantages: it is easy to implement and due to the local

tablish and to know a priori the shape of the fluid/fluid in-

terfaces.

Synchrotron based X-ray microtomography (XMT)
techniques provide high resolution, three-dimensional
digitised images of rocks. By using the LBM approach
in combination with these high resolution images, not
only is it possible to compute macroscopic transport co-
efficients, such as the permeability of the medium, but
information on local fields, such as velocity or fluid den-
sities, can also be obtained at the pore scale, providing
detailed insight into local flow characterisation and aid-
ing the interpretation of experimental measurements [18].

The possibility of simulating fluid flow in real rock sam-

tles allows direct comparisons to be made with experi-

mental results obtained on the same, or similar, pieces of

rock. To achieve a reasonable comparison, the size of the
rock used in LBM simulations should be of the same or-

der of magnitude as the system used in the experiments,
or at least large enough to capture the rock’s morphologi-

features.

A. Lattice Boltzmann theory

The LBM is a technique that permits the study of fluid
behaviour at mesoscopic length and time scales. Instead
of tracking individual atoms or molecules, the LBM de-
scribes the dynamics of the single-particle distribution
function of mesoscopic fluid packets.

In a continuum description, the single-particle distri-
bution function \( f_1(r, v, t) \) represents the density of fluid

particles with position \( r \) and velocity \( v \) at time \( t \), such

that the density and velocity of the macroscopically ob-
servable fluid are given by \( \rho(r, t) = \int f_1(r, v, t) dv \)

and \( u(r, t) = \int f_1(r, v, t) v dv \) respectively. In the non-

interacting, long mean free path limit, with no externally

applied forces, the evolution of this function is described
by the Boltzmann equation

\[
(\partial_t + v \cdot \nabla) f_1 = \Omega[f_1].
\]

While the left hand side describes changes in the dis-

tribution function due to free particle motion, the right hand

side models pairwise collisions.

By discretising the single-particle distribution func-
tion in space and time, one obtains the lattice-Boltzmann
description, where the positions \( r \) on which \( f_1(r, v, t) \)
is defined are restricted to points on a Bravais lattice.
The velocities \( v \) are restricted to a set \( c_i \) joining points
on the lattice and the density of particles at lattice site

\( r \) travelling with velocity \( c_i \), at timestep \( t \) is given by

\[ f_i(r, t) = f(r, c_i, t). \]

The collision operator \( \Omega \) (Equa-
tion (1)) is often simplified to the linear Bhatnagar-Gross-

Krook (BGK) form [19]. It can be shown that distribu-
tions governed by the simple Boltzmann-BGK equation con-
serve mass, momentum, and energy [20]. They obey a
non-equilibrium form of the Second Law of Thermody-
namics [21] and the Navier-Stokes equations for macro-
scopic fluid flow are obeyed on coarse length and time

scales [21, 22].

Algorithmically, the discretised Boltzmann description

can be evolved as a two-step procedure. In the collision
step, particles at each lattice site are redistributed over the

velocity vectors; this process corresponds to the action of
the collision operator. In the advection step, values of the
post-collisional distribution function are propagated to

adjacent lattice sites.

By combining the two steps, one obtains the so-called
lattice Boltzmann equation (LBE)

\[ f_i(\mathbf{r}, t+1) - f_i(\mathbf{r}, t) = \Omega[f] = -\frac{1}{\tau} \left[ f_i(\mathbf{r}, t) - N_i(\rho, \mathbf{u}) \right] , \]

where \( \tau \) is the typical relaxation time (proportional to the fluid viscosity) toward the equilibrium distribution function \( N_i \), which is a polynomial function of the local density and velocity, and can be found by discretising the Maxwell-Boltzmann equilibrium distribution.

To model multiphase flow, our implementation uses the Shan-Chen approach [23], by incorporating an explicit forcing term in the collision operator in order to model multicomponent interacting fluids. Shan and Chen extended the single-particle distribution function \( f_i \) to the form \( f^\sigma_i \), where each component is denoted by a different value \( \sigma \), so that the density and momentum of a single component \( \sigma \) are given by \( \rho^\sigma = \sum_i f^\sigma_i \) and \( \rho^\sigma \mathbf{u}^\sigma = \sum_i f^\sigma_i \mathbf{c}_i \), respectively. In order to produce nearest-neighbour interactions between fluid components, the force term assumes the form

\[ \mathbf{F}^\sigma = -\psi^\sigma(\mathbf{r}) \sum_\sigma g_{\sigma\sigma} \sum_i \psi^\sigma(\mathbf{r} + \mathbf{c}_i) \mathbf{c}_i, \]

where \( \psi^\sigma(\mathbf{r}) = \psi^\sigma(\rho^\sigma(\mathbf{r})) \) is an effective charge for component \( \sigma \), which we have chosen of the form \( \psi^\sigma(\mathbf{r}) = \rho^\sigma(\mathbf{r}) \) [23], and \( g_{\sigma\sigma} \) is a coupling constant controlling the strength of the interaction between two components \( \sigma \) and \( \bar{\sigma} \). If \( g_{\sigma\bar{\sigma}} \) is set to zero for \( \sigma = \bar{\sigma} \), and to a positive value for \( \sigma \neq \bar{\sigma} \) then, in the interfacial region between bulk domains of each component, particles experience a force in the direction away from the interface, producing immiscibility.

\[ \psi^\sigma(\mathbf{r}) = \psi^\sigma(\rho^\sigma(\mathbf{r})) \]

B. Results

The whole set of XMT data set (shown in Figure 4) used for this study describes a Bentheimer sandstone sample of cylindrical shape with diameter 4mm and length 3mm. The XMT data were obtained at the European Synchrotron Research Facility (Grenoble) at a resolution of 4.9\textmu m, resulting in a data set of approximately 816x816x612 voxels. Simulations in subsamples of different size (up to 512\textsuperscript{3} voxels) were carried out using the LBM method. The resources used were NCSC and Lemieux (PSC) on the TeraGrid, the NGS (Oxford and Leeds nodes) for running a large number of simulations and Bezier, the Manchester SGI Onyx2, as the visualisation engine.

We computed the rock permeability using Darcy’s law, a well known relation stating that the flow rate per unit cross sectional area, \( J \), is proportional to the force driving the fluid, the coefficient of proportionality being the permeability of the medium, \( K \), divided by the dynamic viscosity of the fluid \( \mu \). Darcy’s law can be written as

\[ J = -\frac{K}{\mu} (\nabla P - \rho g), \]

where \( \nabla P \) is the pressure drop between inlet and outlet, \( \rho \) is the fluid density and \( g \) is a body force (for example due to gravity). By measuring (or calculating) the flux for different pressure drops (or body force values), and using Equation (4), the permeability \( K \) can be derived. In our simulations we have always set \( \nabla P = 0 \).

For single phase flow, we found a strong dependence of the rock permeability on system size, with a plateau reached only when the system size is equal or greater than 128\textsuperscript{3} voxels. For large system sizes we found a value of permeability of 4 Darcys, which is the same order of magnitude as the experimental value (2 Darcys) [24].

For binary immiscible phase flow in porous media there is no widely accepted macroscopic relation such as Darcy’s law. Coupling between two fluids or any flow-driven change in the interface geometry may be important, and it is unclear why the two-fluid system with non-linear capillary force would obey a linear relation between flux and driving force [17, 25]. However, if two fluids were macroscopically separated in the porous medium, the two-phase flow would satisfy an extended form of Darcy’s equation

\[ J_i = \sum_{j=1,2} k_{ij}(S_w) \frac{K}{\mu_i} X_j, \quad (i = 1, 2) \]

where \( J_i \) is the flux of the \( i \)th component and \( X_j \) is the force acting on the \( j \)th component. The terms \( k_{ij}(S_w) \) are called relative permeabilities, and depend on the mixture composition \( S_w \). \( K \) is the permeability of the medium and \( \mu_i \) the viscosity of component \( i \).

Laboratory measurements of relative permeability are very difficult to perform and are also very time-consuming and costly. An alternative is to obtain multiphase fluid properties through numerical flow simulations. We calculated the relative permeabilities of a binary mixture of two immiscible fluids at different compositions in a subsample of the Bentheimer sandstone of 128x128x256 voxels. The properties of the two fluids are
identical, but the rock walls are made wettable by one of the two fluids (the wetting phase), hence introducing an asymmetry in the system.

We found a linear dependence of the flux on the fluid driving force, with the wetting fluid flow rate smaller than that of the non-wetting one, due to lubrication effects. Similar results have been found in three-dimensional lattice-gas and lattice-Boltzmann studies of binary flow in Fontainebleau sandstone [26–28].

The relative permeability values and snapshots (as two dimensional slices perpendicular to the direction of the fluid driving force) for different saturations of the wetting fluid ($S_{w}$) are shown in Figure 5. The qualitative trend as a function of mixture composition is in agreement with experimental results. It is also interesting to point out that, in spite of a lack of observable phase separation at very low wetting phase saturation ($S_{w}=0.1$), the presence of rock wettability induces the formation of domains, with the wetting fluid adhering to the rock surface (first snapshot on the top left in Figure 5). A more detailed discussion will be presented in a forthcoming paper [24].

C. Advantages of using Grid technologies

There are obvious advantages to be gained from harnessing a large number of supercomputers connected on a high performance computing Grid. Here, we wish to emphasise how the ability to interact with and thereby orchestrate such simulations through computational steering brings added value to Grid computing when compared to performing many independent simulations.

In the LBM simulation of two phase flow in porous media, or in general in complex geometries, it is difficult, if not impossible, to know a priori how long a simulation should run before steady state is reached. The presence of immiscible fluids, and the mechanical dispersion due to the structure of the porous medium, may result in interfaces that change with time, which makes the concept of a steady state virtually meaningless. Also, the stability of the interfaces may depend on the flow rate, i.e. on the strength with which fluid flows through the porous medium. For low flow rates, the interfaces may be stable, while they may change with time if the flow rate is sufficiently high. Moreover, the stability of the interfaces could depend on the parameter controlling the surface tension at the interface between the two immiscible fluids (the coupling parameter in Equation (3)). Also, a dependence on the mixture’s composition may be observed; for example, if one of the two phases is present in low concentration, small bubbles of this phase may form, which can freely flow through the system (see snapshot at bottom right in Figure 5). Steering and visualisation are powerful tools to investigate the effect of such conditions on the behaviour of the flow field and stability of interfaces, thus avoiding wasting CPU time if the steady state is reached or, on the other hand, allowing a simulation to continue if interesting behaviour in the dynamics of the interfaces is found. Remote visualisation makes it possible for the scientist to monitor the running simulations, and explore the system behaviour in real time, as the relevant parameters are changed. This avoids the need to run several test jobs, producing hundreds of gigabytes of data which would have to be analysed a posteriori, with a considerable waste of resources and time, instead providing the scientist with an intuitive feeling for how the system behaves and which parameters are relevant.
V. CONCLUSIONS

Thanks to the extensive efforts we have invested in providing a more robust infrastructure and to the expertise gained in the process by end-users, scientists at the CCS are now able to set up the RealityGrid computational steering framework in a considerably shorter time than before, and launch, steer and visualise applications in a considerably shorter time than before, and launch, steer and visualise applications on Grid resources to perform scientific research.

We are already using RealityGrid infrastructure for large scale lattice-Boltzmann [29, 30] and molecular dynamics applications, such as STIMD (Steered Thermodynamic Integration using Molecular Dynamics) [31, 32] and the SPICE (Simulated Pore Interactive Computing Experiment) component of a Joint US/UK EPSRC/NSF funded High End Computing Project [33], and in the Integrative Biology e-Science Pilot Project [34, 35] and steered coupled models [36].

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[34] Integrative Biology, http://www.integrativebiology.ox.ac.uk/.
