The Application Hosting Environment: Lightweight Middleware for Grid-Based Computational Science

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Abstract

Grid computing is distributed computing performed transparently across multiple administrative domains. Grid middleware, which is meant to enable access to grid resources, is currently widely seen as being too heavyweight and, in consequence, unwieldy for general scientific use. Its heavyweight nature, especially on the clientside, has severely restricted the uptake of grid technology by computational scientists. In this paper, we describe the Application Hosting Environment (AHE) which we have developed to address some of these problems. The AHE is a lightweight, easily deployable environment designed to allow the scientist to quickly and easily run legacy applications on distributed grid resources. It provides a higher level abstraction of a grid than is offered by existing grid middleware schemes such as the Globus Toolkit. As a result the computational scientist does not need to know the details of any particular underlying grid middleware and is isolated from any changes to it on the distributed resources. The functionality provided by the AHE is 'application-centric': applications are exposed as web services with a well-defined standards-compliant interface. This allows the computational scientist to start and manage application instances on a grid in a transparent manner, thus greatly simplifying the user experience. We describe how a range of computational science codes have been hosted within the AHE and how the design of the AHE allows us to implement complex workflows for deployment on grid infrastructure.

Key words: grid computing, scientific workflows, middleware, service oriented architecture, web services *PACS:* 47.11.Mn, 87.57.Ra, 07.05.Tp, 89.20.Ff

1 Introduction

We define grid computing as distributed computing performed transparently across multiple administrative domains [1,2]. By grid computing, we refer to any activity involving digital information - computational processing, visualisation, data collection from instruments and computational analyses, database access, storage and retrieval [1] - performed by utilising computational, visualisation, network and storage resources available on a grid. Grid computing has immense potential for computational scientists. A grid composed of resources belonging to different institutions has the potential to provide a level of service and support that cannot be expected from intra-institutional resources or even an existing set of independent resources which are not integrated into a grid as such. Some of the benefits possible from using grid infrastructure include capacity for increased workload volumes, faster response times/turn-around times for the user, and increasing the frequency of running analyses. Integration of resources into a grid infrastructure allows for better consolidation and workload management and may result in reduction of overall costs for grid resource owners. Grids can be used to solve computational science problems that could not be solved by a single resource either at all or efficiently, possibly due to compute, memory, data or network limitations [3,4]. A grid provides a flexible and dynamic infrastructure based on open standards which scales efficiently as the number of component resources increases. A general computational grid should provide easy access to computational, visualisation, storage, network and other resources, enabling computational scientists to pick and choose those required to achieve their widely varying scientific objectives.

Many emerging grids are in operation around the world, for example, the UK National Grid Service (NGS) [5], US TeraGrid [6], Enabling Grids for E-sciencE (EGEE) [7] and Distributed European Infrastructure For Supercomputing Applications (DEISA) [8] in the EU and the Japanese National Research Grid Initiative (NAREGI) [9], which make capability for computational processing, data storage and visualisation on high speed networks available to computational scientists. The engagement of scientists in grid activities is essential for such grids to mature into genuine productionlevel infrastructure which can deliver the much heralded potential of grid computing to the international computational science community.

2 Motivation for the Application Hosting Environment

Grid architecture consists of various components including grid middleware, application programming interfaces (APIs), software development kits,

protocols, services, system software and hardware [10]. In our efforts over the past four years to utilise grids to address new challenges in computational science and engineering, we have experienced significant barriers, particularly when dealing with heavyweight grid middleware [11]. Transparency, implying minimal complexity for computational scientists using grid technology, has been missing from existing distributed computing infrastructures that might aspire to call themselves grids. In this paper, we present the approach we have taken to address and overcome the heavyweight grid middleware problem.

Grid middleware is the software layer that transforms distributed, heterogeneous resources spanning multiple administrative domains into a single, integrated grid so that the heterogeneity and multiplicity of the distributed resources is transparent to the user. The user interacts with all the heterogeneous resources in the grid through a uniform interface. Thus, middleware is a critical component of grid infrastructure and its lack of usability has been a major barrier to the uptake of grid technology. Many of the current grid middleware solutions can be characterised as what we describe as 'heavyweight', that is they display some or all of the following features: (i) the grid middleware's client-side software, which is what the users/computational scientists have to interact with on their desktops, is difficult to install and configure, (ii) has non-negligible dependencies on supporting software (iii) requires non-standard ports to be opened within client-side firewalls and (iv) the server-side components of the grid middleware exhibit the same heavyweight characteristics as the client-side software; in most cases the situation is worse on the server-side. As a result, the user faces significant obstacles in deploying and using many of the current grid middleware solutions. This has led to reluctance amongst many scientists to actively embrace grid technology [11]. It is important for the development of grid computing as a whole that as many diverse groups of scientists as possible begin to use grids; it is crucial that the uptake of grid technologies occurs beyond specialized grid-centric projects [12,13,14]. While some progress has been made in the field of grid middleware technology [15,16], the prospect of a heterogeneous, on-demand computational grid as ubiquitous as the electrical power grid is still a long way off.

To address these deficiencies, there is now much attention focused on 'lightweight' middleware solutions [17,18,19,20], which attempt to lower the barrier of entry for grid users. Our efforts to address these deficiencies have been concentrated on the development of the Application Hosting Environment (AHE), a lightweight WSRF [21] compliant, web services based environment for hosting scientific applications. The AHE alleviates many of the problems posed by heavyweight grid middleware for computational scientists, who are among those who stand to benefit the most from grid computing. The AHE allows scientists to quickly and easily run unmodified application codes on grid resources, managing the transfer of files to and from the grid resources and allowing the user to monitor the status of application instances that are run on the grid. In the AHE, we adopt a standards-based web services approach to expose scientific applications on the grid as stateful web services.

From a computational scientist's perspective, a web service is simply any computational application functionality that is accessible over a network as a service, that can be invoked in multiple contexts, possibly to form higher-level services. The description of the services provided by the AHE is standards-compliant [22] so that they can be invoked using any web services compliant client (see Appendix B for more details). The AHE design is influenced by our previous work on WEDS (WSRF-based Environment for Distributed Simulation) [18], a hosting environment designed for operation primarily within a single administrative domain. The AHE differs from WEDS in that it is designed to operate seamlessly across multiple administrative domains, in a true grid sense.

3 Design of the Application Hosting Environment

The AHE is an ensemble of programs written in Perl with Java-based command-line and Graphical User Interface (GUI) client tools. The purpose of the AHE is to provide a mechanism for deploying applications onto computational grids that makes it easy for the scientist to start and manage applications on the grid. The AHE has a client-server architecture in which as much of the complexity as possible is moved to the AHE server. This makes the AHE client thinner, with a reduced set of software dependencies, and easy to install. Our approach works better than the conventional and relatively inflexible portal approach as the AHE client is not constrained to being a web browser. The AHE client has been implemented as a desktop GUI application as well as an interoperating set of command-line tools, making it highly flexible and powerful as a tool for constructing lightweight workflows via scripting as described in Section 5. Furthermore, all state persistence occurs on the AHE server, which substantially increases client mobility.

To ensure that the AHE client is easy to install, configure and use, whilst providing maximum functionality, a number of design constraints were set on the overall design of the AHE:

- (1) We do not require the user to install Globus [15], Unicore [16] (or any other grid middleware) clients on his/her machine even if the grid, that he wishes to run applications on, uses such grid middleware.
- (2) We assume that the client device uses NAT (Network Address Translation [23]) and that the device is firewalled to only allow outgoing connections.

This effectively means that the client does not accept any inbound connections: all communication is out-bound and initiated by the client.

- (3) For maximum portability, we require that the client only supports HTTP [24], HTTPS [25] and SOAP [26].
- (4) The client does not have to be installed on a single machine; the user can move between clients on different machines and access the applications that have been launched from any one of them. The user can even employ a combination of different clients - for example, a command line client to launch an application and a GUI client to monitor it. The client therefore must maintain no information about an application instance's state. All state information is maintained as a central service on the AHE server that is queried by the AHE client.
- (5) The client machine needs to be able to upload input files to and download output files from a grid resource, but we assume it does not have GridFTP client software installed. A WebDAV-based intermediate file staging area is therefore used to perform file-staging between the client and the target grid resource.
- (6) The AHE client maintains no knowledge of the location of the application on the target grid resource, or how it should be run, and it maintains no information on specific environment variables that need to be set.
- (7) The client should not be affected by changes to a remote grid resource, for example if its underlying middleware changes to a newer version of the Globus Toolkit [15,27].
- (8) All communication is secured using Transport Layer Security (TLS) [28] with the user's X.509 certificate [29] used for encryption, authentication and authorization.

These design constraints have led us to an architecture in which the AHE client is extremely lightweight and simple to deploy, with no dependencies except for the Java Runtime Environment [30]. It should be noted that this design does not remove the need for middleware solutions such as Globus or Unicore on the grid resource (which may be, for example, a US TeraGrid site or a supercomputer on the DEISA grid); indeed, we provide an interface to run applications on multiple resources with different underlying grid middlewares, so it is essential that the grid resource provides a supported middleware installation on their machines. The AHE uses GridSAM [31], a job submission and monitoring software, as its interface to the grid resources. GridSAM provides the AHE server with a uniform interface to the different type of grid middleware installed on a grid. See Section B and Figure B.1 for a brief discussion of GridSAM's role in the AHE architecture. The AHE removes the requirement to install any other middleware on the user's client machine: the user simply needs to install the lightweight AHE client to interact with the grid resources which may have heavyweight middleware installed on them. The AHE client currently provides a uniform interface to grid resources with installations of Globus Toolkit 2.4.3 [15], Grid Engine 6.0 u4+ [32], Condor v6.4, 6.6 and 6.7 [33] and Unicore [16] while work is in progress to enable interfacing to Globus Toolkit 4.0 [27] based grids. The recently developed Unicore support for AHE fulfils demand for the capability to launch applications on the EU DEISA grid [8] and brings with it the much sought after interoperability between Unicore-based grids and Globus-based grids.

In addition to the state information about all the application instances, the AHE server also stores all the necessary information about how an application should be run on the various computational grid resources and provides a single, uniform interface to the AHE client for running that application across all possible grid resources. This is particularly useful for applications that run on supercomputers which often have unique deployment scenarios and require special runtime environments. Storing this deployment/configuration information on the AHE server as a central application-specific service is an efficient mechanism for making the information available and useful to a large number of users at once.

The AHE design is based around the notion that very often a group of researchers will want to run the same application, but not all of them will possess the skill or inclination to install the application on a remote set of grid resources. In the AHE, we therefore distinguish between experts and endusers. An expert user installs the application and configures the AHE server, so that all participating users can share the same application on the grid at large. The end-user simply needs to download and install the lightweight AHE client and is then able to trivially access such 'centrally installed' applications.

The design of the AHE is novel in its application-centric approach, according to which we treat the computational 'application' as a higher level entity than a computational 'job'. Computational steering applications [34,35], coupled model simulations [36,37] and workflows [38,39,40] are cases where applications and jobs can be clearly distinguished. In the initial AHE release, applications and jobs stand mainly in a one-to-one relationship except for the case of workflow applications. Complex workflow applications have been deployed on grids using the AHE wherein the workflows are composed of simpler computational jobs. This is discussed in more detail in Section 5. By providing a service that will launch a particular application rather than a generic computational job it is possible to reduce the complexity of the client and make the scientist's life easier. The scientist can then concentrate on science rather than spending time understanding and installing middleware and managing individual jobs.

4 Application Hosting

An application is said to be grid-enabled when it is able to run on multiple heterogeneous resources comprising a grid. In the computational science domain, the AHE provides a mechanism to expose an unmodified application as a standards-compliant web service. Appendix A and B provide more technical detail about how this is done.

When an application is launched on a grid resource using the AHE, that instance of the application is referred to as the application instance. In other words, the user can launch many application instances for an application which is hosted in the AHE. Any kind of modelling and simulation application can be hosted within the AHE. To the best of our knowledge, all of the applications currently hosted in the AHE are simulation codes as discussed in Section 4. We therefore use the term simulation instead of application instance in much of the following discussion of the AHE. However, the same discussion is applicable, more generally, to instances of any other type of application hosted in the AHE.

We currently host a number of scientific applications within the AHE including the highly scalable molecular dynamics (MD) codes DL_POLY 3.01 [41], NAMD [42], LAMMPS [43] and GROMACS [44] and the lattice-Boltzmann (LB) code, LB3D [3,45,46]. Scientists can use the AHE client to launch these applications on a grid; in particular, we currently use the AHE to run these applications on the UK NGS and US TeraGrid resources. The AHE does not require the application to be modified as long as the application is reasonably well-behaved with respect to the run parameter specification, file-naming and file-location conventions.

We next describe, how to run such applications on a grid using the AHE. Most of the steps involved are common to all applications. Then we discuss some of the specific applications currently hosted in the AHE. Lastly, we describe how the AHE client and server can be configured to host a new application.

4.1 Running hosted applications

The steps involved in running an application instance on a grid using the AHE are listed below. We present the steps in terms of running application instances of simulation type applications. The AHE GUI client is implemented in the familiar 'wizard' fashion; each step in the launching process is presented to the user as a separate screen in the GUI with controls to navigate between

screens:

- (1) In the AHE client wizard, the user first specifies the particular application that he wishes to run, e.g., DL_POLY, and other constraints such as the number of processors on which to run it, maximum wall time required and so on. The AHE server returns a list of grid resources on which the application is installed and that match the constraints. The user then selects the grid resource on which he wants to run the simulation.
- (2) Next, the AHE client wizard prompts the user to specify the location of the input files and the names of the output files that would be produced at the end of the simulation. In the most general case, the user can manually specify the locations of input files and the names of output files. However, the AHE client has a plug-in parser feature, whereby application-specific plug-in parsers can be integrated into the client automating the file management operations. This is discussed in more detail in Sections 4.2 and 4.3
- (3) The user then uses the AHE client wizard to start the simulation on the grid resource.
- (4) Once the simulation has started, the user can manually check the simulation status or choose either to set the AHE client to poll the status of the simulation or to shut-down the client and return at a later time to retrieve the simulation status. The user can use any machine with an AHE client installation, not necessarily the one from which the simulation was started to monitor his/her simulations. This is ideal in situations where the user would like to access the simulation state, including the input and output files, from different machines.
- (5) Apart from monitoring the status of the simulation, users can also terminate their simulation before normal completion using the AHE client.
- (6) Finally, when the simulation has completed, the user can transfer all the input and output files on the remote grid resource at the click of a button. The task of recovering output files scattered around a (global) grid has been very tedious until now and this feature of the AHE has greatly enhanced the productivity of grid users.
- (7) The user may then destroy all memory of the simulation on the AHE server or can allow the simulation state to persist on the AHE server to review it in the future. Note that a review may involve retrieving the simulation input and output files at a later time.

The combination of the capability to parse configuration files in order to discover input and output files, to automatically stage the files to and from the grid resources, and to review the state of the simulation including associated files long after the simulation has finished, makes the AHE an extremely powerful tool for addressing the challenge of solving the provenance problem especially when one wishes to run a large number of application instances distributed across a grid.

4.2 Example applications

DL_POLY

DL_POLY [41] is a parallel molecular dynamics package for simulations of macromolecules, polymers, ionic systems and solutions. We host DL_POLY within the AHE for users who wish to run molecular dynamics (MD) simulations with DL_POLY on the UK NGS core nodes and the HPCx facility [47]. This makes it trivial to launch DL_POLY simulations on these grid resources using the AHE client wizard.

A DL_POLY specific plug-in parser has been integrated into the AHE client, so that the user simply needs to specify the location of the CONFIG, file on his/her local machine and all the input files, such as CONTROL, FIELD and/or TABLE, etc., automatically get staged to the remote grid resource at the start of the simulation.

Once the simulation has terminated, the user can, at the click of a button, retrieve all the input and output files from his/her DL_POLY simulations, for example, the OUTPUT, REVCON, REVIVE, STATIS files to the local machine.

NAMD and LAMMPS

We host NAMD and LAMMPS within the AHE for users who wish to run MD simulation with these applications on the UK NGS core nodes and US TeraGrid sites. NAMD [42] is a parallel molecular dynamics code primarily used for large-scale bio-molecular simulations. LAMMPS [43] is a parallel molecular dynamics code with optimizations for long-range interactions. It is trivial to launch NAMD and LAMMPS simulations using the AHE client wizard by following the steps described previously.

Plug-in parsers for NAMD and LAMMPS have already been integrated into the AHE client and are supplied with the AHE client download. These plugin-parsers allow the user to specify the location of the NAMD/LAMMPS configuration file from which the AHE automatically discovers and transfers all the input and output files that the application instance will consume and produce.

For example, the NAMD/LAMMPS configuration file along with the force-field paramete file, co-ordinate file, velocity file, and restart files that may be required to run the simulation are automatically staged to the grid resource at the start of the simulation. Since the simulation is run within a single working directory on the remote grid resource, any relative paths in the configuration files are removed. All input and output files that belong to a particular simulation are located in a uniquely associated working directory.

Once the simulation has finished the user can again, at the click of a button, retrieve all the output files from his/her simulation working directory on the remote grid resource.

GROMACS

GROMACS [44] is a highly optimized, parallel molecular dynamics simulation package extensively used for biomolecular simulations. We host GROMACS within the AHE for users who wish to run MD simulations with GROMACS on the UK NGS core nodes. A client parser plug-in makes it trivial to launch the application using either the AHE GUI or command-line clients.

GROMACS differs from most of the other applications currently hosted in the AHE in that it consists of two separate applications, namely a preprocessor (grompp) and the actual simulation code (mdrun). A Perl script has been created which runs on the grid resource and directs the output of the preprocessor to the input of the simulation code. This script is then hosted in the AHE and treated as a single application. A client configuration parser has also been created which takes its input from a 'meta' configuration file, allowing the user to specify parameters for both components of the application.

Once complete, the AHE client stages back both the output from the simulation code and certain important intermediate files created by the preprocessor.

LB3D

LB3D [46] is a massively parallel implementation of the lattice-Boltzmann model for amphiphilic fluid dynamics [3,45] which is able to reproduce the morphological and rheological phenomena observed in ternary amphiphilic mixtures from purely bottom-up mesoscopic interactions. We have hosted LB3D within the AHE to run lattice-Boltzmann simulations on the UK NGS and US TeraGrid nodes. In this case, it was necessary for us to modify the application, as some features of the code were incompatible with the AHE design. LB3D produces output files whose names contain a randomly generated string while relying also on a pre-exisiting output directory at the start of the simulation. In order to be easily hosted within the AHE, it is preferable to know in advance the names of the output files that the code will generate during the execution so as to automate the process of output file retrieval. Moreover, in the AHE design, each independent execution of an application is associated with a unique working directory on the remote grid resource, within which the simulation is run and the staging and de-staging of input and output files occurs. It is, therefore, desirable for the application code to run within a single working directory. In grid environments, where because of the multiplicity of resources, one needs to keep track of output dispersed across various remote grid resources, it is particularly useful to have working directories associated with specific simulations.

4.3 Hosting a new application

To host an application within the AHE, the expert-user needs to configure the AHE server with the following application-specific information:

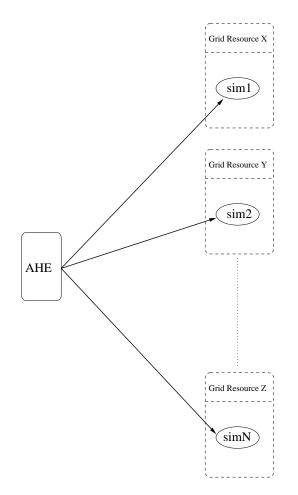
- (1) location of the application executable on the grid resources, e.g., NGS nodes and TeraGrid sites.
- (2) any environment variables that may be required to run the application on the different grid resources such as the path to dynamically linked libraries

The reader should consult the AHE server installation guide [48] for the exact location where this information needs to be stored. After configuring the AHE server with the above information, running a short script provided with the server distribution updates the registry of hosted applications to include the new application. There is no need to restart the AHE server once a new application has been added in this manner.

Once the above changes have been made to the server-side, the user is able to run the application using the AHE client in the generic mode, i.e. the AHE client does not require any modification when a new application is hosted. However, it is possible to write an application-specific plug-in parser for the AHE client which can parse the user-specified application configuration file to automatically discover the input and output files for the particular application instance that the user wishes to launch. The parsing capability allows the user to simply specify the location of the configuration file; the AHE client then automatically parses it to find out all the input file locations and output file names. Thus, when the simulation is started the input files are automatically staged to the remote grid resource and the output files are retrieved at the end of the simulation. Details of writing and integrating such a plug-in parser with the AHE client are specified in the AHE client user guide [49].

5 Scientific Workflows

In addition to the GUI, the AHE client includes a closed set of atomic command-line tools that replicate the essential operations in the AHE GUI client. For example, there are AHE command-line tools to 'prepare' an application instance for running on a grid resource, to 'start', 'monitor', 'terminate' and 'getoutput(files)'. Complex workflows composed of multiple simulations and/or calculations can be realised very simply by writing scripts that combine the command-line tool functionality. Here, we present three examples of how the AHE command-line tools can be combined to compose and deploy complex workflows.



5.1 Ensembles of simulations

Fig. 1. Running ensembles of application instances on a grid using the AHE. Application instances labelled as sim1, sim2,..., simN are started on computational resources on the grid using the AHE. The AHE manages input/output file-staging for each application instance to/from the associated grid resource. The user is able to monitor the status of all the application instances.

In the workflow depicted in Figure 1, the user wishes to launch a large number of independent simulations on the grid and retrieve the results for post-processing. There may be an additional requirement for these simulations to run concurrently. Despite their multiplicity, each simulation may be computationally expensive. For high-end applications, the capabilities needed can only be delivered by resources available on grids such as the UK NGS and US TeraGrid. Computational resources on the grid provide a flexible, low cost alternative to intra-institutional supercomputing resources for running such ensembles of simulations. Provided sufficient computational resources are available on the grid, deployment of the ensemble workflow via the AHE results in shorter turn-around time and greatly enhanced control of provenance for the simulation output data as compared to submitting each simulation individually on a local computational resource.

The ensemble functionality is currently being employed to run an ensemble of molecular dynamics simulations of the HIV-1 protease and inhibitors [38], each with a different starting configuration for the system, in order to obtain better statistics. Within the ensemble of simulations, the initial conditions are identical for the simulations except for the initial atomic velocity distributions, sampled from a Maxwell-Boltzmann distribution and randomised differently for the same system temperature.

Such ensembles of MD simulations are useful for thermodynamic integration (TI) calculations where multiple MD simulations need to be launched at different values of the dual topology parameter λ or where multiple short trajectory simulations can be launched on a grid to give insight into the thermodynamics of a single long trajectory simulation [50]. An alternative way to study TI calculations via chained simulations is discussed in Section 5.2.

Thus the AHE provides a simple way to write scripts in order to start simulations on multiple grid resources. The user needs only to specify the configuration file for each simulation; the AHE automatically discovers and stages input/output files to/from the remote grid resource without the user having to install any complicated grid middleware on his/her local machine. This feature is particularly useful when there are a large number of simulations to be launched on several resources which span multiple administrative domains.

The AHE server maintains a history of all the simulations that have been launched by each user and allows for their monitoring and review in the future. As noted previously, the user has the flexibility to change between client machines while still having a reference to his/her entire simulation history.

5.2 Chained simulations

In the workflow in Figure 2, the user wishes to launch a sequence of chained simulations where one application instance begins execution after the previous instance has finished and may depend on output from the previous instance's execution.

Such a workflow of chained simulations is currently being used by nu-

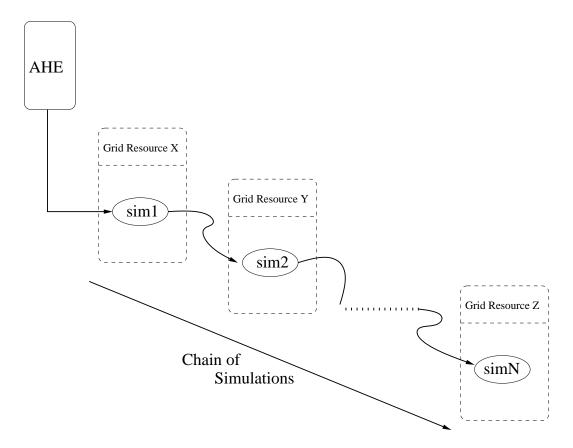


Fig. 2. Running a chain of application instances on a grid using the AHE. Application instances labelled as sim1, sim2,...., simN are started in sequence on computational resources on the grid using the AHE. The AHE manages input/output file-staging to/from the associated grid resources; piping the output from one application instance as input for the next application instance in the chain. The user is able to monitor the status of each application instance as the workflow progresses.

merous AHE users. In particular, the chained simulation capability is being used to study binding affinities of wild-type and mutant HIV-1 proteases with drug inhibitors [39]. In order to obtain a starting structure for the MD production runs, the initial artificially mutated HIV-1 protease wildtype crystal structure is equilibrated by subjecting it to a chain of equilibration simulations, each simulation corresponding to a step in the equilibration procedure. This is illustrated in Figure 3. The AHE is used to automate the

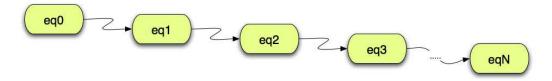
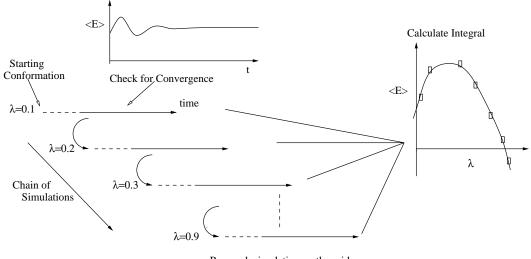


Fig. 3. Running a chain of MD simulations on a grid; each simulation corresponds to a different step in the initial relaxation of the system to equilibrium before production runs can be performed.

entire process of launching and managing the equilibration simulations in sequence on the grid, thus realising the workflow in Figure 3. The automation provided by AHE includes starting each simulation on different grid resources in sequence, transferring input files to the grid resource at the start and retrieval of output files at the end of each simulation. This feature is particularly valuable as it frees the user from the mundane task of keeping track of all the simulation data files and manually transferring them across the grid resources for the next simulation in the chain. Thermodynamic integration



Run each simulation on the grid

Fig. 4. Thermodynamic integration calculation consisting of a chain of simulations at different values of parameter λ is an ideal candidate for grid deployment. See text in Fowler *et al.* [34] for more details.

(TI) calculations [34,40], where each simulation is run at a particular value of the dual topology parameter λ ($0 \le \lambda \le 1$), such that the initial configuration for a simulation at $\lambda_n + 1$ is obtained from a simulation at λ_n , is another example of a workflow of chained simulations that can be deployed via the AHE. This is illustrated in Figure 4. As noted in Section 5.1, TI-type calculations can also be studied using an ensemble workflow. Additionally, one can imagine a chained workflow as in Figure 2 comprising of application instances belonging to different application types.

5.3 Concurrent simulations

In the workflow in Figure 5, the user wishes to launch concurrent and dependent simulations on multiple grid resources. The simulations may need to communicate with each other periodically during their execution. This type of workflow can be used to perform coupled model simulations [37] where the system being simulated spans multiple time-scales and/or

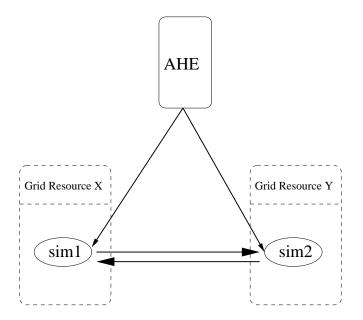


Fig. 5. Running coupled application instances on a grid using the AHE. Each application instance is executed on a separate grid resource via the AHE. The AHE can monitor the individual components as they execute.

length-scales. In order to accurately and efficiently simulate such systems, the different domains of the system are simulated at different levels of detail using distinct applications which communicate at regular intervals. See De Fabritiis *et al.* [36] for a description of such a multiscale computational technique that has successfully coupled molecular dynamics with Landau's fluctuating hydrodynamics to simulate sound waves propagating in bulk water and reflected by a lipid monolayer. Although such coupled models have not been deployed with the AHE yet, the AHE provides the infrastructure to start up the different applications on the grid, and once communication has been established and concurrent execution has begun, the AHE will enable the user to monitor individual applications and/or to terminate them, while at the same time furnishing a high-level overview of the entire coupled model application.

At the time of writing, there is a significant AHE user base with others planning to use it. Favourable experiences have been reported for NAMD and LAMMPS applications hosted within the AHE as compared to alternative strategies [15,18,35] for running jobs on grids [38]. As expected, from the design criteria, the key benefits for users have been:

- (i) minimal installation, configuration and maintenance effort on the clientside;
- (ii) flexibility of restarting or switching between clients so that the client need not be 'attached' to the grid in order to launch or manage jobs;
- (iii) automatic staging in of input files to a grid resource, third party file transfer between resources, and retrieval of distributed files to the local

machine on job completion;

(iv) no need to repeatedly submit individual jobs to many resources and monitor status across multiple grid resources.

Users have expressed the need for the capability to monitor queues on different grid resources. This capability can be provided by the AHE in future if the queue status information is published via a web service by the resource managers installed on the grid resources.

6 Future Developments

Future extensions of the AHE aim to add functionality that enables even more ambitious computational science projects to be undertaken on grids with ease. Globus Toolkit 4 (GT4) [27] and Unicore [16] are able to process jobs specified using the JSDL schema and we are exploring the possibility of future versions of AHE being able to directly submit jobs to Globus Toolkit 4 (GT4) and Unicore without the need for GridSAM (see Appendix B) as a third party tool to provide the web service interface for job submission. Work is underway to integrate the WSRF-compliant RealityGrid steering framework into the AHE [35], which will provide support for starting and managing steerable applications and coupled model applications hosted in the AHE. We plan to extend the current workflow functionality to orchestrate even more complex workflows, using the industry-standard BPEL language [51]. The scientist will be provided with graphical tools to interface with the BPEL workflow engine and easily implement their desired BPEL workflow operations.

We are now looking at new platforms on which the lightweight AHE client can be deployed. For example, work is underway on an AHE client that runs on mobile phones and PDAs [52] allowing scientists to launch and monitor simulations on the move. Co-allocation is one of the major challenges faced by computational scientists trying to perform cross-site runs using multiple concurrently available grid resources [14]. No automated advanced reservation and co-scheduling systems are in place yet within so-called production grids; performing cross-site runs [14] today requires human intervention for booking resources in advance and making sure these are indeed available at the desired time¹. A fault-tolerant web services compliant approach to co-allocation called HARC [55] has recently been proposed and implemented. The attractiveness of this scheduler stems from

¹ Note that the beta version of the NAREGI [9] software stack has a super-scheduler at the heart of its architecture [53] and claims to implement WS-Agreement [54] compliant co-allocation.

its ability to co-allocate (i) compute resources and (ii) lambda networks [56], which are dynamically provisioned optical networks for bandwidth intensive applications. An interface to the HARC system will be developed in the AHE client to provide support for automated, fault-tolerant co-allocation. We hope to provide support for MPICH-G2 [57] enabled applications in the future. Finally, we are also looking into the use of the AHE for accessing campus-based resources, often referred to as 'campus grids'. Ultimately, AHE could become a uniform interface to all computational resources.

7 Conclusions

Our goal in this work has been and continues to be to provide scientists with tools such as command-line interfaces that are simple and familiar, while at the same time furnishing access to a much more powerful set of resources on grids than previously available, allowing scientists to use their own creativity to achieve increasingly complex computational objectives. The AHE allows computational scientists to overcome the barrier of heavyweight, difficult-to-use grid middleware and thereby to take advantage of grid computing with much greater ease than has been possible hitherto. Grid computing has contributed significantly to the scientific programme within isolated, grid-centric computational science projects [3,12,13,58,59] but it still remains under-utilised among wider national and international computational science communities. The involvement of increasing numbers of computational scientists in grid activities is essential for determining best practices in grid scheduling policies, provisioning/orchestration policies and resource configuration. We hope that the AHE will help to realise these goals.

8 Distribution and Installation

The first release of the AHE was made available on 31 March 2006. The AHE (Version 1.0.1) client and server software can be downloaded from the Reality-Grid website at http://www.realitygrid.org/AHE or the NeSCForge website at http://forge.nesc.ac.uk/projects/ahe. Future releases will continue to be available from the RealityGrid website. Documentation, including installation and configuration of the AHE to run applications on the UK NGS and US Tera-Grid, is also available from these websites. Subscription to the AHE mailing list is open at http://www.mailinglists.ucl.ac.uk/mailman/listinfo/ahe-discuss.

A version of the AHE software, Version 1.0.2, has also been developed in which the AHE server can be hosted within the Apache Jakarta Tomcat container [60]. This version of the AHE is distributed via the Open Middleware Infrastructure Institute UK (OMII-UK) [61] within the latest OMII 3.2.0 server and client software which was released on 12 November 2006. This version of the AHE conforms to the OMII Integration Specification and is easily installable and integrated with the rest of the OMII distribution including WSRF::Lite [62] and GridSAM [31] which are pre-requisites for the AHE. OMII 3.2.0 server and client software is available for download at http://www.omii.ac.uk.

9 Acknowledgements

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A Web Services and the Application Hosting Environment

In the AHE, we have adopted the Service Oriented Architecture (SOA) approach to providing applications as services on the grid. Web services are one way of realizing SOA. As mentioned in the main text, from a computational scientist's perspective a web service is simply any computational functionality accessible over a network as a service. The term 'service' implies that the user simply needs to know the description of the service in order to invoke it and does not need to know how the functionality of the service is actually implemented; this is particularly important on a heterogeneous grid. Hence, in order for the web services have standards-compliant interfaces. In the AHE, we use WSRF::Lite [62], a perl library that provides the framework for writing web services. In this Service Oriented Architecture (SOA) approach, the key concept is that of loosely coupled components, i.e., web services, that interact via SOAP messages and whose interface is described by documents conforming to the WSDL standard [22].

There are obvious benefits to the adoption of a standards-based, dynamic and flexible approach to running applications on heterogeneous grid resources and managing the state of the application instances in a uniform, integrated way. Such an approach allows flexible integration of multiple applications to accomplish complex computational tasks on the grid, as we aspire to do with the AHE's workflow functionality. Also, the widespread adoption of the web services approach in industry and academia permits grid computing practitioners to take advantage of numerous existing web services and web services development tools that are independently being made available to the community and to take advantage of the significant standardization and inter-operability efforts which clearly also address significant issues in grid computing.

In the AHE, an application instance is represented as a transient stateful web service Resource WS-Resource [21]. The WS-Resource properties associated with the application instance include

- the application instance's reference handle or the EndPoint Reference(EPR)
- status of the application instance
- a trivial name to refer to the simulation
- date and time when the application instance was started,
- the grid resource on which its running,
- names and URLs of the input files
- names and URLs of the output files.

Each time an application is run on the grid, a WS-Resource [21] is created on the AHE server-side, and is used to represent that instance of the application's execution. This WS-Resource provides an interface for the user to interact with the application instance. The WS-Resource corresponding to the application instance and its WS-Resource properties are stored on the AHE server in a database referred to as the 'App Instance Registry'. This is described in more detail in Appendix B. The WS-Resource properties can be queried at any time using the AHE client or any other web services compliant client. In this way the AHE provides a uniform interface for managing simulations of various scientific application codes deployed on multiple grid resources.

The WS-Resource persists even after the application instance has finished executing, providing information on the location of any output files as well as the input files and configuration parameters used to initially run the application. This is a powerful provenance capability of the AHE, as the user can return at a later time and review the simulation by querying the properties of the associated WS-Resource.

B AHE Architecture

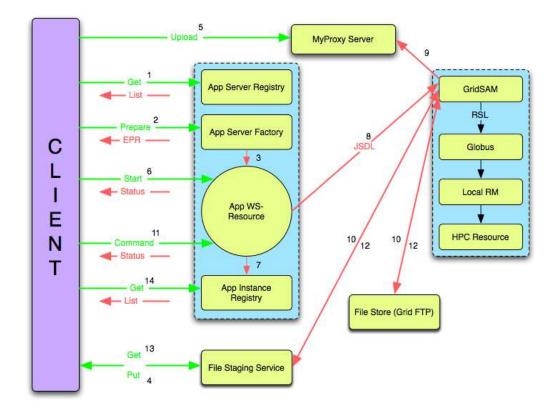


Fig. B.1. Architecture of the Application Hosting Environment; the numbers denote operations performed between the AHE client, AHE server, File Staging Service, File Store, MyProxy server and Grid Resources. See the text in Appendix B for a detailed description of this diagram.

WSRF::Lite

The AHE is developed with WSRF::Lite, a Perl implementation of the Web Service Resource Framework (WSRF [21,63]) specification which has been ratified by the OASIS [64] standards body. WSRF::Lite is the follow-on from OGSI::Lite, the Perl implementation of the Open Grid Service Infrastructure (OGSI [65]) specification from GGF [66]. It is built on SOAP::Lite [67] the Perl module for web services from which it derives its name.

In the current release of the AHE, we host the WS-Resources on the serverside within the Apache web server and store the WS-Resource properties in a PostgreSQL [68] database. The PostgreSQL [68] database storing the simulation's state can be replicated and backed up non-locally to provide fault tolerance.

GridSAM

The AHE currently accesses computational resources on the grids via middleware called GridSAM [31]. GridSAM provides a web services interface, running in an OMII [61] web services container, for submitting and monitoring jobs on grid resources with various Distributed Resource Managers (DRMs) - Globus 2.4.3 [15], Grid Engine 6.0 u4+ [32] and Condor v6.4, v6.6 and v6.7 [33] - via its DRM connector-based plugin-in architecture. GridSAM has a plug-in architecture that allows connectors for different types of DRMs to be integrated into it, thereby adding the functionality to submit and monitor jobs on resources with those DRMs.

Computational jobs submitted to GridSAM are described using another emerging standard, the Job Submission Description Language. GridSAM consumes Job Submission Description Language (JSDL [69]) documents and performs the task of 'job' submission to the target grid resource.

File Staging Area (FSA)

The 'File Staging Area' (FSA) is designed to allow the client to use the Web-DAV [70] file transfer protocol to 'GET' (step 13 in Figure B.1) or 'PUT' (step 4 in Figure B.1) a file on the WebDAV server so that it can be downloaded by GridSAM on to the target grid resource (step 10/12 in Figure B.1). This is designed to handle the case where input files exist on the user's client machine and these need to be transferred to the grid resource. Similarly, the FSA is useful when files need to be retrieved from the remote grid resource to the local client machine. The FSA provides an intermediate file-staging area, albeit one which is accessible via normal HTTP GET and PUT mechanisms and is useful for pulling down the simulation input/output files from anywhere on the grid using nothing more than a web browser or potentially a PDA. We consider this type of file transfer as 'pass by value' since the client actually transports the file to the FSA.

FileStore

For much larger input/output files, which the user may not wish to download to his/her local machine, the AHE supports third-party file transfer using a 'FileStore' mechanism. The FileStore is any place on the grid where files required by the instance of the application are available through GridFTP or HTTP. The FileStore is used to hold large files like checkpoints that would not normally be stored on the client machine. The AHE client passes the URL [71] of the source input file or target output file to the AHE server and the input files automatically get staged from the FileStore to the grid resource on which the simulation is to be run or the output files from the grid resource automatically get staged out to the desired target FileStore. These are steps 10 and 12 in Figure B.1. We call this 'pass by reference' Note that FileStore may be a grid resource providing a storage service such as the data nodes on the UK NGS.

MyProxy

Security is critical in any grid computing environment [1]. We chose not to

use WS-Security [72,73] for the AHE because message level security is not required: we do not have any intermediaries for relaying SOAP messages. In the AHE, communication is via HTTPS to provide Transport Layer Security (TLS [28]); mutual authentication is used between the AHE client and the AHE server using X.509 digital certificates [29]. For users of the UK NGS [5], digital certificates or e-Science certificates can be obtained from the national certification authority [74]. Within the AHE, the App WS-Resource is given access to a proxy certificate [29] stored on a MyProxy [75] server. The AHE server implements fine-grained authorization in that only the owner of the simulation has access to its properties. This can be extended to provide group access or open access analogous to the UNIX file system permissions for collaborative work.

App Server Registry

The 'App Server Registry' maintains a registry of all the applications that are hosted within the AHE, such as, DL_POLY [41], NAMD [42], LAMMPS [43], GROMACS [44] and LB3D [3,45,46]. The user can query the registry (step 1 in Figure B.1) to find the address for the service factory that provides a particular application.

App Server Factory

The 'App Server Factory' is a web service based on the Factory Pattern [76] which creates a new App WS-Resource on the AHE server each time the user invokes the Prepare operation.

App WS-Resource

The 'App WS-Resource' exists on the AHE server and is a WS-Resource representing a particular application instance. The user invokes the Prepare operation of the App Server Factory whenever an application instance needs to be launched on the grid. For each invocation of the Prepare operation, a new App WS-Resource is created on the AHE server and its WS-Resource properties are initialized as per the application instance parameters specified by the user.

App Instance Registry

The AHE server maintains an 'App Instance Registry' which contains the history of all application instances/WS-Resources that the user has launched/created. The App Instance Registry is implemented by a PostgreSQL [68] database. The user can query the App Instance Registry to get a list of all the application instances launched and the associated WS-Resource properties. Collaborative analysis of simulation histories is greatly aided by the stored WS-Resource properties that can be accessed online via the App Instance Registry.

We now briefly describe the numbered operations in Figure B.1:

- (1) User retrieves a list of applications hosted within the AHE from the App Server Registry.
- (2) User invokes the Prepare operation in step 2 on the App Server Factory.
- (3) As a result of the invocation of the Prepare operation, the App Server Factory creates a new App WS-Resource representing the instance of the application. The App Server Factory returns a WS-Addressing [77] End-Point Reference (EPR) to the client which the client uses to communicate with the App WS-Resource.
- (4) The AHE client automatically transfers the user's input files to the File Staging Area.
- (5) The user uploads his/her proxy credential to the MyProxy server. This is then valid for one week by default.
- (6) The user starts the application instance and the AHE returns the initial status of the application instance.
- (7) Once the App WS-Resource is created as a result of the Prepare operation, its reference handle and associated properties are stored in the App Instance Registry (see 3 above).
- (8) The AHE server creates one or more JSDL documents based on the user's specification of the application instance and submits them to GridSAM which then starts the application instance on the target grid resource.
- (9) The App WS-Resource uses the proxy certificate for authentication with the various grid resources that the user wishes to use.
- (10) The input files are staged from the FSA to the target grid resource on which the application instance will be executed.
- (11) The user can use the AHE client to invoke, monitor and terminate commands on the App WS-Resource in order to check the status and, if need be, to terminate the application instance.
- (12) Once the job finishes, the output files are transferred from the grid resource to the FSA.
- (13) The user can use the AHE client to manually or automatically download the output files from the FSA.
- (14) The user can query the App Instance Registry to review the history of application instances.

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