THE UNIVERSITY OF
WARWICK

THE UNIVERSITY OF WARWICK

Research Report 394

# REVIEW OF THE E-SCIENCE DEMONSTRATORS AND THEIR COMPATIBILITY WITH THE WARWICK MIDDLEWARE PROJECT

*Stephen Jarvis, Graham Nudd*

Department of Computer Science
University of Warwick, Coventry CV4 7AL, UK

# Review of the e-Science Demonstrators and their compatibility with the Warwick Middleware Project


**Authors:**

**S A Jarvis, G R Nudd**
High Performance Systems Group,
Department of Computer Science, University of Warwick


**Date:** **31-3-2003**


**Abstract:**

This document reports on the six month survey of the UK e-Science demonstrator projects. The report details the eight project consultations in which we have engaged, and provides a summary of the likely compatibility of these projects with the Warwick middleware research. Two of these eight projects have been identified for further collaboration, details of which are documented. In addition, this consultation has been extended to include UK e-Science pilot projects and the details of planned collaboration with one of these pilot projects also forms part of this report.

**Reference:** **GR/S03058/01** **RR394**
**Performance-based Middleware for Grid Computing**

## Introduction

The e-Science demonstrator projects provide a diverse collection of demonstrations and methodologies that represent tasks which are considered pertinent to e-Science. These projects are at various stages of completion – some have already ended and some are in the initial stages as they rely on key infrastructural support which is currently being installed.

The Warwick Middleware project aims to provide performance services for e-Science and e-Business applications. As part of the e-Science Open Call funding (GR/S03058/01), we have agreed to identify and then deliver results of the application of these middleware performance services to a chosen e-Science demonstrator application.

This document reports on the six month survey of the UK e-Science demonstrator projects. The report details the eight project consultations in which we have engaged, and provides a summary of the likely compatibility of these projects with the Warwick middleware research.

To optimize research compatibility and cooperation within the UK e-Science programme, this six-month study has also included additional consultation:

> The evaluation of UK e-Science demonstrator projects: including the refinement of these to one or a small subset of projects which will be the subject of more detailed scrutiny;
>
> An evaluation of a subset of UK e-Science pilot projects: to investigate whether the middleware performance services might be compatible with some of the larger UK e-Science projects;
>
> An evaluation of the e-Business case studies in light of IBMs involvement in other UK e-Science work.

In order to assess the benefit and appropriateness of the application of the middleware to the demonstrators, a number of broad suitability requirements have been applied:

> Will the Warwick middleware services bring added-value?
>
> Is the demonstrator (language, operating system etc.) compatible with the Warwick middleware tools?
>
> Is specialist equipment needed to run an image of the demonstrator at Warwick?
>
> Are resources available at the partner institution to support the collaboration?

This report contains: a list of the demonstrator consultations which have taken place during the past six months; those demonstrator projects identified for further collaboration; a list of the pilot project consultations which have taken place during the past six months; those pilot projects identified for further collaboration; a list of the supporting research which has been instigated to in order to underline this proposed collaboration.

**Demonstrator Project Consultations**

Consultations have taken place with eight UK e-Science demonstrator projects during the past six months (a summary of these projects, the main contacts with whom we have been involved and their location, are shown in Table 1).

| *Project* | *Contact* | *Location* |
|---|---|---|
| 3D OPT Microscopy Grid | Richard Baldock<br><br>Neil Chue Hong | MRC Human Genetics Unit, Edinburgh<br>EPCC |
| 3D Mouse Grid | Richard Baldock | MRC Human Genetics Unit, Edinburgh |
| Chemical Structures (Comb-e-Chem) | Mike Surridge | University of Southampton (IT Innovation) |
| Dynamic Brain Atlas (IXI) | Derek Hill | King's College London |
| GODIVA | Jochem Marotzke<br>John Stark<br>David Boyds | Southampton Oceanography Centre<br>RAL |
| GRAB (BDWorld) | Alex Gray | Cardiff University |
| NeSC ePortal | Mark Parsons | EPCC |
| SAMD | Keith Cole<br>Stephen Pickles | Manchester University |

Table 1: Overview of demonstrator project consultations

This list of projects can be partitioned in to those for which performance services are not considered important (as the project has already finished, performance is not an important component of the demonstration etc.) – including GODIVA, NeSC ePortal and SAMD – those which might benefit from the introduction of the performance services at a later date – including Comb-e-Chem and GODIVA – and those for which performance services are essential to the success of the project – including Dynamic Brain Atlas and 3D OTP Microscopy Grid.

**Identified Demonstrator Projects for Further Collaboration**

It is possible that projects such as Comb-e-Chem and GODIVA will demonstrate future compatibility with our middleware research, they are however not yet at the stage where we can start to consider how this integration might take place.

Detailed discussion and consultative visits have taken place between Warwick and Edinburgh University (and the MRC Edinburgh) with regard to the 3D OTP Microscopy Grid and also King's College London with regard to the Dynamic Brain Atlas project. An advantage in selecting these two demonstrators for further collaboration is that they both have a considerable image processing content. This area of expertise is supported by the Image Processing Group in the Department of Computer Science at Warwick, and we are well placed therefore to be able to contribute at the necessary level of detail.

*3D OTP Microscopy Grid*

The 3D OPT demonstrator on the reconstruction of mouse embryo data is composed of three tasks – data capture, transfer and parallel reconstruction. Performance is critical to this project; for example, the reconstruction of the 3D image takes about 2-5 hours with a serial version of the algorithm, which for the 3-channel image means an overnight run before the biologists can review the results and reset the parameters as necessary.

The basic algorithm takes a set of projection images, deconstructs them after some preprocessing to sets of sinograms, and then uses these during the reconstruction process; this is equivalent to taking an orthogonal cut through the data. The reconstruction process involves stacking the sections generated by the back-projection processing.

A parallel version of this algorithm has been implemented and demonstrated. This is currently being re-engineered to run on an array of Sun netras at the MRC. The code is written in C and MPI and the Sun Grid Engine is used to handle scheduling. There are plans also to use Globus to connect to remote resources. A stable version of this system is due to be complete by May 2003.

It is likely that our middleware tools will directly benefit this image reconstruction process. Our tools are currently engineered for C MPI-based code and it should be feasible to generate resource models for the hardware at the MRC.

While our performance-based scheduling tools are currently based on a Globus/Condor middleware stack (see below), we plan to investigate whether our performance co-scheduler can be used alongside Sun's Grid Engine.

*Dynamic Brain Atlas*

Although the Dynamic Brain Atlas project has now finished, follow up research funding has been sought, and now granted, during the past six months. We offered partner support in this bid and its success therefore means that there are now resources available at King's to be able to support continued collaboration. The new project, known as IXI, started on the 17th February 2003.

Two work areas have been started at Warwick to facilitate collaboration with this project. The first involves additional support from Dr Chang-Tsun Li (from the Image Processing Group in the Department of Computer Science, Warwick) who is currently working on identifying core image processing kernels which form part of the IXI project. The aim of this is to then test the middleware tools on these image processing kernels, perform some in-house analysis to verify the benefits which they offer, and then transfer these to the demonstrator later in the project.

The second work area is the integration of the performance tools with Condor – the preferred intra-domain scheduler use in IXI. This has formed one of the major areas of research over the past six months and has involved adapting our performance scheduler (known as Titan) so that it can be used as a driver to Condor. By doing this the middleware tools should integrate into the IXI demonstrator platform (and indeed any other that utilizes Condor at the intra-domain level). Progress has already been made on this work area, details of which can be found below.

**Pilot Project Consultations**

Many of the lessons learnt from the prototyping of the demonstrator projects have been transferred to the development platforms of the larger pilot projects (e.g. SAMD and RealityGrid). Indeed the perceived importance of performance services is noticeably greater at the pilot project level than at the demonstrator project level.

This consultation has therefore been extended to include a subset of the UK e-Science pilot projects, whose performance requirements are somewhat compatible (a summary of these projects, the main contacts with whom we have been involved and their location, are shown in Table 2).

| *Project* | *Contact* | *Location* |
|---|---|---|
| RealityGrid | Stephen Pickles<br>Graham Riley | Manchester University |
| EDiamond | Mike Brady<br>David Gavaghan<br>Steve Heisig | Oxford University<br><br>IBM |
| DAME | Karim Djemame | Leeds University |

Table 2: Overview of pilot project consultations

The analysis and development of techniques to address performance issues are clearly already integrated components of these pilot projects. It is important however to build on the research experience gained during the performance engineering of each of these pilot projects, and to use this experience when considering the design and deployment of our own middleware tools.

**Identified Pilot Projects for Further Collaboration**

As part of this process we have been involved in collaborative meetings with the Grid Infrastructure team on the eDiamond project. Through Donna Dillenberger and Steve Heisig (IBM Watson) we are looking to share experience in two specific areas:

> How we define application/request topologies that describe the link between application components. There are two aspects to this work, the language in which these application units should be described (currently the Open Group's ARM API) and then how these work units can be used during the performance analysis of applications.
>
> We are also looking into how user-level service provision can be mapped to these lower-level work units, particularly when these work units are processed across a distributed architecture. This links with the hWLM and eWLM projects that Donna Dillenberger and Steve Heisig are involved in at IBM and also the demonstrator for this work eDiamond.

Experience in this areas is to be shared through conference call meetings and also through meetings at the Oxford e-Science regional centre (organized through David Gavaghan).

## Supporting Research

*Supporting image processing research*

Although our research is to be tested in the context of an e-Science demonstrator project, we are trying to avoid building dependencies that are likely to slow our work down. We have done this by identifying three possible e-Science demonstrators that have similar image processing characteristics (3D OPT Microscopy Grid, IXI and eDiamond). One of our academics from the Image Processing Research Group at Warwick (Dr Chang-Tsun Li) is currently working on identifying core kernel characteristics of these projects, the idea being that if we can test and verify our tools on these core kernels then the integration with the demonstrator/s should be made easier later in the project.

For example, the image segmentation techniques that enable low-level image analysis in projects such as the Dynamic Brain Atlas (IXI), have been the subject of detailed analysis at Warwick, see:

CT Li, Multiresolution Image Segmentation Integrating Gibbs Sampler and Region Merging Algorithm, *Signal Processing*, 83(1):67-78, 2003.

R Wilson, CT Li, A Class of Discrete Multiresolution Random Fields and its Application to Image Segmentation, *IEEE Trans. Pattern Analysis and Machine Intelligence*, 25(1):42-56, 2003.

This approach employs Markov random fields (MRF) defined in a multi-resolution structure to partition the target image into homogeneous regions with distinctive features. By exploiting the local characteristics, known as the Markovianity of the MRFs, the technique allows the local labeling and partitioning process to be carried out in a Grid-enabled environment.

Dr Chang-Tsun Li is analysing this segmentation technique in the context of Grid-applications, with the aim of being able to identify and employ performance analyses to applications that share these core characteristics.

*Integration with standard middleware tools*

We have begun this at the intra-domain level by modifying Titan (our predictive intra-domain scheduler) so that it now acts as a co-scheduling driver to Condor, see figure below.

The advantage of this is that it allows the predictive data derived from PACE to drive the job submission provided by Condor (or indeed any other commodity scheduler). In the case of Condor this is done by auto-generating ClassAds that force Condor to run a task on a designated machine (or set of machines) using the name attribute.

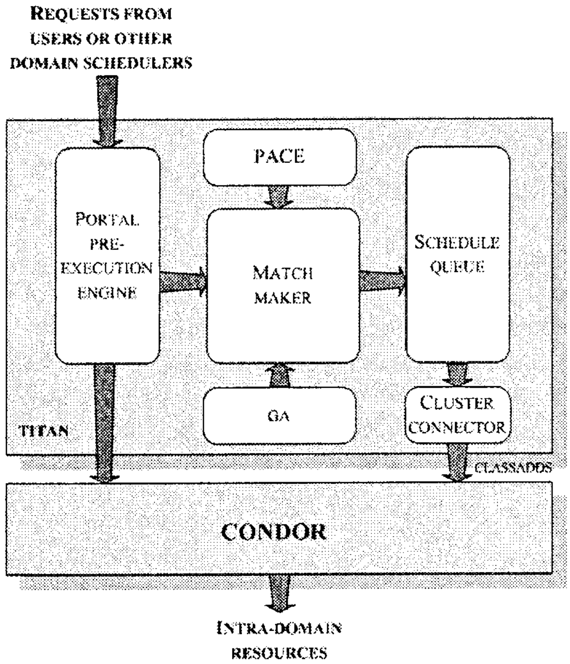


Figure 1: Integration of Warwick middleware tools with standard Grid middleware – phase 1: The Titan predictive scheduler has been modified so that it acts as a predictive co-scheduler to Condor.

We term this *predictive co-scheduling*, and it allows traditional Globus/Condor configurations to utilise performance data at the intra-domain level should it exist; if there is no predictive data then the job passes to Condor in the same way as before.

An additional advantage of the predictive co-scheduling technique described above is the ability to include quality of service criteria into Condor-based intra-domain scheduling. As it stands Condor has no means of reordering tasks or assigning deadlines so as to improve (or indeed guarantee) the service offered to its users. We have currently implemented three metrics into the Titan co-scheduler, these are *makespan* (the time to completion), the *average advance time* (the relationship between a task's execution time and its deadline) and *resource utilisation* (the ability to capture the utilisation of a contributing resource).

By providing these metrics at the co-scheduler level, it is possible to monitor execution and explore execution strategies so that the overall runtime is minimised, the deadlines of tasks are maintained or so that the resources are utilized to best effect.

We are hoping to extend this technique to a multi-domain level using Globus information services.

**Bibliography**

R Baxter, N Chue, Optimisation Plan for 3D OPT Microscopy Grid, EPCC-IS-3DMG-PLAN 1.0, from EPCC Edinburgh.

R Baxter, N Chue, M Parsons, R Baldock, B Hill, J Sharpe, 3D OPT Microscopy Grid – Bringing the Grid to the Biomedical Workbench, from EPCC Edinburgh.

M Brady, eDiamond: Digital Mammography, EPSRC programme GR/S20956/01, 2002.

D Dillenberger, S Heisig, A Martin, D Gavaghan, hWLM/GRID 2002 project proposal, from Oxford e-Science Centre, 2002.

DLG Hill, JV Hajnal, D Rueckert, SM Smith, T Hartkens, K McLeish, A Dynamic Brain Atlas, available from Derek.Hill@kcl.ac.uk

K Mayes, GD Riley, RW Ford, M Lujan, TL Freeman, The design of a performance steering system for component-based Grid applications, from Centre for Novel Computing, University of Manchester, 2003.

GR Nudd, SA Jarvis, Performance-based Middleware for Grid Computing, EPSRC programme GR/S03058/01, 2002.

D Watson, D Gavaghan, M Jirotka, B Collins, A Simpson, M Brady, R Highnam, Critical success factors and high-level requirements for eDiamond, November 2002.