Using the HemeLB parallel Lattice-Boltzmann code on multiple interoperable e-Science infrastructures

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• Context of the GENIUS project
• Modelling bloodflow with HemeLB
• Integrating simulation in to the clinical workflow
• Infrastructure requirements of GENIUS
• The need for interoperability
• Visualising simulation results
• Summary and future work
• ‘Personalized medicine’ - targets the individual, not the average

• Treatments can be assessed for their effectiveness with respect to the patient *before* being administered
  – Saves cost and increases treatment efficacy
  – Reduces animal testing

• Use patient-specific information as input for a simulation, which can help predict the outcome of a course of treatment
Grid Enabled Neurosurgical Imaging Using Simulation

The GENIUS project aims to model large scale patient specific cerebral blood flow in clinically relevant time frames

Objectives:
- To study cerebral blood flow using patient-specific image-based models.
- To provide insights into the cerebral blood flow & anomalies.
- To develop tools and policies by means of which users can better exploit the ability to reserve and co-reserve HPC resources.
- To develop interfaces which permit users to easily deploy and monitor simulations across multiple computational resources.
- To visualize and steer the results of distributed simulations in real time
Clinical Supercomputing

Diagnosis and decision support in surgery

• Provide simulation support from within the operating theatre for neuroradiologists

• Provide new information to surgeons for patient management and therapy:
  1. Diagnosis and risk assessment
  2. Predictive simulation in therapy

• Provide patient-specific information which can help plan embolisation of arterio-venous malformations, coiling of aneurysms, etc.
Modelling blood flow using HemeLB

Efficient fluid solver for modelling brain bloodflow called *HemeLB*:

- Uses the lattice-Boltzmann method
- Efficient fluid solver for sparse geometries, like a vascular tree
- Machine-topology aware graph growing partitioning technique, to help hide cross-site latencies
- Optimized inter- and intra-machine communications
- Full checkpoint capabilities
Current surgical practice relies on a lot of trial and error procedures; success rates fall way short of ideal.

Computational simulation offers insights not previously available to clinicians, and will help to improve success rates of procedures.

Panels showing different flow metrics:
- Pressure
- Stress
- Velocity
Knowledge & discovery

Potentially revolutionizes medical practice

Diagnostics
Whole brain pressure and stress maps

Preventive treatments
Assess risk of vascular rupture

Surgical planning
Giving the clinician whole brain predictive capabilities

A new way of approaching clinical practice
Augmenting clinical expertise and predictive modeling
Book computing resources in advance or have a system by which simulations can be run urgently.

Shift imaging data around quickly over high-bandwidth low-latency dedicated links.

Interactive simulations and real-time visualisation for immediate feedback.
Flexibility and deployability

Beyond the batch job

• Typical computing scenario involves jobs submitted into a queue
  – Submit -> Run -> Post-process

• This won’t work in a clinical scenario since correctness and timeliness are important in clinical computing - late results are useless

Advance reservations
Emergency computing
Grid middleware - the Application Hosting Environment
Blood flow modeling, computational steering and real-time in-situ visualization
Distributed Computing
Lightpaths

The challenge: To incorporate these methodologies into a clinician’s day to day activities, rather than just providing such facilities on an ad hoc basis.
GENIUS requires access to many resources

A single grid infrastructure cannot provide sufficient power in the timescales required to support routine use of the GENIUS technology.
1. Acquire data from scanner
2. Anonymise data
3. Upload data to DICOM server
4. Download data into GENIUS client from DICOM server
5. Build model
6. Upload model to GridFTP staging server
7. Launch simulation
8. Steer and visualise
First step is the conversion of patient-specific MRA or 3DRA data (DICOM format) to a 3D model, vasculature is of high contrast, 300 - 400 μm resolution, 500³ - 700³ voxels.

3DRA - 3-dimensional rotational angiography, vasculature is obtained using digital subtraction imaging with a high-contrast x-ray absorbing fluid.
Acquisition of MRI volume data, $1024^3$ at 0.25 mm resolution.

Reconstruct patient specific cerebral system and boundary condition setup.

Volume rendering corresponding to the reconstructed patient-specific vascular system.
The Application Hosting Environment

- Based on the idea of applications as Web Services
- Lightweight hosting environment for running unmodified applications on grid resources (NGS, TeraGrid, DEISA) and on local resources (departmental clusters, workstations)
- Acts as a client to OGSA-BES submission services using Unicore 6 tools
- Also submits directly to Globus WS-GRAM
- Community model - expert user installs and configures an application and uses the AHE to share it with others
- Simple clients with very limited dependencies - can run from the desktop, command line or PDA
AHE Functionality

- Launch simulations on multiple grid resources
- Single interface to monitor and manipulate all simulations launched on the various grid resource
- Run simulations without manually having to stage files and GSISSH in
- Retrieve files to local machine when simulation is done
- Can use a combination of different clients – PDA, desktop GUI, command line
Scientific Application (e.g. bloodflow simulation HemeLB)

Application Hosting Environment (AHE) as scientific-specific Client technology

OGSA-BES Client

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OGSA-BES Interface

OMII-UK Grid Middleware Stack
GridSAM with Globus GT2

Security Policies with gridmaps

GLUE-based information

Common Environment

massively parallel jobs with HemeLB

GridFTP Interface

HPC Resource within NGS

Storage Resources (e.g. tape archives, robots)

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Grid Middleware
UNICORE with BES

Security Policies (e.g. XACML)

GLUE-based information

Common Environment

massively parallel jobs with HemeLB

DEISA Modules with HemeLB

HPC Resource within DEISA

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Stefan Zasada, Steven Manos, Morris Riedel, Johannes Reetz, Michael Rambadt et al.,
Preparation for the Virtual Physiological Human (VPH) project that requires interoperability of numerous Grids

Slide courtesy Morris Riedel
• GENIUS has been designed to run across multiple machines using MPI-g
• Some problems won’t fit on a single machine, and require the RAM/processors of multiple machines on the grid.
• MPI-g allows for jobs to be turned around faster by using small numbers of processors on several machines - essential for clinician
• HemeLB performs well on cross site runs, and makes use of overlapping communication in MPI-g
• We can reserve multiple resources for specified time periods
• Co-allocation is useful for meta-computing jobs like HemeLB, viz and for workflow applications.
• We use HARC - Highly Available Robust Co-scheduler (developed by Jon Maclaren at LSU).
Highly Available Robust Co-scheduler

• HARC provides a secure co-allocation service
  – Multiple Acceptors are used
  – Works well provided a majority of Acceptors stay alive
  – Paxos Commit keeps everything in sync
  – Gives the (distributed) service high availability
  – Deployment of 7 acceptors --> Mean Time To Failure ~ years
  – Transport-level security using X.509 certificates

• HARC is a good platform on which to build portals/other services
  – XML over HTTPS - simpler than SOAP services
  – Easy to interoperate with
  – Very easy to use with the Java Client API
AHE - HARC integration

- Users can co-reserve resources from the AHE GUI client using HARC
- When submitting a job, users can either run their jobs in normal queues, or use one of their reservations
- AHE passes reservation through to the Globus GRAM
- AHE client uses HARC Java client API to manage reservations
Special PRiority and Urgent Computing Environment

- Applications with dynamic data and *result deadlines* are being deployed
- Late results are useless
  - Wildfire path prediction
  - Storm/Flood prediction
  - Patient specific medical treatment
- Some jobs need priority access “Right-of-Way Token”
SPRUCE Right-of-Way Tokens

Event

1. Automated Trigger

2. First Responder

- Human Trigger

Right-of-Way Token

SPRUCE Gateway / Web Services
JANET Lightpath is a centrally managed service which will help support large research projects on the JANET network by providing end-to-end connectivity, from 100’s of Mb (TDM slices) up to whole fibre wavelengths (10 Gb).

What are we actually using it for?
- Dedicated 1Gb network to connect hospital to national and international HPC infrastructure
- Shifting datasets from the NHNN to UK/US - 0.5 GB - 4 GB in size
- Real-time visualisation
  - 1000\(^2\) pixels @ 30 FPS
- Interactive computational steering
- Cross-site MPI runs (e.g. between NGS2 Manchester and NGS2 Oxford)
• The GENIUS project has developed a lightweight client tool to orchestrate the clinical workflow
• Simulations launched and managed by AHE
Innovative visualization techniques

Real time in situ parallel ray-tracing

- A ray tracer has been incorporated into HemeLB core to efficiently monitor simulation results in real time
- Sub-frames are rendered on each MPI processor/rank and composited before being sent over the network to a (lightweight) viewing client
- Data transmission and post processing is avoided
- Only updated image is sent to the client

- Pressure field
- Velocity field
ReG Interactive visualisation and steering
Impact on HPC resources

• Common requirement for urgent computing; hurricane, earthquake simulations
  – Batch-job submission won’t work
  – Successful patient-specific simulation techniques will likely have 1000’s of cases. The level of compute time required will dwarf current resources.

• Economics of computational treatments
  – Currently available HPC resources would not be able to support routine use of this technique

• Many moral, ethical and policy questions needed to be addressed
  – Resource availability (site policy)
  – Data privacy, data provenance, data assurance, medical ethics.
What have we done so far?

Creation of persistent infrastructure which is available for patient-specific clinical studies

And now…

Validation of the technique in clinical settings
- Retrospective studies using existing patient data
- Prospective study of infantile Vein of Galen malformations

And in the future…

Augment traditional patient imaging data
Big step towards the ‘virtual physiological human’

www.vph-noe.eu
Virtual Physiological Human

• Funded under EU FP 7
• 15 projects: 1 NoE, 3 IPs, 9 STREPs, 2 CAs.

“a methodological and technological framework that, once established, will enable collaborative investigation of the human body as a single complex system ... It is a way to share observations, to derive predictive hypotheses from them, and to integrate them into a constantly improving understanding of human physiology/pathology, by regarding it as a single system.”
Computational experiments integrated seamlessly into current clinical practice

Clinical decisions influenced by patient specific computations: turnaround time for data acquisition, simulation, post-processing, visualisation, final results and reporting.

**Fitting the computational time scale to the clinical time scale:**
- Capture the clinical workflow
- Get results which will influence clinical decisions: 1 day? 1 week?
- This project - *15 to 30 minutes*

Development of procedures and software in consultation with clinicians

Security/Access is a concern

On-demand availability of storage, networking and computational resources
• Clinical relevance of patient specific medicine, both correctness (verification and validation) and **timeliness** are important

• Current emergency computing scenarios are far and few between (hurricane, earthquake simulations).
  – **Batch-job submission + post-processing won’t work here**
  – Successful patient-specific simulation techniques will likely have 1000’s of cases. The level of compute time required will dwarf current resources.

• If HPC is to be exploited by clinicians it needs to be used in a way that fits in with the clinical workflow

• We’ve worked with grids, network providers and the NHS to put in place a system to allow clinicians to use grid resources interactively

• VPH initiative: Likely to increase pressure for non-standard services from resource providers
NGS staff
DEISA staff
TeraGrid Staff
LONI Staff
David Salmon
Simon Clifford
Morris Riedel
Herman Lederer
Brian Toonen
Nicholas Karonis
David Hawkes
Jon Maclaren
Shantenu Jha
Daniel Katz
Shawn Brown
Ken Yoshimoto
Doru Marcusiu