

GPU CLUB

Tuesday 25 November 2014

<http://gpu.manchester.ac.uk>

Agenda

- 14:00 – Introductions
- 14:05 – Neil Morgan, STFC
- 14:30 – Greg Kozikowski, Computer Science
- 14:50 – Pop-ups
 - Dave Topping, Atmospheric Science
 - Malte, Computer Science
 - *From the floor...*
- 15:20 – Next Steps
- 15:30 – Close

Podcast available



UNIVERSITY GPU CLUB

GPU and the Club

- Graphical Processing Unit
 - Graphics cards' increasing ability to undertake specific compute
 - “a few” TFLOPS/sec on a card (CSF Ivybridge: peak of 332 GFLOPS)
 - PCI-e
 - Energy efficiency
- Club / Community
 - Initially set-up to discuss vendor claims of “1000x speed-up”
 - Share real-life experiences, updates/news, solutions!
 - 16 meetings & 1 “GPU Day”
 - Evolving to also consider FPGA, XPhi, EEC

(1): E5-2650 2.6 GHz, 16 cores

Club Successes

- GPU Research
- Vendor involvement
 - AMD, ARM, Intel, NVIDIA speakers & workshops
- CUDA Research Centre
 - %age off certain NVIDIA GPUs
 - Access to experts
- zrek emerging technology cluster
 - K40, K20; XPhi 7120p; FPGA

GPUs Enabling Biological Research

Dr. Andrew Almond, Dr. Ben Sattelle, Life Sciences (MIB).

Almond & Sattelle are running molecular dynamics (MD) simulations of sugars .. Understanding the equilibrium 3D-structure of carbohydrate molecules (e.g. Figure 1) has wide ranging potential applications in medicine and also in the search for sustainable food and energy sources. Equilibrium physical (thermodynamic and kinetic) properties of carbohydrate 3D-structure are not quantifiable using standard biophysics and had not been rigorously explored computationally prior to GPU-accelerated simulations, which allowed simulations to be extended in to the microsecond regime for the first time and convergence of 3D-properties (Figure 2), see [1], [2]. The expanded timeframe has led to new insights into biologically important conformational exchange events (that can now be exploited in molecular design processes. The research group is currently using AceMD software on two workstations with 2 NVIDIA GTX580 GPUs. In future, research will focus on the biophysics of carbohydrate polymers and the bioactivity of chemically modified sugars.

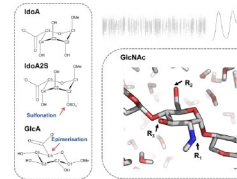
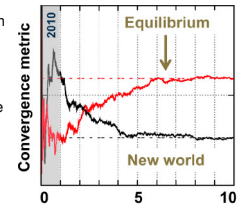


Figure 1: 3D Structure of Modelled Carbohydrates



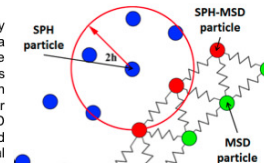
References



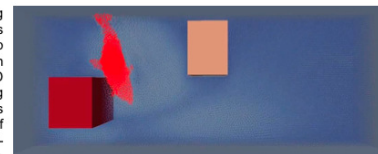
GPU Smoothed Particle Hydrodynamics and Mass-Spring-Damper Modelling

Dr Stephen Longshaw, Dr Benedict Rogers & Prof. Peter Stansby, Mechanical, Aerospace and Civil Engineering (MACE)

Dr Longshaw, Rogers and Prof. Stansby are developing a new method to couple a Mass-Spring-Damper (MSD) technique with Smoothed Particle Hydrodynamics (SPH) to simulate the impact between large sea creatures and underwater energy generating turbines. The MSD method implemented has been designed so that it is possible to define typical elastic engineering properties and the simulation behaves realistically regardless of the number of mass points involved or their physical layout relative to each other. The method is capable of representing 3D deformable bodies with non-homogenous elastic properties as well as membranes.



The work is being performed on GPUs as the size of time-step required to maintain stability with an MSD simulation involving high stiffness values would be unfeasible if performed in a non-accelerated manner.



This has been achieved by extending the GPU and OpenMP based DualSPHysics software to include the coupled MSD capability. Through the

NEIL MORGAN
GREG KOZIKOWSKI

POP UP TALKS

Up to 5 minutes

Up to 2 slides

Community participation

Next Steps

- GPU
 - openACC & “kitchen sink”
 - (access)
- Other architectures
 - Demand for FPGA? For XPhi?
 - For training in these?
- Energy efficiency
 - Interest for subgroup to share ideas & grant proposals?
- Community – rename GPU Club? Help to run?

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