



CUDA
RESEARCH
FAST
FORWARD

Showcase of applications and research by PhD students in top universities of the US doing CUDA research, via "Ignite"-style presentations, 20 slides / 20 seconds each



GPU Technology Theater @ SC11

Monday, November 14, 20:00 pm

Presented by the PASI fellows, moderated by Prof Lorena Barba, Boston University

Christopher Cooper, Boston University

Using GPUs for boundary element methods

The boundary element method is a very convenient method for solving an important family of partial differential equations, because only the boundary needs to be discretized. The BEM is limited by a series of dense matrix-vector multiplications which can be accelerated by using a Fast Multipole Method. The main challenge we address is porting the full BEM algorithm to the GPU, using an available FMM that already runs on the GPU.

Trevor Gokey, San Francisco State University

The glass ceiling of biomolecular computation

Current consumer computer systems top-out at 32 cores, creating a barrier for small computational labs who do not have resources for specialized hardware. Compared to a 32-core machine running the AMBER molecular dynamics package, an Nvidia GTX580 GPU is three times faster, four times less expensive, and consumes half the watts. With the ability to have four GPUs in a single machine, it is possible to attain the computational power of larger labs without the associated overhead.

Olesiy Karpenko, University of Illinois Chicago

Puzzles in massively parallel genome biology await GPU solutions

Millions of uniform genomic events such as gene transcription take place simultaneously in any live cell. The architectures of the regulatory elements that orchestrate these events are extremely complex and largely remain unsolved puzzles. On the bright side, exceptional parallelism and locality of genomic events suggest that massively parallel processing of genomic data with GPUs makes solving these puzzles feasible in the nearest future.

Anush Krishnan, Boston University

Immersed boundary flows on GPU

The immersed boundary method (IBM) is a CFD approach to deal with problems involving

complex geometries in a flow. It has immediate applications in biology, whether it is to study blood flow through heart valves or the lift generated by the flapping wings of a butterfly. We have developed and validated an IBM fluid solver on GPU, which we aim to apply in the study of aerial locomotion in animals such as insects and gliding snakes.

Simon Layton, Boston University

Classical algebraic multigrid for engineering applications

Classical algebraic multigrid can solve general sparse linear systems of equations, with excellent convergence and scaling properties. It is the workhorse in a variety of engineering applications, including unstructured CFD and finite element analysis. We describe what is, as far as we know, the first full-GPU implementation of classical AMG.

Ying-Wai Li, University of Georgia

Speeding up Wang-Landau simulation of lattice model proteins using GPUs

Wang-Landau sampling is a Monte Carlo simulation method in statistical physics, which I have been applying for the study of lattice model protein folding and adsorption problems. In my presentation I will talk about some ideas on parallelizing and speeding up the simulation process making use of GPUs.

Britton Olson, Stanford University

Rocket Science, shock waves and video games: How the evolving GPU will accelerate aeronautical research.

Large-scale calculations of compressible fluid dynamics often require thousands of CPU cores and long run-times. In our studies of an over-expanded nozzle using LES, long integration times are needed to capture the slow unsteady scales at high Reynolds numbers. Using GPU hardware has the potential of making these studies routine in small clusters.

Juan R. Perilla, Johns Hopkins University (currently at University of Illinois at Urbana-Champaign)

Computing transitions in macromolecular systems

A molecular understanding of how protein function is related to protein structure will require an ability to understand large conformational changes between multiple states. We present a novel way to combine information from molecular dynamics using non-linear time series and dimensionality reduction. This new method suggests an implementation for molecular dynamics calculations that may dramatically enhance sampling of intermediate states.

Benjamin Payne, Missouri University of Science and Technology

Transport of light in complex media

Characterizing transport behavior in complex media has applications in fields as varied as medicine, condensed matter physics, and optics. Computational simulations of systems at the boundary between classical and quantum descriptions give new insight to theoretical and experimental investigations. The models developed are used in projecting avenues for future research.

Albert Sidelnik, University of Illinois Urbana-Champaign

High-Level Language Support For GPU Architectures

This talk will focus on work that we have used in supporting (NVIDIA-based) GPUs from a high-level parallel language named Chapel. This work will show that we can get code that is higher-level, more compact, and performs on par as if developing directly in CUDA. Additionally, we will show that the code is also portable and can be targeted towards traditional multicore or clusters.