

## NVIDIA GPU TECHNOLOGY THEATER AT SC13

*\* Information subject to change. All times listed in Mountain Time Zone (GMT-7)*

### Monday, November 18 – Thursday, November 21 during exhibition hours | NVIDIA Booth #613

The NVIDIA GPU Technology Theater is hosting an amazing lineup of industry luminaries, scientists, and developers at SC13, covering a wide range of topics on HPC and accelerated computing.

Come back often for updates!

#### Monday, November 18 | Booth #613

##### **New Features in NVIDIA® CUDA® 6 Make GPU Acceleration Easier**

8:00 PM – 8:30 PM

Mark Harris  
Chief Technologist GPU  
Computing  
NVIDIA

The performance and efficiency of CUDA, combined with a thriving ecosystem of programming languages, libraries, tools, training, and services, have helped make GPU computing a leading HPC technology. Learn how powerful new features in CUDA 6 make GPU computing easier than ever, helping you accelerate more of your application with much less code.

#### Tuesday, November 19 | Booth #613

##### **Towards Performance-Portable Applications Through Kokkos: A Case Study with LAMMPS**

10:30 AM – 11:00 AM

Christian Trott Postdoctoral Appointee  
Sandia National Laboratories

In this talk we demonstrate how LAMMPS uses the many-core device performance portability library Kokkos to implement a single code base for CPUs, NVIDIA GPUs and Intel Xeon Phi co-processors. This portable code base has equal or better performance compared to LAMMPS' current generation of hardware specific add-on packages.

##### **Massively Parallel Computing and the Search for New Physics at the LHC**

11:00 AM – 11:30 AM

Valerie Halyo  
Assistant Professor of Physics  
Princeton University

The quest for rare new physics phenomena at the LHC leads us to evaluate a Graphics Processing Unit (GPU) enhancement of the existing High-Level Trigger (HLT), made possible by the current flexibility of the trigger system, which not only provides faster and more efficient event selection, but also includes the possibility of new complex triggers that were not previously feasible. A new tracking algorithm is evaluated on a NVIDIA Tesla K20c GPU, allowing for the first time the reconstruction of long-lived particles or displaced black holes in the silicon tracker system at real time in the trigger.

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<p><b>Being Very Green with Tsubame 2.5 Towards 3.0 and Beyond to Exascale</b></p> <p>11:30 AM – 12 Noon</p> <p>Satoshi Matsuoka Professor Global Scientific Information and Computing Center (GSIC), Tokyo Institute of Technology</p>	<p>TSUBAME 2.5 succeeded Tsubame 2.0 by upgrading all 4224 Tesla M2050 GPUs to Kepler K20x GPUs, achieving 5.76 / 17.1 Petaflops peak in double / single point precision respectively, latter the fastest in Japan. By overcoming several technical challenges, Tsubame 2.5 exhibits x2-3 speedup and multi-petaflops performance for many applications, leading to Tsubame 3.0 in 2015-16.</p>
<p><b>Efficiency and Programmability: Enablers for Exascale</b></p> <p>12 Noon – 12:30 PM</p> <p>Bill Dally Chief Scientist &amp; SVP Research NVIDIA</p>	<p>HPC and data analytics share challenges of power, programmability, and scalability to realize their potential. The end of Dennard scaling has made all computing power limited, so that performance is determined by energy efficiency. With improvements in process technology offering little increase in efficiency, innovations in architecture and circuits are required to maintain the expected performance scaling. The large scale parallelism and deep storage hierarchy of future machines poses programming challenges. This talk will discuss these challenges in more detail and introduce some of the technologies being developed to address them.</p>
<p><b>Accelerated Computing with OpenACC</b></p> <p>12:30 PM – 1:00 PM</p> <p>Michael Wolfe Compiler Engineer The Portland Group, NVIDIA</p>	<p>The OpenACC API provides a high-level, performance portable programming mechanism for parallel programming accelerated nodes. Learn about the latest additions to the OpenACC specification, and see the PGI Accelerator compilers in action targeting the fastest NVIDIA GPUs.</p>
<p><b>New Features in CUDA 6 Make GPU Acceleration Easier</b></p> <p>1:00 PM – 1:30 PM</p> <p>Mark Harris Chief Technologist, GPU Computing NVIDIA</p>	<p>The performance and efficiency of CUDA, combined with a thriving ecosystem of programming languages, libraries, tools, training, and services, have helped make GPU computing a leading HPC technology. Learn how powerful new features in CUDA 6 make GPU computing easier than ever, helping you accelerate more of your application with much less code.</p>

<p><b>Titan: Accelerating Computational Science and Engineering with Leadership Computing</b></p> <p>1:30 PM – 2:00 PM</p> <p>Jack Wells Director of Science National Center for Computational Science Oak Ridge National Laboratory</p>	<p>Modeling and simulation with petascale computing has supercharged the process of innovation, dramatically accelerating time-to-discovery. This presentation will focus on early science from the Titan supercomputer at the Oak Ridge Leadership Computing Facility, with results from scientific codes discuss, e.g., LAMMPS and WL-LSMS. I will also summarize the lessons we have learned in preparing applications to move from conventional CPU architectures to a hybrid, accelerated architecture, and the implications for the research community as we prepare for exascale computational science.</p>
<p><b>A Productive Framework for Generating High-Performance, Portable, Scalable Applications for Heterogeneous Computing</b></p> <p>2:00 PM – 2:30 PM</p> <p>Wen-mei Hwu Professor and Sanders-AMD Chair, ECE University of Illinois at Urbana-Champaign</p>	<p>I will present two synergistic systems that enable productive development of scalable, Efficient data parallel code. Triplet is a Python-syntax based functional programming system where library implementers direct the compiler to perform parallelization and deep optimization. Tangram is an algorithm framework that supports effective parallelization of linear recurrence computation.</p>
<p><b>Fighting HIV with GPU-Accelerated Petascale Computing</b></p> <p>2:30 PM – 3:00 PM</p> <p>John Stone Senior Research Programmer, Associate Director, CUDA Center of Excellence Theoretical and Computational Biophysics Group, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign</p>	<p>Molecular dynamics simulations provide a powerful tool for probing the dynamics of cellular processes at atomic and nanosecond resolution not achievable by experimental methods alone. We describe how GPU-accelerated petascale supercomputers are enabling studies of large biomolecular systems such as the HIV virus in all-atom detail for the first time.</p>

<p><b>Flying Snakes on GPUs</b></p> <p>3:00 PM – 3:30 PM  <b>Lorena Barba</b>  Associate Professor of  Engineering and Applied  Science  Department of Mechanical and  Aerospace Engineering  The George Washington  University</p>	<p>It would be hard to put a flying snake in a wind tunnel. So we are trying to put them in GPUs instead—via computational fluid dynamics. Our initial success is to see that a flying snake's cross-section can in fact create quite some lift: it even has a favorite angle of attack for which it gives extra lift. We don't know if this is the secret of flying snakes, but we do know that looking at nature can teach engineers some new tricks.</p>
<p><b>Exploring Emerging  Technologies in the HPC Co-  Design Space</b></p> <p>4:00 PM – 4:30 PM  <b>Jeff Vetter</b>  Future Technologies Group  Leader and Professor  Oak Ridge National Laboratory  and Georgia Tech</p>	<p>New architectures, such as novel heterogeneous cores and NV-RAM memory systems, are often radically different from today's systems. Our team has recently developed a number of techniques for modeling, simulating, and measuring these future systems. Aspen, our performance modeling language, allows users to compose and answer modeling questions quickly.</p>
<p><b>Using a Hybrid Cray  Supercomputer to Model Non-  Icing Surfaces for Cold-Climate  Wind Turbines</b></p> <p>5:00 PM – 5:30 PM  <b>Masako Yamada</b>  Physicist  Advanced Computing Lab  GE Global Research</p>	<p>We have been awarded 80 million CPU hours on Titan, a hybrid Cray supercomputer, to model the freezing behavior of water droplets. By optimizing the three-body mW water potential in LAMMPS, we have achieved 5x acceleration in the hybrid CPU/GPU environment, relative to previous Jaguar performance.</p>

## **20 Petaflops Simulation of Protein Suspensions in Crowding Conditions**

5:30 PM – 6:00 PM

Simone Melchionna  
Researcher  
IPCF - National Research Council of Italy

This talk describes the recent simulation of ~18,000 proteins in suspension, reproducing the crowding conditions of the cell interior. The simulations were obtained with MUPHY, a computational platform for multi-scale simulations of real-life biofluidic problems. The same software has been used in the past to simulate blood flows through the human coronary arteries and DNA translocation across nanopores. The simulations were performed on the Titan system at the Oak Ridge National Laboratory, and exhibits excellent scalability up to 18, 000 K20X NVIDIA GPUs, reaching 20 Petaflops of aggregate sustained performance with a peak performance of 27.5 Petaflops for the most intensive computing component. In this talk I will describe how the combination of novel mathematical models, computational algorithms, hardware technology and parallelization techniques allowed reproducing for the first time such a massive amount of proteins.

*ACM Gordon Bell Finalist*

**Wednesday, November 20 | Booth #613**

### **Skin-Barrier Investigation Using GPU-Enhanced Molecular Dynamics**

10:30 AM – 11:00 AM

Russell Devane  
Scientist  
Proctor & Gamble

GPU enabled molecular dynamics are being used to investigate permanent crossing of the primary skin barrier, the stratum corneum (SC). This work is helping to identify the molecular characteristics that dictate the ability of a compound to cross the SC barrier in order to build more accurate skin penetration models.

### **Emerging Technologies for High-Performance Computing**

11:00 AM – 11:30 AM

Jack Dongarra  
Professor  
University of Tennessee

This talk will highlight the emerging technologies in high performance computing. We will look at the development of accelerators and some of the accomplishments in the Matrix Algebra on GPU and Multicore Architectures (MAGMA) project. We use a hybridization methodology that is built on representing linear algebra algorithms as collections of tasks and data dependencies, as well as properly scheduling the tasks' execution over the available multicore and GPU hardware components.

### **New Features in CUDA 6 Make GPU Acceleration Easier**

11:30 AM – 12 Noon

Mark Harris  
Chief Technologist, GPU Computing  
NVIDIA

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<p><b>Applications of Programming the GPU Directly from Python Using NumbaPro</b></p> <p>12 Noon – 12:30 PM</p> <p>Travis Oliphant Co-Founder and CEO Continuum Analytics</p>	<p>NumbaPro is a powerful compiler that takes high-level Python code directly to the GPU producing fast-code that is the equivalent of programming in a lower-level language. It contains an implementation of CUDA Python as well as higher-level constructs that make it easy to map array-oriented code to the parallel architecture of the GPU.</p>
<p><b>Twinkle, Twinkle Little Star - Using 18.000 GPUs to Simulate Jets in the Cosmos</b></p> <p>12:30 PM – 1:00 PM</p> <p>Michael Bussmann Junior Group Leader Computational Radiation Physics Helmholtz-Zentrum Dresden-Rossendorf</p>	<p>In order to understand what happens when jets of hot, streaming gas are ejected at high speed into the cosmos, we are bound to rely on measuring the radiation emitted by the particles in the jet. Astrophysical jets can originate from a variety of sources such as stars, black holes and even galaxies. In such jets, the plasma flow can become unstable, generating characteristic patterns of particle flows. Using our particle-in-cell code PICoGPU utilizing the complete TITAN supercomputer system at Oak Ridge National Laboratory, we were able, for the first time, to not only simulate the particle dynamics but also the radiation emitted during the formation of such an instability, the Kelvin-Helmholtz instability.</p> <p><i>ACM Gordon Bell Finalist</i></p>
<p><b>AMR Based on Space-Filling Curve for Stencil Applications</b></p> <p>1:00 PM – 1:30 PM</p> <p>Takayuki Aoki Professor/Deputy Director Global Scientific Information and Computing Center (GSIC)/ Tokyo Institute of Technology</p>	<p>AMR is an efficient method to assign a mesh with a proper resolution to any local areas. By using bigger leaves than those of CPU, we can assign a CUDA block to a leaf with enough thread numbers. We show a GPU implementation in which the leaves are connected by a space-filling curve.</p>
<p><b>Can You Really Learn To Use Accelerators in One Morning?</b></p> <p>1:30 PM – 2:00 PM</p> <p>John Urbanic Information Technology Manager Pittsburgh Supercomputing Center</p>	<p>OpenACC provides a friendly learning curve for using GPUs and other accelerators. We describe how we have been able to create hundreds of capable new users with half-day and two-day hands-on workshops. Come knowing nothing about accelerators, leave knowing how you and your colleagues can get in on this important new paradigm.</p>

<p><b>Tomorrow's Exascale Systems: Not Just Bigger Versions of Today's Peta-Computers</b></p> <p>2:00 PM – 2:30 PM</p> <p>Thomas Sterling Executive Associate Director &amp; Chief Scientist Indiana University</p>	<p>To get to Exascale is going to require more innovation than simply extending Petaflops machine structures with Moore's Law. Power, reliability, user productivity, generality, and cost all demand dramatic advances in all aspects of supercomputer design, operation, and programming. A new synergy of dynamic adaptive techniques, architecture, and programming interfaces are driving research towards a new generation of HPC. This talk will introduce these emerging ideas and illustrate how they will impact the future of our field.</p>
<p><b>Piz Daint: A Productive, Energy Efficient Supercomputer with Hybrid CPU-GPU Nodes</b></p> <p>2:30 PM – 3:00 PM</p> <p>Thomas Schulthess Professor of Computational Physics &amp; Directors CSCS ETH Zurich, Swiss National Supercomputing Center (CSCS)</p>	<p>Piz Daint: a productive, energy efficient supercomputer with hybrid CPU-GPU nodes We will discuss the makings of Piz Daint, a Cray XC30 supercomputer with hybrid CPU-GPU nodes. The presentation will focus on quantitative improvements in time and energy to solution due to the use of GPU technology in full climate, materials science and chemistry simulations.</p>
<p><b>Deploying Clusters with NVIDIA® Tesla® GPUs</b></p> <p>3:30 PM – 4:00 PM</p> <p>Dale Southard Senior Solution Architect HPC/Cloud NVIDIA</p>	<p>Tips and techniques for deploying high-performance computing clusters using NVIDIA® Tesla® GPUs.</p>
<p><b>Pinning Down the Superconducting Transition Temperature in the Hubbard Model</b></p> <p>4:00 PM – 4:30 PM</p> <p>Peter Staar PhD Student ETH Zurich</p>	<p>With massive improvement in algorithms and how they map onto modern hardware platforms, as well as availability of efficient multi-petaflops supercomputers like Titan, simulation-based solution of one of the most sought after problems in condensed matter theory has become possible. Implications on studies of high-temperature superconductivity will be discussed.</p> <p><i>ACM Gordon Bell Finalist</i></p>

<p><b>The NVIDIA Co-Design Lab for Hybrid Multicore Computing at ETH</b></p> <p>4:30 PM – 5:00 PM</p> <p>Peter Messmer Professor of Computational Physics &amp; Directors CSCS NVIDIA</p>	<p>Developing successful scientific software becomes increasingly a collaborative endeavor, joining the talents of from a multitude of disciplines. NVIDIA and ETH Zurich are forming a Co-Design Lab for Hybrid Multicore Computing as a joint effort to develop and optimize scientific applications for hybrid computing architectures. In this talk, I will introduce the lab and present some early successes of this new collaboration.</p>
<p><b>PARALUTION - Library for Iterative Sparse Methods on Multi-core CPU and GPU Devices</b></p> <p>5:00 PM – 5:30 PM</p> <p>Dimitar Lukarski Post-Doctoral Researcher Dept. of Information Technology, Div. of Scientific Computing Uppsala University</p>	<p>PARALUTION is a library which enables you to perform various sparse iterative solvers and preconditioners on multi/many-core CPU and GPU devices. Based on C++, it provides generic and flexible design which allows seamless integration with other scientific software packages, and gives you full portability of your code.</p>
<p><b>Common Use Cases and Performance for NVAMG: A Fast Linear Solver Toolkit on the GPU</b></p> <p>5:30 PM – 6:00 PM</p> <p>Joe Eaton Manager, NVAMG CUDA Library NVIDIA</p>	<p>We discuss some of common use cases for NVAMG, our toolkit for fast linear solvers on the GPU. NVAMG includes Algebraic Multi-Grid methods, Krylov methods, nesting preconditioners, and allows complex composition of the solvers and preconditioners. We also present some recent performance results on NVIDIA® Tesla® K20 and K40 GPUs for large-scale CFD problems of industrial relevance.</p>

Thursday, November 21 | Booth #613

<p><b>From Brain Research to High-Energy Physics: GPU-Accelerated Applications in Jülich</b></p> <p>11:00 AM – 11:30 AM</p> <p>Dirk Pleiter Leading Scientist Jülich Supercomputing Centre</p>	<p>In 2012 the NVIDIA Application Lab at Jülich has been established to work with application developers on GPU enablement. In this talk we will tour through a variety of applications and evaluate opportunities of new GPU architectures and GPU-accelerated HPC systems, in particular for data-intensive applications.</p>
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<p><b>Accessing New NVIDIA® CUDA® Features from CUDA Fortran</b></p> <p>11:30 AM – 12 Noon</p> <p>Brent Leback Compiler Engineering Manager The Portland Group, NVIDIA</p>	<p>This talk will present examples of how to take advantage of new CUDA features, specifically those introduced in CUDA 5.0 and CUDA 5.5, from CUDA Fortran. Details of overloading one specific Fortran intrinsic function which obtains near peak performance will be given. A preview of CUDA 6.0 features and how CUDA Fortran will evolve to enable them for Fortran programmers will also be shown.</p>
<p><b>Earthquake Simulations with AWP-ODC on Titan, Blue Waters and Keeneland</b></p> <p>12 Noon – 12:30 PM</p> <p>Yifeng Cui Lab Director, HPGeoC San Diego Supercomputer Center/UC San Diego</p>	<p>We simulate realistic 0-10 Hz earthquake ground motions relevant to building engineering design, and accelerate SCEC CyberShake key strain tensor calculations on Titan and Blue Waters. Performance improvements of AWP-ODC, coupled with co-scheduling CPUs and GPUs, make a California statewide seismic hazard model a goal reachable with existing supercomputers.</p>
<p><b>Running the FIM and NIM Weather Models on the Titan Supercomputer</b></p> <p>12:30 PM – 1:00 PM</p> <p>Mark Govett Chief, Advanced Computing Section NOAA Earth System Research Laboratory</p>	<p>Session description to come.</p>
<p><b>HACC: Extreme Scaling and Performance Across Architectures</b></p> <p>1:00 PM – 1:30 PM</p> <p>Salman Habib Senior Scientist Argonne National Laboratory</p>	<p>Cosmological simulations of the evolution of structure in the universe are among the most challenging of supercomputing tasks. Running on Titan, we use HACC (Hardware/Hybrid Accelerated Cosmology Code) to demonstrate how the use of GPUs to accelerate the force evaluations can lead to significantly improved performance.</p> <p><i>ACM Gordon Bell Finalist</i></p>

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