

# Scientific Computing

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## CBC Workshop on CBC Key Topics - August 25-26, 2011

Total number of participants: 23  
 Total number of guests outside of CBC: 5  
 Number of different nationalities represented: 7  
 Total number of speakers: 7  
 Total number of talks: 7

### Agenda

#### Thursday, August 25

##### **1300-1345: Low-complexity finite element methods for the de Rham complex on simplices via Bernstein polynomials** by Robert C. Kirby, Texas Tech University

Place: Bakrommet@Simula

###### **Abstract:**

In recent work, we have shown how special structure of the Bernstein polynomials on a d-simplex gives rise to low-complexity finite element algorithms. I will survey our techniques, based on sparsity of differentiation and dimensional recursion in evaluating B-form polynomials at special quadrature points. Then, I will present new work demonstrating how to express the exterior calculus bases of Arnold, Falk, and Winther in terms of short linear combinations of Bernstein polynomials. So, evaluating bilinear forms for  $H(\text{div})$  and  $H(\text{curl})$  with optimal complexity simply requires a very sparse linear transformation plus established techniques for Bernstein polynomials. This work is still preliminary, but I will present basic numerical results for Bernstein polynomials, show some pictures of exterior calculus basis functions, and describe the ramifications of Bernstein polynomials for software (say, as compared to FIAT).

##### **1400-1430: Why blood flow in the vicinity of aneurysms is difficult to compute** by Kristian-Valen Sendstad, University of Toronto and Simula

Place: Bakrommet@Simula

###### **Abstract:**

Aneurysms are balloon-shaped structures on the walls of blood vessels, which may rupture and cause stroke. Understanding aneurysm formation and rupture, and the relation to the properties of blood flow, is fundamental to diagnostics and clinical treatment. Blood flow is commonly assumed to be laminar with pulsations in the range 1-3 Hz. Through direct numerical simulations of fluid flow, using very high spatial and temporal resolution, we have recently discovered that blood flow in the vicinity of aneurysms may undergo transition to turbulence and hence become very complex, with oscillations of the order of 100 Hz. The consequences are two-fold: first, previously performed blood flow simulations may be qualitatively inadequate due to too coarse resolution; and second, high-frequency oscillations in the flow may have serious impact on the medical understanding of aneurysm and rupture.

##### **1445-1530: Right through the heart: biophysically-based strategies for modeling cells and tissues** by Molly Maleckar, Simula

Place: Bakrommet@Simula

###### **Abstract:**

Cardiac modeling activities at Simula Research Laboratory feature a range of competencies including the development of methods to study electrophysiology and mechanics in heart tissue, and the use of these tools to study selected questions related to cardiac dysfunction and arrhythmia. This talk will present some perspectives on biophysically-based modeling and simulation and their application in the context of cardiac research.

#### Friday, August 26

##### **0930-1015: Developing GPU-enabled scientific libraries** by Matthew Knepley, University of Chicago

Place: Storstua@Simula

###### **Abstract:**

A central challenge for the use of GPU hardware for computational science is the integration of code optimized for manycore execution into existing scientific libraries. The most successful paradigm for several decades has been the development of high quality libraries, such as the PETSc library for parallel linear algebra and scalable linear and nonlinear solvers. We will demonstrate the steps taken to augment PETSc with GPU code for linear and nonlinear solvers. However, the fragility of GPU with respect to performance necessitates the extension of the library approach with code generation facilities. We will present both template metaprogramming and domain specific language (DSL) generation schemes for code generation and discuss the tradeoffs for both library developers and users. We will discuss

the development of a library for finite element computations on the GPU, compatible with PETSc solvers, and also with the FEniCS toolkit which allows flexible specification of weak forms using a DSL.

**1030-1115: Run-time code generation for heterogeneous computing: methods and applications in high-order PDE solvers** by Andreas Klockner, Courant

Place: Storstua@Simula

**Abstract:**

Creating peak-performance and scalable compute codes on graphics processors is a challenge that is aggravated by complicated and constantly changing hardware. In this talk, I will describe techniques and tools to tap the enormous performance potential of GPUs for discontinuous Galerkin finite element solvers. Particular emphasis will be on the advantages that high-order discretizations offer on modern SIMD-like architectures. I will explain a few of the design considerations and tricks that enabled sustained single-chip floating point performance of above 200 GFlops/s across a wide range of discretization parameters and equation types. I will introduce tools for run-time code generation and empirical optimization from a high-level language that were crucial to the present effort. With the infrastructure in place, further discussion will concern some potential applications and perspectives on how this technology might change requirements of algorithms that work alongside PDE solvers, such as time steppers or linear solvers.

**1130-1200: Scientific computing applied to investment finance**

Place: Storstua@Simula

**Abstract:**

This talk gives a very basic introduction to the problem settings in investment finance. Scientific computing has grown to be a significant tool in the investment business, and examples of computations and challenges will be presented.

**Lunch 12-13**

**1300-1345: Challenges in computational geosciences** by Stuart Clark, Simula

Place: Mellomrommet@Simula

**Abstract:**

*not available*

<b>What</b>	▪ Workshop
<b>When</b>	Aug 25, 2011 01:00 PM to Aug 26, 2011 02:00 PM
<b>Where</b>	Bakrommet & Storstua @ Simula
<b>Contact Name</b>	Hans Petter Langtangen
<b>Attendees</b>	Anders Logg Andre Massing Andreas Klockner Benjamin Kehlet Bernardo Lino de Oliveira Glenn Lines Hans Petter Langtangen Ida Norderhaug Drøsdal Jussi Koivumaki Joakim Sundnes Karen Støverud Kent-Andre Mardal Kristian Valen-Sendstad Marie Rognes Martin Alnæs Matt Knepley Molly Maleckar Ola Skavhaug Rob Kirby Sam Wall Svein Linge Xing Cai
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