Confirmed talks FEniCS 14, Paris
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When more than one author is listed, the speaker's name is in boldface.

Martin Sandve Alnæs, Simula
Title: *TBA*

David Bernstein, Garth Wells, Chris Richardson, Axel Gerstenberger
Title: *The XFEM in FEniCS with an Application in Fracture Mechanics*
Abstract: (Key Words: *extended finite element method, partition of unity method, fracture mechanics*) The extended finite element (partition of unity) method was first proposed in 1999 for the simulation of systems with strong discontinuities. In continuum mechanics this enables the description of a fracture (a displacement discontinuity) in a body without explicitly meshing the fracture surface. Using this method, quasi-static fracture propagation can be simulated without a fracture surface conforming mesh and with no need for remeshing during fracture propagation. We describe an implementation of this method in the FEniCS project for unstructured three dimensional simplicial meshes. A generic surface class admits a variety of concrete representations, including implicit surfaces, which may be flat or curved. We show results from static, mode I fractures in bodies which are externally loaded as well as those resulting from a normal traction on the fracture surface.

Erik Burman, **Susanne Claus**, Peter Hansbo, Mats G. Larson, Andre Massing,
Title: *Level-set based unfitted finite element methods in FEniCS*
Abstract: In this presentation, we will give an overview of CutFEM, a novel stabilised unfitted finite element method, and its implementation in FEniCS. In our CutFEM approach, the discretisation of the boundary of a given domain is represented by a level set function and this level set function is allowed to cut arbitrarily through the elements of a fixed and regular background mesh. The background mesh is then also used to represent the approximate solution of the governing PDEs. This enables a discretisation of the PDEs independent of the geometric description of the domain and the associated mesh generation and therefore provides means to efficiently solve problems involving complex and evolving geometries. This is

especially important in situations where the computational cost for preprocessing of acquired geometry descriptions into representations suitable for the computational method at hand are prohibitively expensive. For example, the simulation of blood flow dynamics in vessel geometries requires a series of highly non-trivial steps to generate a high quality, full 3D finite element mesh from biomedical image data. CutFEM eases the burden of mesh generation by requiring only a low-quality and even non-conforming surface mesh representation of the computational geometry. However, in order to ensure an accurate and stable scheme independent of the boundary location, stabilisation techniques have to be employed. In our presentation, we will detail such a stabilisation technique involving so-called ghost penalties across element edges that are intersected by the interface and we will give details of how this CutFEM approach combined with Nitsche's method is implemented in FEniCS. We will finalise this discussion with computational results for a range of problems both in the bulk and on surfaces with increasing complexity.

Colin Cotter, Department of Mathematics, Imperial College London
Title: *Mixed finite element methods on curved meshes*
Abstract: In this talk I will discuss how I write Dolfin code for solving mixed finite element problems on curved meshes, despite the fact that only affine transformations are currently supported. In particular, I will concentrate on "compatible" mixed finite element spaces that correspond to a discrete de Rham complex. In this case, many terms in PDEs often become "topological" in the sense that distorting the element does not change the local matrix for those terms. It then becomes tractable to alter the metric in the remaining terms purely at the UFL level; I will show how to do this. To obtain the correct convergence rate for solving problems with higher-order spaces (such as (V,Q) = (BDM(k),P(k-1)) or (RT(k),P(k)), using the FEniCS enumeration) on curved meshes such as the sphere, it is necessary to use elements that are kth-order approximations to the manifold surface. In numerical weather prediction, the strong timescale separation between divergence-free and divergent motions means that classical approaches have used the C-grid finite difference method (which corresponds to a particular implementation of Discrete Exterior Calculus (DEC)), which provides a discrete Helmholtz decomposition. The requirement of great flexibility in mesh structure has recently led us to develop extensions of this approach

based on compatible mixed finite element spaces, which also have a discrete Helmholtz decomposition. In these problems, it turns out that even if one is using lower order spaces, it is necessary to use higher-order approximations of the sphere since the error in initialising the model from data due to the flat approximation of the sphere can spuriously project onto the fast divergent modes where they wreak havoc with the weather forecast. Hence, implementing compatible finite element methods on curved elements is a problem that I care about. To show stability and convergence for the discrete Poisson equation, for example, use is made of the property that the divergence operator maps from V to Q. On curved meshes, this causes a problem one has to include a factor of 1/det(J) in all of the functions in Q, which degrades the approximation order. Bochev and Ridzal (SIAM Journal on Numerical Analysis, 2008) suggested a fix for the case of RT1 on non-affine quadrilaterals, namely to replace the div operator with the DIV operator which is used in DEC. I will explain that this idea extends easily to any other compatible mixed finite element spaces, since it is simply the usual div operator followed by L2 projection into Q. With this modification, the correct high-order convergence rate can be obtained, which I will illustrate with numerical tests (I will also show Dolfin code). If there is time then I will also show numerical results from nonlinear models used in numerical weather prediction, based on the same approach.

Simon W. Funke and M Nordaas, Simula Research Laboratory
Title: *Optimisation algorithms in Hilbert spaces for PDE-constrained problems*
Abstract: The solution of optimisation problems constrained by partial differential equations becomes more and more feasible due to the increase in computational resources, the development of efficient algorithms and the advance in automated frameworks such as FEniCS and dolfin-adjoint. Nevertheless, practical optimisation problems still raise a significant challenge due the large number of degrees of freedoms and the computational cost of the resulting PDE solves. Hence special attention on using effective algorithms is required when solving practical problems. A key property for an efficient optimisation algorithm is that the required iteration numbers are independent on the problem discretisation - in particular with respect to mesh resolution and partial refinement. However, a straight-forward application of optimisation algorithms on the reduced problem results in

mesh-size dependent iteration numbers and a degrading performance on non-homogeneous meshes. In this talk we present how mesh-independent convergence can be recovered by formulating standard optimisation algorithms in a Hilbert space setting based on the continuous optimisation problem. In particular, the optimisation algorithms are designed to respect the inner products and induced norms of the underlying function spaces of the control and state spaces. Based on this idea we develop a new optimisation framework, Moola, which honors the underlying Hilbert spaces and the inner products. Moola is written in Python and uses an abstract algebra interface to combine easy code readability while maintaining full parallelisation of the algebraic operations. Currently common unconstrained optimisation algorithms are implemented and Moola integrates seamlessly with FEniCS and dolfin-adjoint. We show that this strategy is equivalent to a preconditioned conjugate gradient methods, and for the BFGS method a user defined initial estimate of the Hessian matrix and demonstrate the effectiveness of the proposed approach by numerical experiments.

Axel Gerstenberger, Garth Wells, Chris Richardson, David Bernstein

Title: *An algebraic multi-grid implementation in FEniCS for solving 3D fracture problems using the extended finite element method*

Abstract: The eXtended Finite Element Method (XFEM) is a valuable tool for simulating crack propagation, fluid- structure interaction and multiphase/multimaterial problems, which is evident by the vast literature on this method. As problem sizes grow, the wish to apply iterative Algebraic Multi-Grid (AMG) methods to XFEM problem arises. However, the introduction of additional degrees of freedom with special approximation functions, which is the main ingredient of XFEM, poses a number of challenges that hamper the straightforward application of existing AMG. Examples of such difficulties are increased condition numbers of the system matrix, varying number of unknowns per node, and matrix graphs, that do not reflect physical properties of the system. This presentation revisits the main difficulties of using AMG methods for XFEM and how these diffi- culties can be overcome to again reach the performance that one expects from using AMG for standard Finite Element Methods [1]. Beyond the theoretical aspects, the presentation demonstrates the relative ease of implementing this method into the FEniCS framework and gives 3d simulations results using both Trilinos and PETSc linear backends. REFERENCES [1] A. Gerstenberger and R. Tuminaro. An algebraic multigrid approach to solve extended finite element method based fracture problems. Int. J. Numer. Meth. Engng., Vol. 94(3), 248272, 2013, DOI:10.1002/nme.4442

Johan Hoffman, KTH, Stockholm

Title: *High Performance Computing with FEniCS*

Abstract: PRACE (Partnership for advanced computing in Europe) is the organization that is responsible for coordination of European supercomputing infrastructure. In the PRACE 8th Regular Call for 2014-2015, the only project that was awarded access to the most powerful (Tier-0) resources in the field of Mathematics and Computer Sciences was the project FEniCS-HPC - High performance adaptive finite element methods for turbulent flow and multiphysics with applications to aerodynamics, aeroacoustics, biomedicine and geophysics. The project includes researchers at the KTH Royal Institute of Technology in Sweden, the Basque Center for Applied Mathematics in Spain, and the RIKEN Advanced Institute for Computational Science in Japan. In this talk we describe the method and software development at the center of FEniCS-HPC, and highlight application projects based on the FEniCS-HPC computational technology, including simulation of the aerodynamics of airplanes, blood flow in the human heart, and human phonation. References: [1] PRACE 8th Regular Call, http://www.prace-ri.eu/PRACE-8th-Regular-Call [2] J. Hoffman, J. Jansson, R. Vilela De Abreu, Time-resolved adaptive FEM simulation of the DLR F-11 aircraft model at high Reynolds number, AIAA 2014-0917, Proc. 52nd Aerospace Sciences Meeting, AIAA SciTech, 2014. [3] J. Hoffman, J. Jansson, R. Vilela de Abreu, N. C. Degirmenci, N. Jansson, K. Muller, M. Nazarov and J. Hiromi Spuhler, Unicorn: parallel adaptive finite element simulation of turbulent flow and fluid-structure interaction for deforming domains and complex geometry, Computers and Fluids, Vol.80, pp.310-319, 2013. [4] The Eunison project, http://www.eunison.eu [5] CTL Forge, http://dryad.csc.kth.se

Bärbel Janssen, KTH, Stockholm

Title: *Quadrature for flexible interface representation in Dolfin-HPC*

Abstract: In fluid-structure interaction problems as well as in multiphase flows the interface is typically not aligned with the mesh, so that a separate representation of the interface is needed. Given an interface representation

we want to be able to integrate over a single phase in the mesh, for which we need special local quadrature rules. Dolfin-HCP is a branch of Dolfin focused on high performance computing for massive parallel hardware architectures, where we typically want to avoid Python dependencies. Since no access from the C++ side in Dolfin-HPC to the quadrature has been available so far, the implementation of quadrature rules in 2D and 3D was necessary. In this talk we will focus on the extensions and changes to ufc, ufl and Dolfin-HPC which were unavoidable to allow for local integration.

Johan Jansson, KTH, Stockholm and Basque Center for Applied Mathematics, Bilbao
Title: *Adaptive high-performance methods and applications in the FEniCS-HPC framework*
Abstract: We present a new adaptive finite element method (FEM) directly using the a posteriori error representation as a local error indicator, and representing the primal and dual solutions in the same finite element space (here piecewise continuous linear functions on the same mesh). Since this approach gives a global a posteriori error estimate that is zero (due to Galerkin orthogonality), the error representation has traditionally been thought to contain no information about the error. However, we show the opposite, that locally, the orthogonal error representation behaves very similar to the non-orthogonal error representation using a quadratic approximation of the dual. This method is completely automated, cheap and easy to implement, which makes it suitable in a high-performance computing setting, such as the FEniCS-HPC framework. We also present applications in FEniCS-HPC, such as self-oscillating vocal folds in a turbulent fluid-structure interaction setting with contact in the EUNISON project and adaptive simulation of a full aircraft at take-off and landing conditions as a contribution to the HiLiftPW-2 workshop organized by NASA and Boeing among others. This research is mainly supported by a Severo Ochoa Center of Excellence grant (Spain) for BCAM, a PRACE Tier-0 HPC grant (EU) for FEniCS-HPC and an EU FP7 grant (EU) for the EUNISON project.

Kristian Ejlebjerg Jensen, Gerard J. Gorman, Imperial College London,
Title: *Anisotropic Mesh Adaptation and Topology Optimization*
Abstract: Mesh adaptation is a well recognized tool for achieving a near pareto-optimal compromise between computational cost and accuracy, and

it is critical for performance, when multiscale phenomena are to be resolved. Such problems are often characterised by weak elliptic character and highly directional features; the latter calling for anisotropic elements, if the discretisation is to truly match the physics. We have combined a thread-parallel anisotropic mesh generator (PRAgMaTIc) with FeniCS and, staying true to the spirit of the UFL language, we can adapt the mesh to describe a variable with a single python statement. Within the field of topology optimization the number of design variables is normally scaled with the number of degrees of freedom for the forward problem. These optimization problems are typically solved on a fixed structured mesh due to ease of implementation and compatibility with mathematical optimizers. The method is widely used in the automotive and aerospace industries for structural optimization as it can give an excellent starting point for light and stiff components. In this context, a p-norm of the von Mises stress is often used for converting between local and global stress constraints, but this function poses a problem for isotropic meshes as it tends to increase rapidly over a small length scale near the boundary of the structure. In other words: candidates for stiff and light structures can be found, but a manual post processing step is required to ensure that these structures do not fail under load. Currently optimization with stress constraints are plagued by infeasible starting points as well as local minima. We have been successful in compliance minimization, by using topological derivatives in a continuous approach as well as using a transformation of the discrete sensitivity and internal optimizer variables to continuous fields.

Benjamin Kehlet, Simula

Title: `mshr` — *mesh generation in FEniCS*

Abstract: Lately an effort has been made to improve the mesh generation features in FEniCS with respect to robustness and functionality. The result is a new component, `mshr`, which replaces the mesh generation code in Dolfin. `mshr` can generate meshes from CSG geometries or boundary descriptions in various file format and supports `cgal` and `tetgen` as mesh generation backends. In this talk we present new functionality and give examples of use.

Rob Kirby, Baylor Univ., Waco, TX

Title: *Recent results on Bernstein polynomials*

Abstract: Bernstein polynomials provide a general geometrically decomposed arbitrary-order simplicial finite element basis. They also give "spectrally efficient" algorithms – much like using high order tensor product bases on rectangular domains. They also can be used to generate bases for H(div) and H(curl) spaces. For high degree, the Bernstein algorithms far outperform the FEniCS implementation. I will survey results and also talk about challenges that the Bernstein polynomials would present to full integration with FEniCS.

Fabio Luporini, Paul H. J. Kelly, and David A. Ham, Imperial College London

Title: *COFFEE: an Optimizing Compiler for Finite Element Local Assembly (COFFEE stands for COmpiler For FinitE Element local assembly)*

Abstract: Local assembly is the characteristic operation of the finite element method, which entails the numerical evaluation of a problem-specific integral for each element in the discretized equation domain. Since the domain size can be huge, efficient computation of such integrals is fundamental. Many approaches are possible: in addition to the conventional quadrature representation, the introduction of DSLs and the adoption of run-time code generation has led to novel methods based on tensor contraction [1] and symbolic manipulation [2]. It has been demonstrated, however, that quadrature representation remains the optimal choice for a wide class of problems [3]. Low-level optimization of routines based on quadrature representation is, in general, a challenging issue. Even though an affine, typically non-perfect loop nest is generally present, the short trip counts and the complexity of mathematical expressions make it hard to determine a single or unique sequence of successful transformations. In this context, we present the design and systematic evaluation of COFFEE, a domain-specific compiler for local assembly integrated with the FEniCS-compatible system Firedrake. COFFEE manipulates abstract syntax trees produced by a modified version of the FEniCS Form Compiler (FFC), introducing composable optimizations aimed at improving instruction-level parallelism, especially SIMD vectorization, and register locality. It then generates C code including vector intrinsics. Experiments using a range of finite-element forms of increasing complexity show that significant performance improvement over

FFC-optimized problems is achieved. In this talk, we also mention two optimizations, which are currently under development in COFFEE, that are of general interest for the FEniCS community: inter-kernel vectorization and generation of specialised code for small linear algebra operations. The former enables SIMD vectorization in problems in which the amount of loop-invariant code, inherently unstructured, represents the bulk of the computation, for example those based on hyperelasticity; the latter centers on transforming the quadrature code into a sequence of calls to optimized BLAS routines. References [1] Robert C. Kirby and Anders Logg. A compiler for variational forms. ACM Trans. Math. Softw., 32(3):417444, September 2006. [2] Francis P. Russell and Paul H. J. Kelly. Optimized code generation for finite element local assembly using symbolic manipulation. ACM Transactions on Mathematical Software (TOMS), 39(4), 2013. [3] Kristian B. Olgaard and Garth N. Wells. Optimizations for quadrature representations of finite element tensors through automated code generation. ACM TOMS, 37(1):8:18:23, January 2010.

Corrado Maurini, Andres Leon Baldelli, and Tianyi Li, Univ. Pierre and Marie Curie
Title: *Variational inequalities solvers and their application to variational damage and fracture mechanics*
Abstract: Many non-linear problems imply the minimisation of functionals under unilateral constraints. In these problems, the optimality conditions are expressed by a set of variational inequalities. Two major examples in solid mechanics are contact and damage problems. Although robust scalable solvers for convex problems including bound-constraints on the unknowns are now available, they are rarely accessible in finite element software. In this talk I will briefly describe the FEniCS interface to the solvers for bound-constrained problems recently included in PETSc and discuss more in detail their application to my specialised field of research: damage and fracture mechanics. I will show how FEniCS allows us to write with few lines of python code a solver for a generic class of gradient damage models used to approach crack evolution in brittle materials in the framework of the variational approach to fracture. In this approach, cracks are regularised through a smeared damage field which should respect an irreversibility condition forbidding crack self-healing. The nucleation, shape, and quasi-static evolution of cracks is obtained by solving a non-

linear problem including a variational inequality on the damage field.

Hartmut Monien, Bethe Center for Theoretical Physics, Bonn
Title: *Using FEniCS to solve problems in algebraic geometry*
Abstract: Algebraic geometry is concerned with finding the locus of zeros of sets of polynomial equations in a commutative ring. In my talk I will show how some hard questions in that field can in fact be answered by explicitly solving a 2D partial differential equation on a Riemann surface. I will present two nontrivial examples which can already be solved using FEniCS and will discuss the current limitations and technical requirements for making FEniCS fully usable for this kind of application.

Andrew T. T. McRae, Gheorghe-Teodor Bercea, Lawrence Mitchell, David A. Ham, and Colin J. Cotter, Imperial College London,
Title: *Firedrake: extruded meshes and outer-product elements*
Abstract: At the time of writing, FEniCS's DOLFIN only supports fully unstructured meshes with simplicial elements—intervals, triangles and tetrahedra. There are many examples where a partially-structured mesh, with non-simplicial cells, is more appropriate. This is especially true if the domain (or the PDE) is far from isotropic. A classic example is in geophysical contexts, where the vertical thickness of the atmosphere or ocean is several orders of magnitude smaller than the horizontal scales. In Firedrake, we label these meshes extruded: a 'base' mesh is extruded upwards or outwards to form a new mesh with a regular layered structure. This partial structure also helps to offset the efficiency losses that arise from using an unstructured base mesh. The geometric cells are the product of a 'base' cell a 2D triangle or 1D interval with an interval: giving a 3D triangular prism or 2D quadrilateral, respectively. We also require finite element spaces on such cells. At a local level, these can often be expressed in terms of products of existing elements. The simplest example is a CG element on a prism. This is just the outer product of the CG elements on a triangle and on an interval. However, far more unusual finite element spaces can also be constructed in the same way, including those compatible with the principles of FEEC[1]. In this talk, we will give some details of how extruded meshes are implemented within Firedrake. This includes modifications made to FIAT and FFC in order to automatically generate these new types of elements, and corresponding additions to UFL. Reference: [1] Douglas N. Arnold and

Richard S. Falk and Ragnar Winther. Finite element exterior calculus, homological techniques, and applications. Acta Numerica, Vol. 15, 1155, 2006.

Jean-Claude Nedelec, Ecole Polytechnique
Title: *TBA*

Florian Rathgeber, Imperial College London,
Title: *Firedrake: Re-imagining FEniCS by Composing Domain-specific Abstractions*
Abstract: In an ideal world, scientific applications are computationally efficient, maintainable, composable and allow scientists to work very productively. The FEniCS project has demonstrated that these goals are achievable for the domain of finite element computations. In this talk we demonstrate the composition of the domain-specific abstractions Firedrake and PyOP2 into a FEniCS-compatible system for the portable solution of partial differential equations using the finite element method on unstructured meshes. Domain knowledge is used to deconstruct the problem into a series of lower level operations which can be solved by composing existing tools and contributions from different scientific communities to solve sophisticated problems. Firedrake exposes a DOLFIN-compatible interface allowing scientists to describe variational forms and discretisations for linear and non-linear finite-element problems symbolically using the Unified Form Language UFL. Forms are translated into computational kernels by a modified version of the FEniCS Form Compiler FFC. Assembly operations are transformed into local computations over the mesh and passed to PyOP2 for efficient parallel execution. Variational problems are solved using PETSc's SNES interface. PyOP2 abstracts away the performance-portable parallel execution of computational kernels on a range of hardware architectures, targeting multi-core CPUs, GPUs and accelerators and distributed parallel computations with MPI. Backend-specific code tailored to each specific computation is generated, just-in-time compiled and efficiently scheduled for parallel execution at runtime. The composability of the Firedrake and PyOP2 abstractions allows optimised implementations for different hardware architectures to be automatically generated without any changes to a single high-level source. A separation of concerns is achieved, where the reasoning about the variational form is separated from the computations over

the mesh. Firedrake is freed from handling any field data or parallelism, whereas PyOP2 is agnostic to the fact it is executing a finite element local assembly kernel.

Laurent Rineau, Geometry Factory
Title: *CGAL mesh generation*

Marie E. Rognes, Simula Research Laboratory
Title: *An adjoint-enabled simulation framework for cardiac electrophysiology*
Abstract: TBA

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