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Preconditioning for large scale micro finite element analysis of 3D poroelasticity

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Keywords: Bone structure analysis, Biot model of poroelasticity, Krylov space solver, multigrid preconditioning.

ABSTRACT

Poroelasticity investigates the deformation of porous media under the influence of the fluid contained within the body. The foundations of the classical theory of poroelasticity has been stated by Biot. In his theory, Biot coupled a porous Hookean solid with Darcy's law in conjunction with continuity to model the fluid passing through the pores of the solid matrix. Poroelasticity is used in a wide range of disciplines. Our interest in poroelasticity originates in osteoporosis, a disease that is a major health problem in developed countries where the risk for an osteoporotic fracture for women above 50 years is about 50%, for men it is about 20%. In this connection, we have developed a solver called ParFE to model linear *elastic* response of realistic bone structures to exterior forces. The code is highly adapted to voxel-based models generated by CT scans. It is used by researchers that focus on bone remodeling which investigates the changes on the bone structure exposed to cyclic load.

A linear *poroelastic* problem requires the simultaneous solution of elasticity equations and Darcy's law along with mass conservation where the coupling between the solid and fluid content is realized. We present a solver for large scale poroelasticity problems considering voxel models on the micro level which will later be used as a tool to analyze bone poroelasticity. The governing equations are discretized using mixed finite elements considering a formulation which uses displacements $\mathbf{u}$, flux $\mathbf{f}$, and pressure p as primary unknowns, respectively. The geometry is modeled with equal size hexagonal elements, so-called voxels, in which the approximations are piecewise trilinear (Q_1) for displacements and piecewise constant (P_0) for the pressure. The flux is approximated by lowest order Raviart-Thomas (RT_0) elements.

This mixed finite element discretization leads to a linear system of equations with a 3-by-3 block structure. All diagonal blocks are symmetric definite. The system as a whole is indefinite.

We solve the linear system by (flexible) GMRES, with block-diagonal and block-triangular preconditioners. A solve with the diagonal blocks of the preconditioner is replaced by a number of AMG V-cycles or by AMG preconditioned CG. We investigate how the iteration count of the outer iteration is affected by the accuracy of the inner iteration.

Our present highly parallel solver, an extension of ParFE, relies heavily on the Trilinos framework which defines distributed vectors and sparse matrices for parallel environments and provides state-of-the-art packages for iterative solvers as well as for preconditioners and partitioning tools. The solver is tested against benchmark problems on artificial domains and realistic bone structures, all of them composed of voxels. We report on the parallel performance observed on the Cray XT-5 at the Swiss National Supercomputing Center (CSCS).

Domain Decomposition Methods for Cardiac Electro-Mechanics

Christoph Augustin

SFB Workshop on Efficient Solvers in Biomedical Applications

ABSTRACT

In this talk we will present a structural model for the nonlinear elastic behavior of cardiac tissue and outline the main equations of strongly and weakly coupled electro-mechanics. The resulting nonlinear models lead to very complex and time-consuming algorithms. Hence parallel methods are very well suited to treat such problems. We outline the main ideas of domain decomposition methods and show their application to the cardiac model. Numerical examples are included where we compare different solution strategies for the elasticity problem. Finally, we give first examples of the coupled problem.

Fast boundary-integral methods for modeling drug-protein interactions and drug design

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ABSTRACT

Computer simulation of drug-protein interactions play important roles aiding in the design and improvement of therapeutics. Many simulations employ continuum models based on the Poisson equation, which offer a computationally fast alternative to atomistic models (e.g. molecular dynamics). As a result, boundary-integral methods of potential theory are widely used in computational chemistry, particularly to model how biological water mediates drug-protein binding. In this talk, I will provide an overview of fast boundary-integral approaches for molecular modeling and drug design, recent theoretical advances, and the main modeling challenges that the community still faces. Specific topics will include fast boundary-element method solvers, high-order methods, approximation theories and more advanced continuum theories, and fast algorithms for inverse problems associated with optimizing drug affinity for molecular targets.

Scalable Numerical Solution of PDEs with the Distributed and Unified Numerics Environment

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ABSTRACT

The Distributed and Unified Numerics Environment (DUNE) is a software framework for the grid-based numerical solution of partial differential equations developed by several groups in Germany. It is based on a strict separation of algorithms and data structures by abstract interfaces and the consequent use of static polymorphism to achieve performance. The sparse linear algebra and iterative solver part features in particular recursive block structuring and a scalable agglomeration-based algebraic multigrid method. The performance of DUNE and its solvers will be demonstrated with respect to different applications including elliptic model problems, multiphase compositional flow in porous media and Maxwell's equations using up to 300000 cores. This is joint work with Markus Blatt, Jorrit Fahlke, Olaf Ippisch, Steffen Müthing and Rebecca Neumann.

From h to p efficiently: What is the appropriate accuracy for biomedical simulations?

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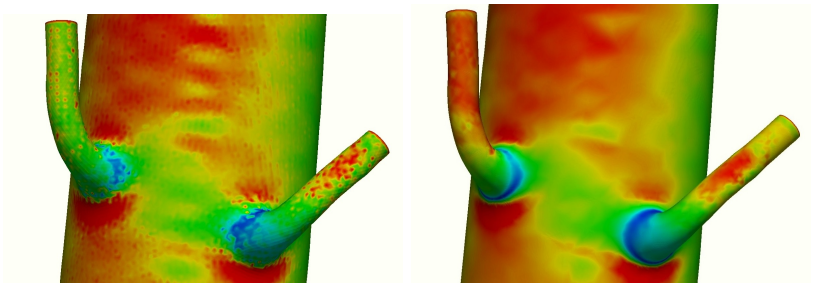

Atherosclerosis is the leading cause of morbidity and mortality in the developed world. The prevalence of this disease has an immense social and economic impact. The disease is characterised by the progressive narrowing and hardening of medium-sized and large arteries, which can lead to ischemia of the heart, brain, or extremities; ultimately, by triggering blood clots, the disease can give rise to myocardial or cerebrovascular infarctions (heart attacks and strokes). A striking feature of the disease is its characteristic, patchy distribution within the arterial system; some sites become severely affected whilst other remain free of disease. Because of this feature, much research has focused on the role of locally-varying haemodynamic factors, particularly wall shear stress (WSS), in the development of atherosclerotic lesions; however, despite the plethora of research there is, to date, no consensus on the issue.

A pertinent question to ask when modelling the governing partial differential equation (PDE) in such a problem is: What is the ideal discretisation order for a desired computational error? Although, typically the answer is understood in rather general terms there are comparatively little quantitive results. The issues behind this question are demonstrated in the figure above where the wall shear stress pattern around two small branching vessels in and anatomically realistic aorta model is compared. The left hand image is a linear finite element approximation on a fine mesh and the right image is a coarse mesh approximation using a 6th order polynomial expansion. The high order discretisation is much smoother but this accuracy typically is associated with a higher computational cost. Although the low order approximation looks more pixelated it does however capture all the salient features of the wall shear stress patterns.

The spectral/hp finite element method can be considered as bridging the gap between the traditionally low-order finite element method on one side and spectral methods on the other side. Consequently, a major challenge which arises in implementing the spectral/hp element methods is to design algorithms that perform efficiently for the entire range of discretisations. Additionally, the choice of discretisation controls the solution accuracy. In solving a given PDE using the spectral/hp element method, it is desirable to achieve a certain level of accuracy at minimal runtime cost. In this talk, an overview of the strategy for aortic blood flow modelling will be given.

Interface operators, domain decomposition and applications

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Heterogeneous problems characterized by different differential operators in subregions of the computational domain can be equivalently expressed in terms of suitable pseudo-differential operators, defined on the interfaces between the subdomains.
In this way, the given coupled problems can be reformulated as interface equations and the local pseudo-differential operators can be used to characterize possible preconditioners for the interface problems themselves.
In this talk, we show how this approach can be applied to some problems of interest in biomedical applications, e.g., fluid-structure interaction and filtration problems. We introduce suitable interface operators and we propose possible preconditioners to solve the systems arising from the finite element approximation of such problems. Finally, we present some numerical tests to prove the effectiveness of this technique.

Fine-grained Parallel Solvers and Preconditioners on Multi-core CPUs and GPUs - The Next Steps in the Biomedical Engineering

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ABSTRACT

The core of many biomedical simulation software packages (or systems) is based on different iterative linear and non-linear solvers. Due to the fact that large fraction of the computation time is spend for this tasks, their performance depends significant on the hardware utilization of the modern multi- and many-core devices. A critical problem arises from the fact that the classical legacy codes are usually not able to automatically take advantage of the new hardware technologies. Due to the growing peak performance gap between single core and multi-/many-core devices, the single-threaded programs tend to perform in non-optimally on the emerging platforms.

In this talk, we detail a generic adaptation process of Krylov-subspace and multi-grid solvers. Special focus goes to different fine-grained parallel preconditioners and smoothers based on additive and multiplicative decompositions. In order to provide the necessary level of parallelism, we tread the additive splitting scheme with a multi-coloring technique. For the incomplete LU factorization, we show a novel method for controlling the fill-in entries during the factorization process - called the power(q)-pattern method.

All of the fine-grained parallel numerical methods are embedded in the finite element software package HiFlow3. The efficiency of proposed schemes will be shown in two test scenarios - preconditioned Krylov subspace methods and matrix-based multi-grid methods. In addition, we present our on going work on integrating the proposed methods in specific biomedical applications based on HiFlow3.

On the preconditioning of the Navier–Stokes equations with applications in arterial blood flow

Efficient Solvers in Biomedical Applications, Mariatrost, July 2-5, 2012

Lorenz John[1] Olaf Steinbach[2]

We present an overview on different preconditioners for the Navier–Stokes equations. In particular we focus on preconditioning techniques for high Reynolds number flows, which arise in problems for arterial blood flow. Further, preconditioners for stabilized finite element methods and optimal control problems for the Navier–Stokes equations are discussed. Some numerical results will be given.

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Abstract

SFB Workshop: Efficient Solvers in Biomedical Application

Mixed cG/dG Finite Element Methods for Solving the Bidomain Equations

In this talk we present a mixed cG/dG finite element method which is continuous in space and discontinuous in time for the solution of the cardiac bidomain equations. To this end we use existing results on existence and uniqueness for the quasi-stationary case, and apply them for the parabolic system. Further we will focus on a stability and error analysis and we present some first numerical results. Such an approach allows for rather general discretization in space and time including adaptive refinements, and the coupling with other physical fields such as mechano-electric feedback.

Efficient Solution of the Laplace Equation during Mesh Generation

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ABSTRACT

When generating a mesh for large scale applications, the solution of the Laplace-equation is an important topic. Here the contradiction of "needing a mesh to generate a mesh" occurs. Within this talk a method of solving laplace-equation with a non-mesh based approach will be presented. As the storage of the matrix is also a topic to be memory efficient, an implementation will be proposed which works without having the matrix in memory, but allows multigrid acceleration in the iterative solution algorithm. The parallel aspects of this algorithm working on shared memory architectures are discussed.

Domain decomposition methods for almost incompressible elasticity problems within the simulation of biological soft tissue

Axel Klawonn* Oliver Rheinbach†

Abstract

The treatment of atherosclerosis by a balloon angioplasty involves large deformations of the arterial walls. The mechanical behavior of arterial walls in the physiological range can be described by anisotropic, almost incompressible hyperelastic elasticity. Discretization of the three dimensional models by the finite element method usually results in a large number of equations which are solved using a domain decomposition methods suitable for parallel computing. In this talk, departing from the framework for the solution of the anisotropic, almost incompressible nonlinear elasticity problem, we will concentrate on the incompressibility aspect of the elastic material and the development and analysis of robust solvers for these type of problems.

This talk is based on results obtained in different joint projects with Andreas Fischle and Sabrina Gippert, Department of Mathematics, University of Duisburg-Essen and Daniel Balzani, Dominik Brands, Sarah Brinkhues, and Jörg Schröder, Institute of Mechanics, University of Duisburg-Essen.

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Identification of objects: high resolution imaging

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ABSTRACT

The problem of identification of geometric objects (defects, obstacles, scatterers) and reconstruction of its geometric and physical parameters from given boundary measurements has numerous applications in the biomedical sciences in the context of nondestructive testing with acoustic, elastic, electromagnetic waves. We consider a class of inverse problems for identification of unknown objects within multiple measurements concept. Based on optimality conditions and level sets we provide high resolution properties of the object imaging and its stability to discretization and noise errors. For the analysis and numerical realization of the problem, the methods of topology optimization, generalized singular perturbations endowed with variational techniques, and a Petrov-Galerkin enrichment method within GFEM are used. In example configuration, we focus on the Helmholtz problem for identification of the position of objects of arbitrary shape and unknown boundary conditions. We present the result of numerical tests.

Inherently parallel solution methods for problems in nonlinear biomechanics

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ABSTRACT

The parallel solution of large scale -and possibly constrained- problems in nonlinear mechanics and biomechanics puts a high demand on the used solution method. A standard strategy is to employ Newton-like techniques on the global nonlinear problems, leading to a sequence of global linear problems which then are solved in parallel. The approach to be discussed here is based on a different paradigm: Instead of linearizing the global problem, we divide the original nonlinear problem into many small nonlinear subproblems, which are then solved independently. On major point to be addressed here is, of course, the convergence of the resulting distributed iteration scheme. Strategies like ASPIN, for example, also pursue the idea of solving local nonlinear problems, but do not provide convergence control strategy. One unique feature of our algorithm is that we actually can prove global convergence. This is done by exploiting the fact that for hyperelastic materials the equilibrium conditions are actually the first order necessary conditions of a (non-convex) minimization problem. Borrowing ideas from Trust-Region strategies, we will show how to construct an efficient and inherently parallel method, which converges to first order critical points for arbitrary start iterates. With stronger smoothness assumptions, also convergence to second order critical points can be shown. We will present this approach and discuss it along example from mechanics and biomechanics. Numerical examples on up to 2000 cores will be shown and discussed. Furthermore, we will explain how to incorporate constraints and in what way this ideas can be extended in order to modify the ASPIN strategy such that it becomes globally convergent (G-ASPIN), thus showing the flexibility of our theoretical framework.

Computational modeling of chemo-electro-mechanical coupling

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ABSTRACT

Computational modeling of the human heart allows us to predict how chemical, electrical, and mechanical fields interact throughout a cardiac cycle. Pharmacological treatment of cardiac disease has advanced significantly over the past decades, yet it remains unclear how the local biochemistry of individual heart cells translates into global cardiac function. Here we propose a novel, unified strategy to simulate excitable biological systems across three biological scales; from the molecular level via the cellular level to the organ level. To discretize the governing chemical, electrical, and mechanical equations in space, we propose a monolithic finite element scheme. We apply a global-local split, in which the deformation of the mechanical problem and the transmembrane potential and electrical problems are introduced globally as a nodal degrees of freedom, while the state variables of the chemical problem are treated locally as internal variables on the integration point level. This particular discretization scheme is highly efficient and inherently modular, since it allows us to combine a variety of different cell types through only minor local modifications on the constitutive level. To ensure unconditional algorithmic stability, we apply an implicit backward Euler finite difference scheme to discretize the resulting system in time. To increase algorithmic robustness and guarantee optimal quadratic convergence, we suggest an incremental iterative Newton-Raphson scheme. The proposed algorithm allows us to simulate the interaction of chemical, electrical, and mechanical fields during a representative cardiac cycle on a real patient-specific geometry, robust and stable, with calculation times on the order of four days on a standard desktop computer. More importantly, for real time clinical applications, the plain electrical problem only requires simulation times of less then ten seconds.

Domain Decomposition Solvers for some Fluid-Structure Interaction Problems

Ulrich Langer* and Huidong Yang†

April 26, 2012

Abstract

In this talk, we present some analysis and numerical studies of two partitioned fluid-structure interaction solvers: a preconditioned GMRES solver and a Newton based solver. The structure part in the fluid-structure interaction problems considered consists of a nearly incompressible elasticity model in a classical mixed displacement-pressure formulation. Both solvers are highly relying on robust and efficient solvers for the fluid and structure sub-problems obtained from an extended and stabilized finite element discretization on hybrid meshes. For solving the discretized sub-problems with incompressible and nearly incompressible models, a special algebraic multigrid method capable of handling such general saddle point systems is investigated.

In addition, a two-layer coupled fluid-structure-structure interaction model is considered, which incorporates an anisotropic structure model into the fluid-structure interaction problems. We propose two domain decomposition solvers for such a class of coupled problems: a Robin-Robin preconditioned GMRES solver combined with an inner Dirichlet-Neumann iterative solver, and a Robin-Robin preconditioned GMRES solver combined with an inner monolithic algebraic multigrid solver capable of handling an anisotropic compressible and nearly incompressible sub-problem.

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Parallelization of a PCG-AMG Solver in Multi-CPU/GPU Environments

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ABSTRACT

We present a parallel conjugate gradient solver with an algebraic multigrid preconditioner for second-order elliptic PDEs called: Parallel Toolbox (PT). The PT is designed for multi-CPU and multi-GPU environments and uses non-overlapping-elements domain decomposition as parallelization approach. We discuss in detail the parallelization strategy, the resulting parallel performance properties, and recent optimizations in the communication pattern. Strong scalability benchmarks are presented for the bidomain equations of a state-of-the-art model of rabbit ventricles using the CARP (Cardiac Arrhythmias Research Package) simulator.

An adaptive DG finite element method in space and time

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For evolution equations we present a space-time method based on Discontinuous Galerkin finite elements. Space-time methods have advantages when we have to deal with moving domains and if we need to do local refinement in the space-time domain. For this we use a residual based error estimator. This method will be applied to the heat equation and to the Navier Stokes equations as model problems. Numerical examples and some applications will be given.

An efficient multigrid solver based on aggregation

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ABSTRACT

Modeling in biomedical applications often leads to complex coupled systems of PDEs that can only be solved numerically. After discretization, one is left with a huge set of linear or nonlinear equations, whose solution requires proper techniques. And the latter often need as building block an inner procedure able to quickly solve discrete Poisson-like or convection-diffusion equations, sometimes with complex geometries and highly varying coefficients.

n this talk, we present a solver having these capabilities. It is of algebraic multigrid type, but uses a somehow nonstandard coarsening based on the aggregation of the unknowns. Among its attractive features, it offers stable performances without parameter tuning or variant switch; that is, using the code in a purely black box fashion. It also scales well in parallel. This is illustrated with numerical results obtained on a set of examples that includes symmetric and highly nonsymmetric 2D and 3D problems, with both structured and unstructured grids, some of them with local refinement and/or higher order finite element discretization, and possible strong jumps or anisotropies in the coefficients. Results in parallel with many cores are also presented. Eventually, a numerical comparison with other solvers, suggests that the aggregation-based method can be significantly faster, especially on ”difficult” 3D examples.

Challenges in simulations of arterial blood flow

Petra Pustejovska
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Efficient Solvers in Biomedical Applications, Mariatrost, July 2-5, 2012

We consider blood flow in human arteries of middle diameter. For this real–life application, we demonstrate main aspects that should be considered in the mathematical modeling and following computational simulations of such flows, mainly the importance of real geometry, pulsative boundary conditions and reasonable hemodynamical models. The talk will be mainly introductory, focused on application, pointing out interesting challenges in numerical computations.

PDE tools to study evolution in spatially structured populations

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ABSTRACT

Evolutionary plays a role in chronicle infections, epidemics or cancer. Many theoretical tools exist to understand evolutionary phenomena, but most of them fail when the spatial structure of the population has to be taken into account. A way to deal with such situations is to use kinetic equations, that have been used successfully in other fields (fluid mechanics, chemistry...). The models can then be written quite easily, but numerical simulations are time consuming, and qualitative analysis is challenging. We show however that kinetic equations can be useful to study evolution in spatially structured populations.

A Heterogeneous Model of the Human Knee Joint

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ABSTRACT

We construct a patient-specific forward-dynamic finite element model of the human knee joint, comprising bones, cartilage layers, and the major ligaments. The ligaments are modeled with one-dimensional rods with director triads (Cosserat rods), and the rods are combined with 3D continuum mechanics models for the bones and cartilage. Cartilage is assumed to be linear viscoelastic of Kelvin-Voigt type, and we model the contact between the articular cartilage layers in the tibiofemoral joint. The numerical method uses the contact-stabilized Newmark method for a stable time discretization of the contact problems, and an energy–momentum method for the time discretization of the rods. The spatial coupled problems are solved using Steklov-Poincaré-type methods, with a multigrid solver for the fast solution of the cartilage contact problems. Together we obtain a procedure that delivers, within the limits of the model, precise and reliable time-dependent stress distributions at a low cost of computer power.

Numerical methods for strongly coupled simulations of cardiac electro-mechanics

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ABSTRACT

he rhythmic contraction and relaxation of the heart muscle is controlled by an electrical signal originating from pacemaker cells in the sino-atrial node. This electrical signal may in turn be affected by the mechanical deformations of the tissue through a number of mechanisms collectively referred to as mechano-electric feedback (MEF). Known mechanisms of MEF include stretch dependent binding and detachment rates, stretch activated ion channels, and deformation dependent tissue conductivities. Although the significance of individual MEF processes remains unclear, their existence motivate modeling the electrical and mechanical activity of the heart as a single, coupled system. Computer simulations based on these coupled models are commonly referred to as strongly coupled simulations, in contrast to earlier simulation methods that were based on pre-computing the electrical potentials and using them as input to models of tissue mechanics. However, the increased physiological realism of strongly coupled simulations comes at the expense of a number of computational challenges. Examples of specific challenges include the complexity of the involved mathematical models, strict temporal and spatial resolution requirements dictated by the rapid dynamics of the electro-physiology models, and the strong non-linearity of the mechanical problem. In this presentation we discuss alternative strategies for discretization and linearization of the coupled electro-mechanical problem. We present numerical results to investigate the stability and accuracy of the methods, with particular emphasis on comparing operator splitting methods with fully coupled approaches.

Efficient solvers based on manycore computers and adaptive techniques for cardiac modeling

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ABSTRACT

Computer models have become valuable tools for the study and comprehension of the complex phenomena of cardiac electrophysiology. However, the high complexity of the biophysical processes translates into complex mathematical and computational models. In this paper we evaluate different parallel and numerical techniques to accelerate these simulations. At tissue level we have used mesh adaptivity and finite volume method, which is a very attractive approach since the spreading electrical wavefront corresponds only to a small fraction of the cardiac tissue. Usually, the numerical solution of the partial differential equations that model the phenomenon requires very fine spatial discretization to follow the wavefront. Therefore, the use of uniform meshes leads to high computational costs. In this sense, the tests reported in this work show that simulations of two-dimensional models of cardiac tissue have been accelerated by 250 times when using an adaptive mesh algorithm together with a time step adaptive algorithm. In addition, we have started to parallelize this new numerical schemes for manycore computers using OpenMP and CUDA. Preliminary results show that these adaptive techniques together with parallel algorithms for manycore computers are a powerful combination for solvers of cardiac models that reduce the execution time of the simulations without significant loss in accuracy.

Modelling and Simulation of Biological Systems

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ABSTRACT

Biological systems are distinguished by their enormous complexity and variability. That is why mathematical modelling and computational simulation of those systems is very difficult, in particular thinking of detailed models which are based on first principles. The difficulties start with geometric modelling which needs to extract basic structures from highly complex and variable phenotypes, on the other hand also has to take the statistic variability into account. Moreover, the models of the processes running on these geometries are not yet well established, since these are equally complex and often couple many scales in space and time. Thus, simulating such systems always means to put the whole frame to test, from modelling to the numerical methods and software tools used for simulation. These need to be advanced in connection with validating simulation results by comparing them to experiments.

To treat problems of this complexity, novel mathematical models, methods and software tools are necessary . In recent years, such models, numerical methods and tools have been developed, allowing to attack these problems. In the talk we consider two examples as paradigms for the process of modelling and simulation in biosciences. The first example is the diffusion of xenobiotics through human skin, the second one is the automatic reconstruction of neurons and nueclei by means of numerical methods for partial differential equations.

Preparing Algebraic Multigrid Solvers for Future Supercomputers

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ABSTRACT

Algebraic Multigrid (AMG) solvers are an essential component of many large-scale scientific simulation codes. Their continued numerical scalability and efficient implementation is critical for preparing these codes for future computer architectures. Multi-core processors are now standard on commodity clusters and high-end supercomputers alike, and core counts are increasing rapidly. With exascale machines expected to have hundreds of millions or billions of tasks and hundreds of tasks per node, programming models will necessarily be hierarchical, with local shared-memory nodes in a larger distributed-memory message-passing environment.

AMG has demonstrated good weak scalability in distributed-memory environments, but our investigation of its use on multicore architectures has shown that non-uniform memory access (NUMA) latency between sockets, deep cache hierarchies, multiple memory controllers, and reduced on-node bandwidth can negatively affect its performance. To achieve high performance on exascale machines, we will need to ensure numerical scalability and an efficient implementation as core counts increase, memory capacity per core decreases, and on-node cache architectures become more complex. Some components of AMG that lead to very good convergence do not parallelize well or depend on the number of processors.

We examine the effect of high level parallelism involving large numbers of cores on one of AMGs most important components, smoothers. We also develop a performance model of the AMG solve cycle to better understand AMGs performance bottlenecks, and use it to evaluate new AMG variants. Since our investigations show that the increasing communication complexity on coarser grids combined with the effects of increasing numbers of cores lead to severe performance bottlenecks for AMG on various multicore architectures, we investigate two different approaches to reduce communication in AMG: the the development of AMG variants, which require less messages, and the use of a hybrid MPI/OpenMP programming model.

Simulation of the effect of sodium and potassium blockers on the electrical activity of the heart: Modelling from ion-channels to the body surface.

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ABSTRACT

Prediction of drug-induced cardiotoxicity is a major concern for regulatory agencies, pharmaceutical industry and society. A number of preclinical and clinical methods and biomarkers have been proposed to detect possible drug cardio-toxic effects as early as possible during drug development. However, approval of drug compounds is decided based on evaluation of the QT interval in the Electrocardiogram (ECG), as conducted thorough QT studies. Therefore, early and improved prediction of potential drug-induced prolongation of QT interval from preclinical assays is one of the major goals in safety pharmacology. In the present work, we describe novel tools based on advanced computational techniques "Chaste" (www.cs.ox.ac.uk/chaste) allowing simulation of alterations in the human ECG induced by drug-induced effects on specific ionic currents. Chaste is a parallel finite element library, containing a bidomain solver. Chaste's parallelisation is based on the message-passing standard Message Passing Interface (MPI) and it uses ParMETIS to ensure optimal domain decomposition. A shared-memory aware MPI implementation was used to improve intra-node communications.

A 3D anatomically-based model of the whole human body is presented with biophysically-detailed representation of human membrane kinetics, realistic cardiac geometry, fibre orientation and heterogeneity in electrophysiological properties of cardiac ventricles. The 3D multiscale model is used to simulate the effect of specific drug concentrations of fast sodium and hERG current blocker on the action potential at the cell level, on activation and repolarization maps at the heart level, and on the Qt interval at the body surface level. The simulation of drugs effect is also shown on different biomarkers.