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Abstracts Posters

Coupling MFS and FCM for the simulation of settling particles at low Reynolds number

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Abstract

We present a numerical model for the simulation of settling particles at low Reynolds number. The flow is modelled as a quasi-stationary Stokes flow driven by localized time-dependent body forces due to the presence of particles. The particles are modelled with the Force Coupling Method (FCM; Maxey & Patel, Int. J. Multiphase Flow, 2001). The resulting governing equations for the flow are solved with a multilayer version of the Method of Fundamental Solutions (multilayer MFS; Boselli et al., PAMM, 2009). As an application, we present a model for benign paroxismal positional vertigo (BPPV). BPPV is a disease of the vestibular system of the inner ear closely related to the presence of small calcite particles (canaliths) which settle inside the semicircular canals (SCC). The anatomy of the SCC is suitable to be split into subdomains with different typical flow features. Therefore we use a domain decomposition method in order to reduce the computational effort and extend the applicability of MFS.

LONG TIME BEHAVIOUR OF PARTITIONED MULTISTEP METHODS

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1 Introduction

The purpose of this work is the study of the partitioned multistep methods with focus on the preservation of the Hamiltonian for long time integrations.
Our interest is in problems that cannot be written in the form

$$\ddot{q} = -\nabla U(q).$$

In this work we present numerical experiments that confirm the excellent performance of explicit, symmetric partitioned multistep methods when applied to the equations of motion for the spherical pendulum and for the double pendulum. By studying the parasitic solution components we analyze the linear case (leading to a surprising result) and we obtain a heuristic explanation for the non-linear problems.

2 Results

We show that applying a partitioned multistep method to an Hamiltonian system, the error on the energy remains bounded for long times integrations.
In Fig. 1 there is the comparison of the error on the energies obtained with the method

$$\begin{array}{ll} (A): & p_{n+3} - p_{n+2} + p_{n+1} - p_n = h\left(f_{n+2} + f_{n+1}\right) \\ (B): & q_{n+3} - q_{n+1} = 2hg_{n+2} \end{array} \tag{1}$$

and the explicit Adams method of order 2 applied on the equations of the Spherical Pendulum

$$\left\{ \begin{array}{rcl} \dot{p}_\theta & = & p_\varphi^2 \frac{\cos\theta}{\sin^3\theta} - \sin\theta \\ \dot{p}_\varphi & = & 0 \\ \dot{\theta} & = & p_\theta \\ \dot{\varphi} & = & \frac{p_\varphi}{\sin^2\theta} \end{array} \right.$$

We introduce the parasitic components, that are connected to the preservation of the Hamiltonian: in the Fig. 2 are reported the error on the Hamiltonian obtained with the partitioned multistep method, and the corresponding parasitic components; in the Fig. 3 are reported the parasitic components and the error on the Hamiltonian for the Equations of the Double Pendulum whose Hamiltonian is

$$H(p,q) = \frac{p_1^2 + 2p_2^2 - 2p_1p_2\cos(\theta_1 - \theta_2)}{2\left(1 + \sin^2(\theta_1 - \theta_2)\right)} - 2g\cos(\theta_1) - g\cos(\theta_2).$$

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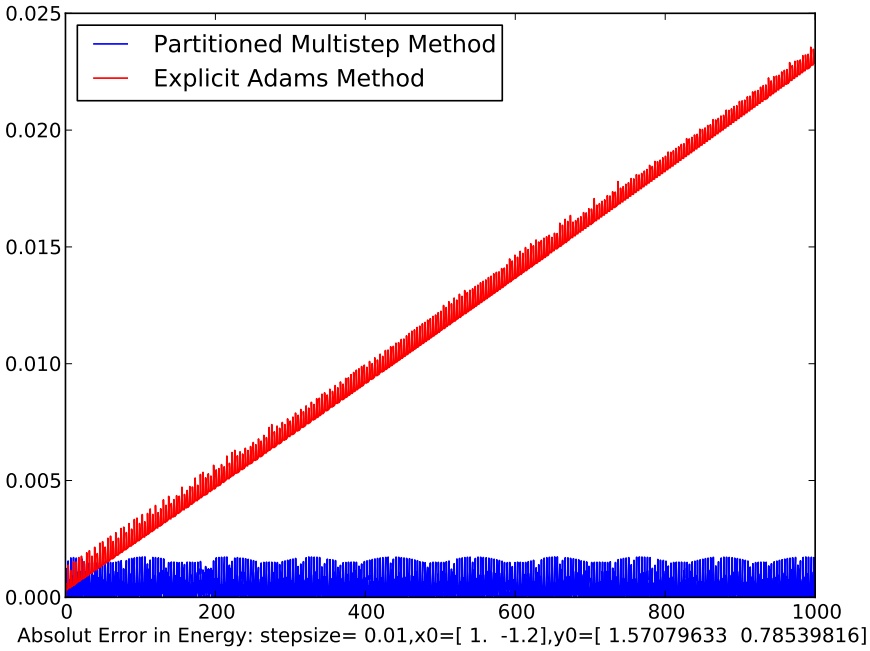

Figure 1: Comparison of the errors on the Hamiltonian obtained with Partitioned Multistep method and Explicit Adams Method

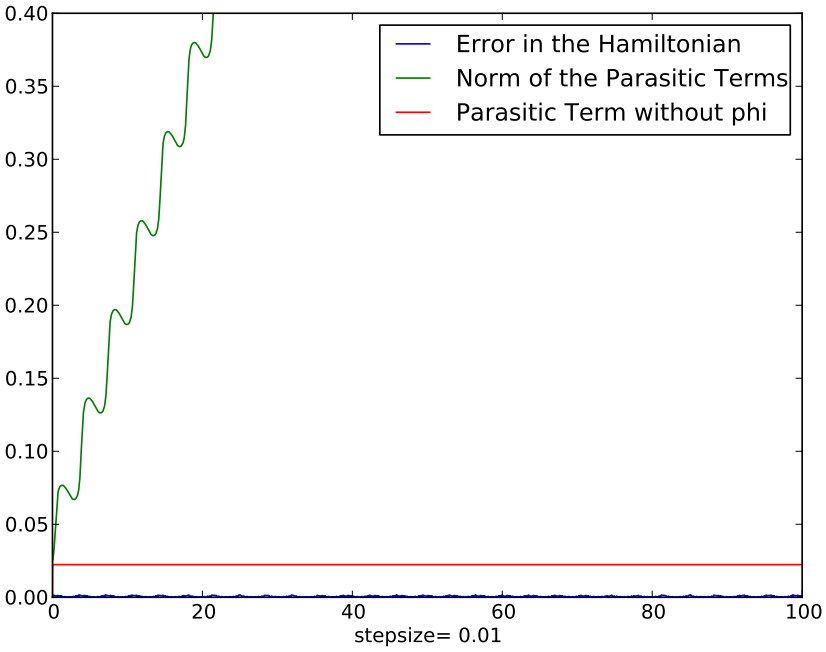

Figure 2: The Spherical Pendulum: error on the energy and parasitic terms

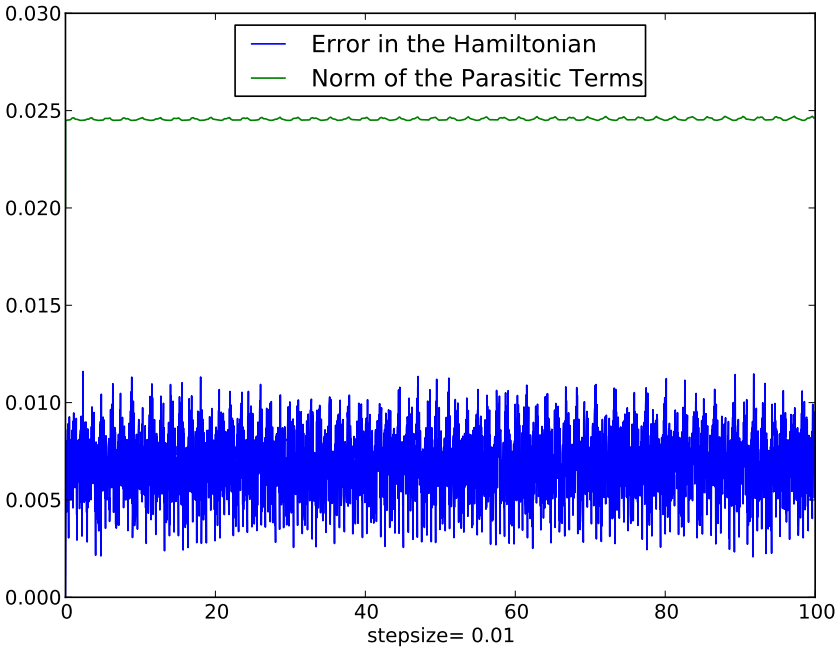

Figure 3: The Double Pendulum: error on the energy and parasitic terms

Mechanical model of plant cell tissue

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Abstract

Recent advances in molecular biology and genetics provide an insight into physiological mechanisms involved in maintenance and growth of plant cells. However, the functional complexity of plant cell tissue is such, that one cannot single-out one phenomenon and experiment with it. Therefore, all biological hypotheses explaining *in vivo* observations have to be analysed and verified on theoretical models *in silico*. In order to link physiology and growth in these computer models, the mechanical state of cells in the tissue has to be taken into account. First mechanical models of a plant cell tissue [**?**, **?**] consist usually of a mass spring network simulating the mechanics of cell walls only on the epidermis (plant skin). More refined models [**?**, **?**] represent the elastic response of cell walls in 3D by a system of membranes or shells. The common feature of these two approaches, however, is that the symplastic compartment of a cell (the cell interior) is simulated only by a given constant turgor pressure applied in normal direction to cell walls. Since the material constants and constitutive laws for these models cannot be measured directly, they are usually inferred from some standard stress-strain experiments like atomic force microscopy (AFM) or micro-electro-mechanical (MEMS) "poking". Experimental data are then usually collected over relatively short time periods on osmotically treated cells. While the "constant turgor pressure" approximation appears to be quite precise when considering slow growth, on the short time scale of a "poking" experiment it does no longer apply. Moreover, due to osmotic treatments which are usually applied in the "poking" experiments, the hydrostatic pressure might no longer be dominated by osmotic pressure. Hence, a complete model of cell mechanics including the cytoplasm is needed in this case.

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Comparison of a Radial Basis Function Eigenvalue Solver and High-Order Finite Elements

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Meshless methods are an emerging class of numerical schemes with interesting characteristics in computational sciences. No explicit mesh configuration is required to solve physical problems with a meshless method. Instead a node distribution $\mathcal{N}_c = \{\vec{\zeta}_1, \ldots, \vec{\zeta}_n\} \subset \mathbb{R}^d$ is used in a collocation approach, thus avoiding the computational overhead of dealing with mesh elements. This advantage is especially helpful in adaptive grid refinement. The interpolation is carried out by Radial Basis Functions (RBFs) [1] centered at $\vec{\zeta}_k$ as $\vec{x} \mapsto \varphi(||\vec{x} - \vec{\zeta}_k||_2), \mathbf{x} \in \mathbb{R}^d, k = [1, \ldots, n]$. In the current implementation these are Gaussians $\varphi(r) = e^{-cr}$, which are expected to provide exponential spatial convergence [2] when $c \to 0$ or $\max_{i,j}(||\vec{\zeta}_i - \vec{\zeta}_j||_2) \to 0$. Due to their radial nature of the basis functions, a 3D implementation is straightforward. On the negative side, this type of functions are generally globally supported and poorly conditioned. The latter point is manifested in a gradually increased condition number for decreasing shape parameters c, i.e. the matrix solver eventually breaks down. We circumvent this by applying a "leave one out cross validation" (LOOCV) algorithm [3] which yields an optimized shape parameter c for a given node distribution in order to realizing stable simulations. In this work a scalar Laplace eigenvalue problem in strong form is solved in $d = 2$ with Dirichlet boundary conditions. As an illustration we calculate eigenvalues in the unit disc.

The node adaptivity algorithm is based on the initial set of collocation nodes $\mathcal{N}_c$. A Delaunay tessellation is performed on $\mathcal{N}_c$ and a new set of test nodes $\mathcal{N}_t = [\vec{\xi}_1, \ldots, \vec{\xi}_m]$ is generated by placing new nodes on the edge centers of the Delaunay cells. An error function is calculated based on the residual error and the

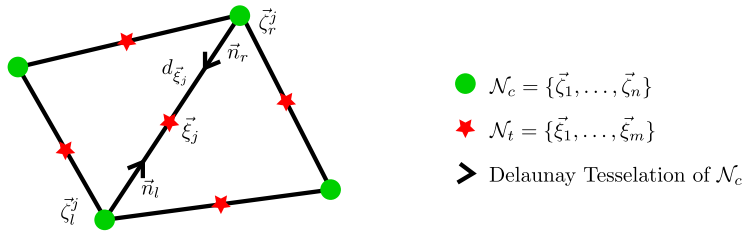

Figure 1: Collocation and test nodes for the adaptive refinement algorithm.

jump in the numerical gradient between two nodes. For given approximative eigenpair (U, λ) the local residual error is computed as

$$\eta(\vec{\xi}_j) = d_{\vec{\xi}_1}^2 ||\lambda U(\vec{\xi}_j) - \Delta U(\vec{\xi}_j)||_2 + d_{\vec{\xi}_1}^2 ||\nabla U(\vec{\zeta}_l^j) \cdot \vec{n}_l - \nabla U(\vec{\zeta}_r^j) \cdot \vec{n}_r||_2 \tag{1}$$

with the test node $\vec{\xi}_j$ between the collocation nodes $\vec{\zeta}_l^j$ and $\vec{\zeta}_r^j$. The distance between these nodes is $d_{\vec{\xi}_j}$ and the unit vectors $\vec{n}_l, \vec{n}_r$ point from the collocation nodes to the test node (Fig. 1). All test nodes for which the error function lies above a certain limit are added to the set of collocations subsequently:

$$\mathcal{N}_c = \{\vec{\zeta}_1, \ldots, \vec{\zeta}_n\} \cup \{\vec{\xi}_k : J(\vec{\xi}_k) \geq \beta \max_j J(\vec{\xi}_j)\} \tag{2}$$

for a given $\beta \in [0, 1]$. Several refinement iterations with the error estimator (1) are conducted. The result of a refinement of the TM_{02} mode is shown in Fig. 2.

A study is performed to compare the performance of the presented method with a high-order finite-element method. The adaptive refinement algorithm is performed for several eigenmodes and compared with discontinuous p-FEM with curved elements using 6 triangular elements and $p \leq 18$.

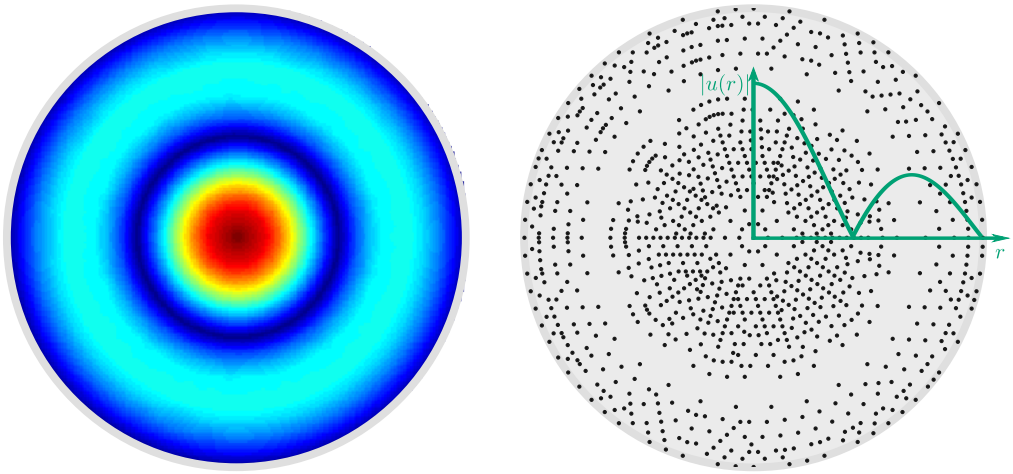

Figure 2: Solution and node distribution $\mathcal{N}_c$ after refinement for TM_{02} mode.

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Optimized Schwarz method for problems with cross points

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When performing large-scale physical simulations, one often encounters linear systems that are so large that the they must be subdivided and solved in parallel using many processors. In optimized Schwarz methods, this is done by dividing the computational domain into many subdomains, solving the smaller subdomain problems in parallel, and iterating until one obtains a global solution that is consistent across subdomain boundaries. Fast convergence can be obtained if Robin conditions are used along subdomain boundaries, provided that the Robin parameters p are chosen correctly. It is well known that for two-subdomain problems with no overlap, the optimal choice is $p = O(h^{-1/2})$ (where h is the mesh size), with the resulting method having a convergence factor of $\rho = 1 - O(h^{1/2})$. However, when cross points are present, i.e., when several subdomains meet at a single point, this choice leads to a divergent method. In this work, we use a simple model problem to show that convergence can only occur if $p = O(h^{-1})$ at the cross point. In addition, this choice of p allows us to recover the $1 - O(h^{1/2})$ convergence factor in the resulting method.

Observables and Models of Stellar Explosions

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1 Introduction

Knowledge in astrophysics originates from a synthesis of astronomical observation, knowledge of terrestrial physics and theoretical models of astrophysical scenarios. The extraction of information about the laws of physics in the universe is most efficient, if the degree of detail and quality in the observation can be matched by corresponding astrophysical models. However, it is a long-standing problem to perform reliable three-dimensional computer models of astrophysical scenarios due to the typically enormeous scale differences in time and space that need to be covered, due to the technically challenging radiative transfer that determines the long-distance observation, and due to the often fundamental three-dimensional nature of the local interaction between fluid instabilities, the radiation field and the magnetic fields in gravitationally bound objects. We focus on stellar core-collapse supernova explosions, which still pose open proof-of-principle questions regarding their explosion mechanism, for which detailed observations are available in almost all astronomical windows (optical, electromagnetic, neutrinos, cosmic rays, in future hopefully gravitational waves), which probe matter under interesting conditions that are not accessible in terrestrial experiments, and whose nucleosynthetic yields provide a key to the understanding of Galactic evolution.

2 Results

We use our spherically symmetric general relativistic hydrodynamics code AGILE with Boltzmann neutrino transport [**?**] or, alternatively, our multi-dimensional magneto-hydrodynamics code FISH [**?**] together with the isotropic neutrino diffusion source approximation (IDSA) [**?**] to build models of stellar core collapse and postbounce evolution. We show that the neutrino signature of a galactic supernova is likely to reveal detailed information about the explosion mechanism [**?**] and that gravitational waves can be expected to be detected [**?**] at the LIGO detector. We try to visualise the dynamics and fluid instabilities of supernova explosions by presenting the results of first three-dimensional models with spectral neutrino transport and 600^3 zones resolution. These models serve as foundation for further improvements of the numerical algorithms in the HP2C project 'Stellar Explosions' and as platform for the investigation of the interesting and uncertain microscopic input physics.

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Adaptive finite element heterogeneous multiscale method for homogenization problems

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1 Abstract

We discuss *a posteriori* error estimates for elliptic homogenization problems discretized by the finite-element heterogeneous multiscale method [**?**, **?**]. Unlike standard finite element methods, our method is based upon a macro-to-micro formulation where the macroscopic finite element method discretizes the physical problem while the unknown macroscopic data is recovered on the fly by a microscopic method.

We derive a framework which builds upon the well-developed *a posteriori* analysis for single-scale problems [**?**, **?**]. As the effective macroscopic data (such as the effective conductivity tensor) are not readily available due to the multiscale nature of the problem, appropriate new error indicators have to be defined. These indicators are used to derive *a posteriori* estimates for the upper and lower bound in the energy norm. The macroscopic mesh refinement strategy is thus proven to be both reliable and efficient [**?**, **?**]. Furthermore as these indicators only depend on the already computed macro and micro solutions, the computational overhead for adaptivity is minimal.

Up to a modeling error, our estimates do not need any assumption on the spatial structure for the oscillating tensor. In the case of a uniformly oscillating tensor, our estimates are consistent with the classical single-scale *a posteriori* error estimates applied to the homogenized problem.

We highlight algorithmic differences with single-scale adaptive FE methods and confirm the efficiency and reliability of our adaptive multiscale method with numerical experiments.

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Towards Massively Parallel Numerical Methods in a Biomedical Application

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Abstract

As the landscape of compute architectures is constantly evolving allowing us to deal with applications of increasing problem size with billions of unknowns, it is equally important to address both numerical methods and software issues due to many levels of parallelism. Hyperthermia treatment is a promising option in oncology. By heating the tumor using electro-magnetic energy to about 45°C, it is made more susceptible to an accompanying radio- or chemo-therapy. In treatment planning two objectives are of interest: simulating the temperature distribution within the patient's body and determining the therapeutically optimal applicator antenna parameters given the patient's geometry and target temperature distribution. The first leads to solving Pennes's bioheat equation, a parabolic PDE, the latter to solving a large-scale nonlinear nonconvex PDE-constrained optimization problem. The PDE is discretized using a finite volume discretization. To solve the forward problem, an explicit integration scheme is used. The code for the arising stencil computations is generated by our evolving stencil framework. The benefit of the framework is its ability to generate parallel code for multi- and many-core architectures including multi-core CPUs and GPUs. The hardware characteristics are exploited by adapting the code for optimal performance by using autotuning techniques that range from architecture-specific parameter determination to choosing parallelization strategies [1,2]. For solving the inverse problem we are using a primal-dual inexact interior point method combined with our recently developed highly-scalable hybrid solver "PSPIKE" [3,4].
In order to tackle large-scale optimization problems we are facing with several challenges such as inexactness, krylov-subspace methods, preconditioning, outer/inner convergence, HPC cluster machines, and different programming paradigms. The massively parallel optimization framework is able to solve PDE-constrained optimization problems with millions of variables and constraints within a few minutes.

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A Geometric Integrator for Solving Stochastic Oscillators

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In solving stochastic wave equations numerically, stochastic oscillators play an important role. The pseudo-spectral semi-discretization in space of the considered partial differential equation leads to a large system of coupled stochastic oscillators. We could just use an Euler-Maruyama method to solve the system, but since the oscillators can be highly oscillatory, the time restrictions would be very stringent. We consider a one-dimensional problem which describes a stochastic oscillator. The exact solution of this second-order stochastic differential equation satisfies some properties such as the linear growth of the second moment. Therefore, we propose a geometric integrator which is based on the variation-of-constants formula and which solves the equation efficiently and reproduces these properties exactly.

Robust PML for Nonlinear Wave Equations

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Abstract

Nonlinear wave problems in unbounded domains have in many fields of application, such as ultrasound surgery, molecular biology, oceanography and nano optics. The perfectly matched layer (PML) method has proved a flexible and accurate method for the simulation of waves. It consists in surrounding the computational domain by an absorbing layer, which generates no reflections at its interface with the computational domain. We propose a simple PML formulation directly for the nonlinear wave equations. Inside the absorbing layer, our formulation requires few variables, such that it is cheap to implement. Since our formulation requires no higher derivatives, it is also easily coupled with standard finite difference or finite element methods. Strong stability is proved in linearized problem while numerical examples in two and three space dimensions illustrate the accuracy and long time stability of our PML formulation.

Wave Propagation in Heterogeneous Media: A Multiscale Finite Element Method

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The simulation of time dependent waves propagating through a medium with rapidly varying propagation speed can be prohibitively expensive with a standard finite element (FE) approach, because it requires a resolution down to the findest scales of the medium. We propose a FE-scheme for solving the wave equation numerically within the framework of heterogeneous multiscale methods (HMM), as introduced by E and Engquist [5], which overcomes these problems. Here we adapt the method described by Abdulle [1, 3] to the time dependent wave equation and derive optimal error estimates. Numerical experiments in periodic and non-periodic heterogeneous media in one and two space dimensions illustrate the usefulness of our approach.

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Solution of parameter-dependent linear systems by tensor methods

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Consider a parameter-dependent linear system

$$A(\alpha)x(\alpha) = b(\alpha),$$

where α is a vector of p parameters. We assume that the parameter space is discretized with a regular grid and aim at computing the solution $x(\alpha)$ for each grid point. This becomes rather expensive for larger p as the number of grid points grows exponentially in p. We therefore propose the use of low tensor rank approximations to reduce the computational cost significantly. For this purpose, we treat the right hand side b and the solution x evaluated at all grid points as tensors of dimension $p + 1$. Assuming that b admits a low tensor rank approximation and A is sufficiently smooth, one can show that x also admits a low tensor rank approximation. We present algorithms which exploit this fact and demonstrate their efficiency with a number of examples.

Partitioned Runge-Kutta-Chebyshev methods

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Abstract

Current research on stabilized methods focus on the time integration of advection-diffusion-reaction problems [**?**, **?**]. The advection terms introduce eigenvalues with imaginary parts which complicate the selections of the temporal step size, the number of stages and the damping parameter of the method.

This poster introduces a new one-step, stabilized method of second-order which treats stiff and non-stiff terms separately. The method, called PRKC (Partitioned Runge-Kutta-Chebyshev), reduces the number of function evaluations of the non-stiff terms and embeds a thin long rectangle inside its stability regions that facilitates the integration of advection-diffusion problems.

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Anisotropic finite element adaptation for 3D aerodynamic flows

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1 Introduction

In the field of numerical simulations, the accuracy of the solution depends on the quality of the mesh. A 3D adaptive finite element algorithm was developed to solve the compressible Euler and Navier-Stokes equations, with goal to reduce the CPU time and to reach a desired level of precision. The refinement and coarsening criterion is based on an a posteriori error estimator suitable for meshes with large aspect ratio. Moreover, an anisotropic error estimator for goal oriented a posteriori error estimates is developed. This project is supported by Dassault Aviation.

2 Results

Numerical simulations have been carried out for an inviscid flow around a complete supersonic aircraft and a transonic viscous flow around the ONERA M6 wing.

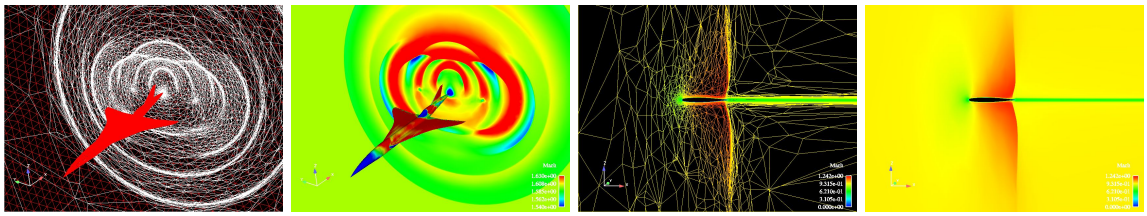

Figure 1: Adapted meshes and the associated local Mach number for the flows around the aircraft (left) and the ONERA M6 wing (right).

References

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