Adaptive Modeling and Simulation 2013

Edited by:
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Parés

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PREFACE

This book contains the Abstracts of the papers presented at ADMOS 2013, the sixth International Conference on Adaptive Modeling and Simulation, held at Instituto Superior Técnico, Technical University of Lisbon, Portugal, from June 3 to 5, 2013.

Numerical Modeling and Simulation is increasingly used as a complement to Experimental Modeling and Analysis and as a design or certification tool in engineering applications. However, after more than thirty years of worldwide research efforts around Adaptive Modeling and Simulation, the problem of properly assessing and controlling the quality of the numerical solutions is still relevant, as the design of sophisticated engineering systems requires increasingly complex and coupled modeling, which leads to increasingly time-consuming computations. Adaptive approaches, which provide reliable and cost efficient modeling and coherent coupling of different scales and mechanisms in a unique model, are more strategic and indispensable than ever.

The objective of the ADMOS 2013 conference is to provide a forum for presenting and discussing the current state-of-the-art achievements on Adaptive Modeling and Simulation, including theoretical models, numerical methods, algorithmic strategies and challenging engineering applications.

This book collects the contributions presented by the participants in the conference, which address a wide range of topics in adaptive modeling, from the classical theoretical aspects and numerical techniques to cutting edge problems and formulations, such as the determination of guaranteed error bounds and adaptive strategies for non-linear, transient or coupled problems, the application of adaptive techniques to reduced order models, the use of goal-oriented anisotropic error estimators and remeshing, as well as the application of adaptive techniques in the stochastic framework.

Advanced numerical techniques are also considered, for example XFEM, Discrete Galerkin, Meshless and Domain Decomposition, as well as the more classical methods. The domain of the applications covers a wide range of problems, from the traditional areas of structural and fluid mechanics, to quantum mechanics or biomechanics, with scales ranging from the nanoparticles, via the mesoscopic level, to those of industrial structures and civil engineering constructions, all studied with a focus on the main goal of adaptivity, seeking reliable and cost efficient modeling.

This book includes Abstracts sent directly by the authors, and the editors cannot accept responsibility for any inaccuracies, comments and opinions contained in the text. The organizers would like to take this opportunity to thank all the authors for submitting their contributions.

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CONTENTS

PLENARY LECTURES

GENERAL CONTRIBUTIONS

PLENARY LECTURES

VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

VIRTUAL CHART BASED DESIGN, INVERSE ANALYSIS AND CONTROL

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Key words: Parametric modeling, Model order reduction, PGD, Virtual charts

Abstract. Virtual chart constitutes an appealing tool for performing efficient design, real time simulations, efficient optimization, inverse analysis and control of systems and processes. When such charts are available, no more on-line simulation are needed, because everything reduces to a dialog between the designer or controller and the chart. The chart contains all the required information, that is, the solution of the physical model for each choice of the model parameters. These parameters can correspond to the applied loads, initial or boundary conditions, material or process parameters, parameters defining the geometry of the domain in which the model is defined, ... The main difficulty related to the construction of such a chart lies in the fact that the parametric space must be accurately explored in order to define an accurate chart. When the number of parameters increases, the sampling of such high-dimensional parametric space becomes unaffordable when standard discretization techniques apply for each possible scenario. Model order reduction makes possible the off-line construction of virtual charts in two ways. First, by constructing an adaptive reduced basis, from which the solution of each direct problem can be performed very fast, reaching several order of magnitude of CPU time savings. Second, by introducing the parameters as extra-coordinates and then addressing the solution of the resulting multidimensional problem by invoking the PGD, one can have access to the solution of innumerable scenarios, all those represented by the discretization of the extra-coordinates related of the model parameters. Again the question of adaptivity is crucial. From these virtual charts, simulation, optimization, inverse analysis, control, ... can be performed on-line, many times in real time and by using light computing devices like smartphones or tablets.

DIRECT FEM-SIMULATION OF TURBULENT FLOW

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Abstract. Turbulent fluid flow has been considered as the main unsolved problem of classical mechanics beyond theoretical description and also beyond computational simulation, because of thin no-slip boundary layers requiring trillions of mesh points to be resolved. In recent work we have discovered that using a slip boundary condition as a model of the small skin friction of slightly viscous turbulent flow, allows predictive simulation of mean value quantities such as drag and lift of turbulent flow with instead millions of mesh points. Basic aspects of turbulent flow from applications point of view thus show to be computable by stabilized finite element methods without turbulence modeling referred to as Direct FEM-Simulation, which opens large areas for exploration. As a key example the turbulent flow around a wing and complete airplane is computable and inspecting the solutions leads to a new theory flight essentially different from the accepted theory by Kutta-Zhukovsky-Prandtl developed 100 years ago.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

PARALLEL MESH MULTIPLICATION AND GENERATION: TOWARDS PETASCALE SIMULATIONS

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Abstract. In this talk we review our current efforts in the development of enabling technologies for parallel large-scale simulations. We begin by revisiting the concept of what is large, given the current capabilities of today's high performance computers and high resolution visualisation devices. In the sequel we discuss a very efficient parallel procedure to produce high resolution models, the mesh multiplication (MM). MM recursively refines your mesh until a preset level is reached. Implementation issues, associated to mesh partition and unknown reordering are addressed. We then show a parallel implementation and performance analysis of a linear octree-based mesh generation scheme designed to create reasonable-quality, geometry-adapted unstructured hexahedral meshes automatically from triangulated surface models. We present algorithms for the construction, 2:1 balancing and meshing large linear octrees. Our scheme uses efficient computer graphics algorithms for surface detection, allowing us to represent complex geometries. We show that our implementation is able to execute the 2:1 balancing operations over 3.4 billion octants in less than 10 seconds per 1.6 million octants per CPU core. Next we examine the performance impact from tetrahedralization of non- conforming meshes generated by our parallel octree mesh generation scheme. We end our talk with a discussion of the applicability of these enabling technologies in challenging new applications in science and engineering.

VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

ERROR-CONTROLLED ADAPTIVE MULTISCALE ANALYSIS FOR CRACK INITIATION AND PROPAGATION IN BRITTLE MATERIALS

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Abstract. The addressed research is based on linear elastic fracture mechanics for the macro-scale, so far, and on non-local continuum damage mechanics with linear kinematics until micro-cracking on micro-scale. The material considered is alloyed ceramics (Yttria (3Y) stabilized (with 2%-3%) tetragonal Zirconia-Oxide -- a polycrystalline ceramic 3Y-TZP). The main goals are: error-controlled adaptive modeling and numerical approximations on both scales, including error estimators for quantities of interest. This also needs energy consistent projections from micro- to macro-scale and backwards. The final objective is defined as coupled micro-macro damage and crack propagation processes for technologically interesting problems. This is scheduled in an overall adaptive scheme, trying to realize step by step verification and validation of this coupled process.

Our current results are based on new explicit and implicit residual error estimators for the eXtended Finite Element Method (XFEM), including goal-oriented error estimation [1,2]. Special features of singular enrichment functions within XFEM are also discussed. In particular, it is shown that a significant reduction of the discretization error in crack tip element is achieved by using a statically admissible asymptotic displacement field in the XFEM discretizations. Alternative to XFEM, the adaptive Singular Function Method (SFM) is considered, including new explicit residual (constant-free) error estimator for low order triangles [3], yielding very good effectivity indices between 1 and 2.

Modeling of microcrack nucleation and coalescence in ceramic specimen is realized within the framework of Continuum Damage Mechanics (CDM), in particular in terms of a non-local damage model using the enhanced gradient formulation [4]. Error estimation analysis for this coupled problem and results of adaptive mesh refinements are presented. A major point is the transition from continuous damage to equivalent micro-cracks, using energetic equivalence between damage and fracture [5].

GENERAL CONTRIBUTIONS

VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

HIERARCHICAL MOMENT CLOSURE APPROXIMATION OF THE BOLTZMANN EQUATION

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Abstract. The Boltzmann equation (BE) is the classical model in the kinetic theory of (monoatomic) fluids, describing rarefied flow by modeling deviations of the velocity distribution from a local equilibrium, thus, accounting for the transitional molecular/continuum regime. The BE provides an evolution equation for the one-particle marginal, viz., the probability density of particles in phase (position/velocity) space. The BE has several fundamental structural properties, notably, conservation of mass, momentum and energy, Galilean invariance and decay of an entropy functional (the celebrated H-theorem). These structural properties underly the connection between the BE and conventional continuum models: all conventional continuum models, such as the Navier-Stokes-Fourier system [1], can be derived as limits of the BE.

The BE poses a formidable challenge for numerical approximation methods, on account of its high dimensional phase-space setting: for a problem in N spatial dimensions, the single molecule phase-space is 2N dimensional. Away from the fluid dynamical regime numerical approximations of kinetic systems are predominantly based on particle methods, such as the Direct Simulation Monte Carlo (DSMC) method. However, the phase-space description of the system results in the prohibitive computational cost of DSMC in the fluid dynamical limit. Moreover, from an approximation perspective, DSMC can be inefficient since it is inherent to the Monte-Carlo process that the approximation error decays only as $n^{-1/2}$ for the number of simulation molecules n [2]. Hence, efficiently modeling gases in the transition regime between the free molecular flow and fluid dynamics remains difficult.

An alternative strategy to describe deviations from fluid dynamics is by means of moment-closure approximations [3, 4]. In moment-closure approximations, the BE is projected onto a polynomial space, in the velocity dependence, and the system is closed by providing an approximation to the one-particle marginal based on the same polynomial space. This procedure can in fact be conceived of as a Galerkin approximation. The closure is chosen such that the structural properties of the BE are retained. From an adaptive approximation standpoint, the resulting hierarchical structure of the the moment closure system presents promising potential for rigorous model adaptivity. However, fundamental challenges remain to be addressed.

This work applies the moment method onto the BE to derive a closed hierarchy of moment systems that retain structural features of the system in question and address the aforementioned issues. In addition opportunities pertaining to goal-oriented adaptive modeling provided by the hierarchical structure exhibited by the resulting closed systems of moment equations will be discussed.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

DEIM-BASED PGD FOR PARAMETRIC NONLINEAR MODEL ORDER REDUCTION

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Key words: Model Reduction; Nonlinear; DEIM; Proper Generalized Decomposition

Abstract. A new technique for efficiently solving parametric nonlinear reduced order models in the Proper Generalized Decomposition (PGD) framework is presented here. This technique is based on the Discrete Empirical Interpolation Method (DEIM)[1], and thus the nonlinear term is interpolated using the reduced basis instead of being fully evaluated. The DEIM has already been demonstrated to provide satisfactory results in terms of computational complexity decrease when combined with the Proper Orthogonal Decomposition (POD). However, in the POD case the reduced basis is *a posteriori* known as it comes from several pre-computed snapshots. On the contrary, the PGD is an *a priori* model reduction method. This makes the DEIM-PGD coupling rather delicate, because different choices are possible as it is analyzed in this work.

1 INTRODUCTION

The efficient resolution of complex models (in the dimensionality sense) is probably the essential objective of any model reduction method. This objective has been clearly reached for many linear models encountered in physics and engineering [2, 3]. However, model order reduction of nonlinear models, and specially, of parametric nonlinear models, remains as an open issue. Using classic linearization techniques such Newton method, both the nonlinear term and its Jacobian must be evaluated at a cost that still depends on

the dimension of the non-reduced model [1]. The Discrete Empirical Interpolation Method (DEIM), which the discrete version of the Empirical Interpolation Method (EIM) [4], proposes to overcome this difficulty by using the reduced basis to interpolate the nonlinear term. The DEIM has been used with Proper Orthogonal Decomposition (POD) [5, 1] where the reduced basis is *a priori* known as it comes from several pre-computed snapshots. In this work, we propose to use the DEIM in the Proper Generalized Decomposition (PGD) framework [5, 6], which is an *a priori* model reduction technique, and thus the nonlinear term is interpolated using the reduced basis that is being constructed during the resolution.

2 DEIM-based PGD FOR NONLINEAR MODELS

Consider a certain model in the general form:

$$\mathcal{L}(u) + \mathcal{F}_{NL}(u) = 0 \tag{1}$$

where $\mathcal{L}$ is a linear differential operator and $\mathcal{F}_{NL}$ is a nonlinear function, both applying over the unknown $u(\boldsymbol{x}), \boldsymbol{x} \in \Omega = \Omega_1 \times \ldots \times \Omega_d \subset \mathbb{R}^d$, which belongs to the appropriate functional space and respects some boundary and/or initial conditions. Using the PGD method implies constructing a basis $\mathcal{B} = \{\phi_1, \ldots, \phi_N\}$ such that the solution can be written as:

$$u(\boldsymbol{x}) \approx \sum_{i=1}^{N} \alpha_i \cdot \phi_i(\boldsymbol{x})$$

where α_i are coefficients, and

$$\phi_i(\boldsymbol{x}) = P_{i1}(x_1) \cdot \ldots \cdot P_{id}(x_d) \ , \ i = 1, \ldots, N$$

being $P_{ij}(x_j), j = 1, \ldots, d$, functions of a certain coordinate $x_j \in \Omega_j$. In the linear case, the basis $\mathcal{B}$ can be constructed sequentially by solving a nonlinear problem at each step in order to find functions P_{ij}. In the nonlinear case a linearization scheme for Eq. (1) is compulsory, but evaluating the nonlinear term is still as costly as in the non-reduced model. The DEIM method proposes to circumvent this inconvenient by performing an interpolation of the nonlinear term using the basis functions. In a POD framework, these functions come from the precomputed snapshots, but in a PGD framework these functions are constructed by using the PGD algorithm. Here we propose to proceed as follows:

1. Solve the linear problem: find u^0 such that $\mathcal{L}(u^0) = 0 \rightarrow \mathcal{B}^0 = \{\phi_1^0, \ldots, \phi_{N_0}^0\}$
2. Select a set of points $\mathcal{X}^0 = \{\boldsymbol{x}_1^0, \ldots, \boldsymbol{x}_{N_0}^0\}$. Later on we explain how to make an appropriate choice.
3. Interpolate the nonlinear term $\mathcal{F}_{NL}$ using functions $\mathcal{B}^0$ in the points $\mathcal{X}^0$. Or in other words, find the coefficients φ_i^0 such as:

$$\mathcal{F}_{NL}\left(u_m^0\right) \equiv \mathcal{F}_{NL}\left(u^0(\boldsymbol{x}_m^0)\right) = \sum_{i=1}^{N_0} \varphi_i^0 \cdot \phi_i^0(\boldsymbol{x}_m^0) \ , \ m = 1, \ldots, N_0$$

The previous equation represents a linear system which will be invertible if $\mathcal{B}^0$ is linearly independent (and it is because it comes from the solution of the linear problem) and all points of $\mathcal{X}^0$ are different.

4. Once we have computed $\{\varphi_1^0, \dots, \varphi_{N_0}^0\}$, the interpolation of the nonlinear term reads:

$$\mathcal{F}_{NL}(u) \approx b_0 = -\sum_{i=1}^{N_0} \varphi_i^0 \cdot \phi_i^0$$

And therefore, the linearized problem writes:

$$\mathcal{L}(u) = b_0 \tag{2}$$

5. At this point, three options can be thought:

   (a) Restart the separated representation, i.e., find u^1 such that:

   $$\mathcal{L}(u^1) - b_0 = 0$$

   Applying the PGD method we will obtain a new reduced basis $\mathcal{B}^1 = \{\phi_1^1, \dots, \phi_{N_1}^1\}$.

   (b) Reuse the solution u^0, i.e. $u^1 = u^0 + \widetilde{u}$. Then, we seek $\widetilde{u}$ such that:

   $$\mathcal{L}(\widetilde{u}) = b_0 - \mathcal{L}(u^0)$$

   We solve this problem by applying the PGD method, i.e. $\widetilde{\mathcal{B}} = \{\widetilde{\phi}_1, \dots, \widetilde{\phi}_{\widetilde{N}}\}$ and then $\mathcal{B}^1 = \mathcal{B}^0 \oplus \widetilde{\mathcal{B}}$ and $N_1 = N_0 + \widetilde{N}$.

   (c) Reuse by projecting. In this case we consider

   $$u^{0,1}(\boldsymbol{x}) = \sum_{i=1}^{N_0} \eta_i^0 \cdot \phi_i^0(\boldsymbol{x})$$

   which introduced into Eq. (2) allows computing coefficients η_i^0. Then the approximation is enriched by considering $u^1 = u^{0,1} + \widetilde{u}$. In this case, we seek $\widetilde{u}$ such that:

   $$\mathcal{L}(\widetilde{u}) = b_0 - \mathcal{L}(u^{0,1})$$

   Once this problem is solved by applying the PGD method, i.e. $\widetilde{\mathcal{B}} = \{\widetilde{\phi}_1, \dots, \widetilde{\phi}_{\widetilde{N}}\}$ and then $\mathcal{B}^1 = \mathcal{B}^0 \oplus \widetilde{\mathcal{B}}$ and $N_1 = N_0 + \widetilde{N}$.

6. From this point we repeat the precedent steps: let us assume that we have already computed u^k. Then select a set of points $\mathcal{X}^k = \{\boldsymbol{x}_1^k, \dots, \boldsymbol{x}_{N_k}^k\}$, interpolate the nonlinear term using $\mathcal{B}^k$, and find u^{k+1}, until a certain convergence criteria is reached.

3 ELECTION OF THE INTERPOLATION POINTS

An open question is how to choose the points $\mathcal{X}^k = \{\boldsymbol{x}_1^k, \ldots, \boldsymbol{x}_{N_k}^k\}$. Consider that a certain computation step we know the reduced approximation basis:

$$\mathcal{B}^k = \{\phi_1^k, \ldots, \phi_{N_k}^k\}$$

Following [1, 4], we consider:

$$\boldsymbol{x}_1^k = \arg\max_{\boldsymbol{x}\in\Omega} |\phi_1^k(\boldsymbol{x})|$$

Then we compute c_1 from

$$c_1 \cdot \phi_1^k(\boldsymbol{x}_1^k) = \phi_2^k(\boldsymbol{x}_1^k)$$

which allows defining:

$$r_2(\boldsymbol{x}) = \phi_2^k(\boldsymbol{x}) - c_1 \cdot \phi_1^k(\boldsymbol{x})$$

from where we can compute the following point, $\boldsymbol{x}_2^k$ as:

$$\boldsymbol{x}_2^k = \arg\max_{\boldsymbol{x}\in\Omega} |r_2(\boldsymbol{x})|$$

As by construction $r_2(\boldsymbol{x}_1^k) = 0$, we can ensure that $\boldsymbol{x}_1^k \neq \boldsymbol{x}_2^k$. This process can be generalized and thus, if we are looking for $\boldsymbol{x}_j^k, j \leq k$, the following function can be constructed:

$$r_j(\boldsymbol{x}) = \phi_j^k(\boldsymbol{x}) - \sum_{i=1}^{j-1} c_i \cdot \phi_i^k(\boldsymbol{x})$$

where coefficients $c_i, 1 \leq i \leq j-1$, need to be computed. It can be done by imposing that:

$$r_j(\boldsymbol{x}_l^k) = 0 = \phi_j^k(\boldsymbol{x}_l^k) - \sum_{i=1}^{j-1} c_i \cdot \phi_i^k(\boldsymbol{x}_l^k) \ , \ l = 1, \ldots, j-1$$

that constitutes a linear system whose solution results the coefficients c_i. And then we compute the sought point:

$$\boldsymbol{x}_j^k = \arg\max_{\boldsymbol{x}\in\Omega} |r_j(\boldsymbol{x})| \tag{3}$$

It must be pointed out that, in principle, Eq. (3) implies reconstructing the solution, that is to say, to compute explicitly the functions $\phi_l^k, l = 2, \ldots, j-1$ from the separated functions $P_{l,s}^k(x_s)$ with $s = 1, \ldots, d$. For $l = 1$, notice that things are much simpler:

$$\boldsymbol{x}_1^k = \left(x_{1,1}^k, \ldots, x_{1,d}^k\right)$$

with

$$x_{1,s}^k = \arg\max_{x_s\in\Omega_s} |P_{1,s}^k(x_s)| \ , \ s = 1, \ldots, d$$

For $l > 1$ some simplifying procedures must be defined for avoiding the solution reconstruction and improve the performance in the multi-parametric case. The analysis of such procedures constitutes a work in progress.

4 NUMERICAL EXAMPLE

Aiming to prove the ability of the DEIM-based PGD method for solving nonlinear problems, we consider the transient heat equation with a quadratic nonlinearity:

$$\frac{\partial u}{\partial t} - \Delta u + u^2 = 0 \ , \ (\boldsymbol{x}, t) \in \Omega \times (0, T] \tag{4}$$

being $\Omega = [0,1]\times[0,1] \subset \mathbb{R}^2$. The initial condition reads $u(\boldsymbol{x}, t=0) = 0$ and the boundary conditions are given by $u(x=0, y=0, t) = u(x=1, y=0, t) = 0$ and $\nabla u \cdot \boldsymbol{n}\,(x=0.5, y=1, t) = 1$. Outside these boundaries, a zero-flux condition is considered.

A space-time separated representation is sought in this case:

$$u(\boldsymbol{x}, t) = \sum_{i=1}^{N} X_i(\boldsymbol{x}) \cdot T_i(t) \tag{5}$$

We use here the reuse option, that is to say, the reduced basis is enriched without projection. Using the notation introduced in the previous section the convergence was reached after the construction of $k = 4$ reduced bases in which the nonlinear term was interpolated, for a relative error less than 1% to the reference solution. However, a relative error of 0.5% cannot be attained in spite of the number of basis enrichment. The final solution involved $N = 52$ functional products $\phi_i = X_i(\boldsymbol{x}) \cdot T_i(t)$. Fig. 1 compares the time evolution at different locations obtained with the DEIM based PGD and the exact solution. Then Fig. 2 and 3 depict the four fist space and time modes respectively. From these results we can conclude on the potentiality of the proposed technology for solving non-linear eventually multi-parametric models.

5 CONCLUSIONS

This work presents the DEIM-based PGD technique for solving efficiently reduced nonlinear models. The improvement is achieved by interpolating the nonlinear term using the reduced basis, computed as usual with the PGD method, instead of performing its complete evaluation. As the PGD is an *a priori* model reduction technique, a progressive reduced basis enrichment must be considered, and thus up to three different choices can be done: restart the reduced basis, reuse the previous reduced basis by enrichment and reuse the reduced basis by projecting. A deep analysis of the different alternatives is in progress.

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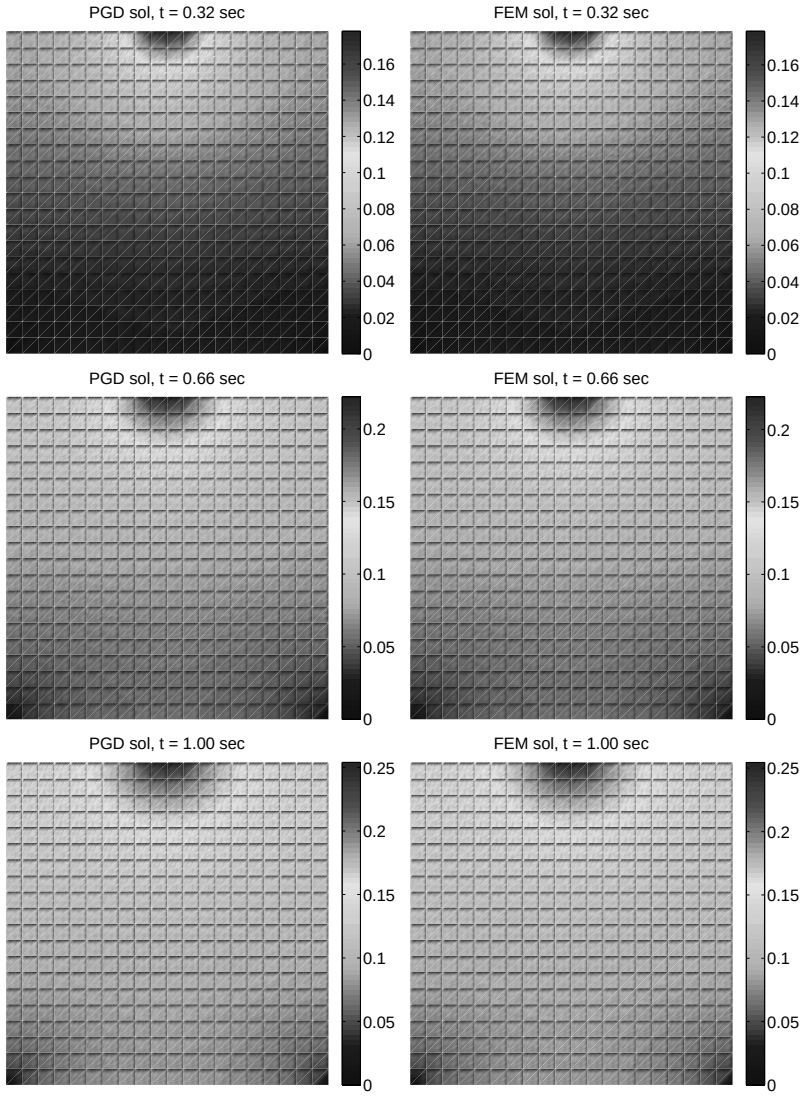

Figure 1: Comparison of the DEIM-based PGD solution (on the left) to the FEM reference solution (on the right), for three different times, $t = 0.32, 0.66, 1.00$ sec

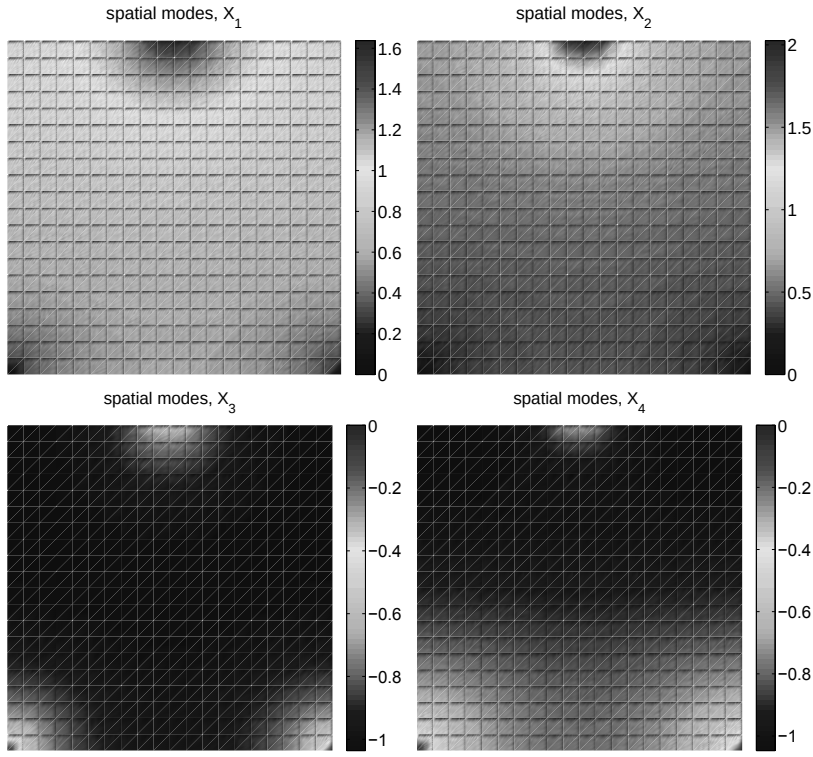

Figure 2: First four space normalized modes of the DEIM-based PGD solution

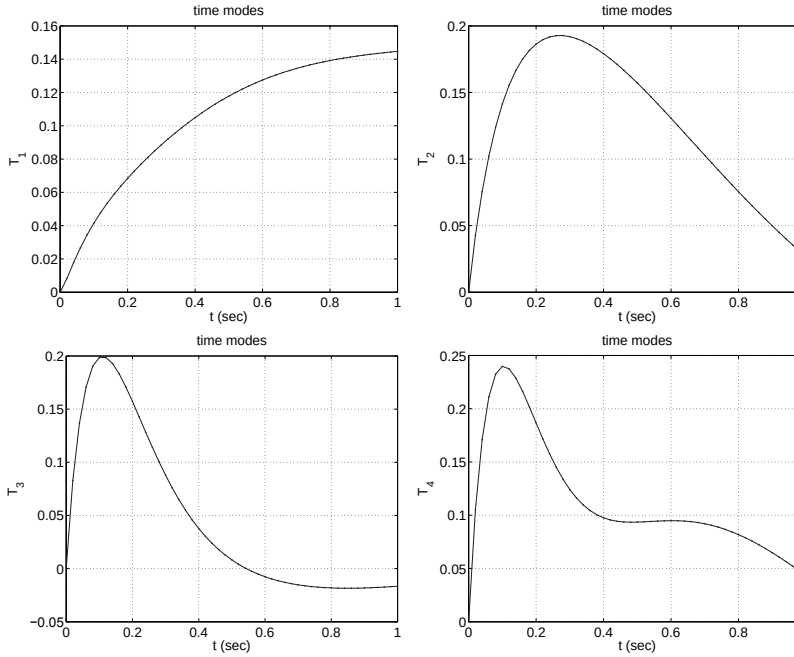

Figure 3: First four time normalized modes of the DEIM-based PGD solution

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ADMOS 2013
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AN UNSTRUCTURED FINITE VOLUME SOLVER FOR A NEW CONSERVATION LAW IN FAST TRANSIENT DYNAMICS

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Abstract. Since the advent of computational mechanics, the numerical modelling of fast structural dynamics has been a major field of interest in industry. Traditionally, a Lagrangian formulation is employed for the numerical simulation of these problems and low order spatial interpolation is preferred for computational workload convenience. The well known second order solid dynamics formulation, where the primary variable is the displacement, is typically discretised in space by using the Finite Element Method (FEM) and discretised in the time domain by means of a Newmark (trapezoidal) time integrator [1]. However, it has been reported that the resulting space-time discretised formulation presents a series of shortcomings. From the time discretisation point of view, the Newmark method has a tendency to introduce high frequency noise in the solution field, especially in the vicinity of sharp spatial gradients. From the space discretisation point of view, the use of isoparametric linear finite elements leads to second order convergence in displacements, but only first order convergence for stresses and strains. It is also known that these elements exhibit locking phenomena in incompressible or nearly incompressible scenarios.
Recently, a new mixed methodology [2] has been developed in the form of a system of first order conservation laws, where the linear momentum and the deformation gradient tensor are regarded as the two main conservation variables. The current paper will present and compare different techniques used for solving this methodology. Specifically, cell centred Finite Volume, Two Step Taylor Galerkin, Stream Upwind Petrov Galerkin (SUPG) and the Jameson-Schmidt-Turkel (JST) will be presented. The paper will focus on new developments towards the efficient implementation on unstructured meshes.

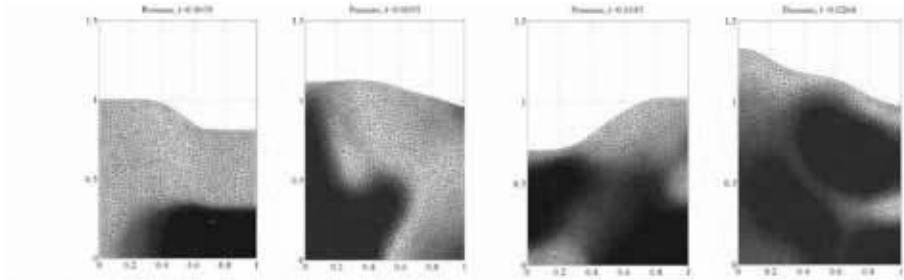

Figure 1 An example of fast dynamics solved using the JST method on unstructured meshes.

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A NEW RESIDUAL LEAST SQUARES ERROR ESTIMATOR FOR FINITE VOLUME METHODS – APPLICATIONS TO LAMINAR FLOWS

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Abstract. Adaptive refinement is an important technique to reduce the computation time of flows in very refined meshes and increasing the local accuracy of the simulation.
A new a-posteriori error estimator, suitable for h-adaptive methods on unstructured grids, is based on the residual evaluation and a high-order polynomial reconstruction.The results are performed by the authors own Navier-Stokes code, which has been used to solve different adaptive problems [1, 2, 3].
The residual least squares (RLS) estimator is applied to different problems with a known analytic solution to study the numerical error decay with the adaptive algorithm and it is compared with the classic Taylor Series estimator [4, 5]. The proposed adaptive procedure is also applied to 3D flows around a sphere for two different types of grids.

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A CLASS OF PIOLA-KIRCHHOFF HYBRID STRESS FINITE ELEMENTS FOR ELASTODYNAMICS

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Abstract. We introduce a novel hybrid stress finite element formulation for two-dimensional linear electrodynamics. This approach is an extension of the Piola-Kirchhoff hybrid stress formulation that we have recently proposed for linear elastostatics [1], and is applied in this communication to problems in the frequency domain. The formulation is consistent with a complementary form of the Hamiltonian variational principle, which involves, as fundamental unknown variables, the stress field components and boundary displacements. The approximate stress fields are split into two parts: a divergence-free (static) part, taken as the solution of the homogeneous momentum equations, and a dynamic part, taken as the particular solution of the momentum equations. The key ingredient of the formulation is to explicitly approximate, in the parent domain, either the second Piola-Kirchhoff stresses, the first Piola-Kirchhoff stresses, the Cauchy stresses, or rather their combination, and to enforce the divergence-free condition in the physical domain by means of a suitable projection. The main advantage of this formulation over traditional hybrid stress formulations [2] is that it allows to consider arbitrarily shaped elements without necessarily compromising static admissibility. Feasibility and effectiveness of the proposed formulation will be numerically demonstrated through the analysis of benchmark tests, which will also consider the problem of characterizing the properties of the error of these solutions.

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THREE DIMENSIONAL RE-MESHING FOR REAL TIME MODELING OF ADVANCING PROCESS IN MECHANIZED TUNNELING

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Abstract. The simulation of the advancing process for arbitrary alignments during shield tunnelling requires a continuous adaption of the finite element mesh in the vicinity of the tunnel face in conjunction with a steering algorithm for the Tunnel Boring Machine (TBM) advance. Moreover, the finite element mesh should match the actual motion path of the shield machine resulting from the FE-analysis in each excavation step. For this purpose, a technique to automatize the process of mesh generation based on hybrid mesh approach in which a new computational mesh in the vicinity of the tunnel face will be automatically generated within the advancing process is introduced.

This contribution is concerned with the 3D automatic mesh generation of finite element models for numerical simulations of shield driven tunnelling processes [1]. Automating the remeshing procedure of the tunnel geometry would reduce the effort required for generating a 3D model and improve the quality of the mesh dramatically. A novel approach for hybrid mesh generation is proposed, which adapts the spatial discretization in the vicinity of the tunnel face according to the actual position of the TBM. This hybrid mesh attempts to combine full advantage of the numerical accuracy and practical aspects of structured hexahedra meshes, while the numerical error can be controlled by the chosen density and interpolation order of the unstructured tetrahedral mesh (generated by the tool TetGen [2]) within the excavation region denoted as region of interest. An appropriate algorithm based on Superconvergent Patch Recovery (SPR) for the transfer of internal variables is adopted. In addition, mesh refinement based on a suitable combined error indicator for elasto-plastic models is introduced. During the generation of an adapted discretization according to the actual stage of excavation, this indicator enables the remeshing technique to be driven by a set of criteria that are function of both the current position of the TBM and the discretization error. The developed adaptive FE-model for mechanized tunnelling is implemented into the object-oriented FE-code KRATOS. The applicability of the proposed approach for capturing the projected excavation path and to perform a large-scale simulation of a tunnelling process along curved alignments is demonstrated by means of selected examples.

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GLUE-CONCRETE INTERFACE OF BONDED ANCHOR

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Key words: Bonded anchor, Tensile load, Bond stress, Experiments, Numerical Modeling, , Contact.

1 INTRODUCTION

This paper considers the practical application of nonlinear models in the analysis of an anchor bolt additionally placed in a concrete specimen. The model also considers epoxy surface. The results of analyses performed using the concrete model of specialized Atena 2D and Atena 3D finite element code are presented and discussed. The mesh density and convergence stability are compared in single anchor case study. All model results are compared with experimentally obtained data. There are also experiments focused on bond stress presented which are very important for verification of model assessment.
The article is focused on problems of post-installed steel bonded anchors real behaviour. Experiments and numerical models described in this paper are focused on problems of bond stress quality, on anchor joint loaded by tension force. There are progress and configuration of each experiment described.

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ROBUST ERROR CONTROL FOR PHASE FIELD MODELS PAST TOPOLOGICAL CHANGES

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Abstract. Phase field models are often used to describe the evolution of submanifolds, e.g., the Allen-Cahn equation approximates motion by mean curvature and more sophisticated phase field models provide regularizations of the Willmore flow and other geometric evolution problems. The models involve small regularization parameters and we discuss the dependence of a priori and a posteriori error estimates for the numerical solution of the regularized problems on this parameter. In particular, we address the question whether robust error estimation is possible past topological changes. We provide an affirmative answer for a priori error estimates assuming a logarithmic scaling law of the time averaged principal eigenvalue of the linearized Allen-Cahn or Ginzburg-Landau operator about the exact solution. This scaling law is confirmed by numerical experiments for generic topological changes. The averaged eigenvalue about the approximate solution enters a posteriori error estimates exponentially and therefore, critical scenarios are detected automatically by related adaptive finite element methods. The devised scheme extracts information about the stability of the evolution from the approximate solution and thereby allows for a rigorous a posteriori error analysis.

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ADMOS 2013
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GOAL-ORIENTED ERROR ESTIMATION AND ADAPTIVITY FOR THE TIME-DEPENDENT LOW-MACH NAVIER-STOKES

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Abstract. We present a goal-oriented algorithm for error control and adaptivity, targeting the low-mach compressible Navier-Stokes equations. The algorithm, using the GRINS computational framework, is illustrated first for stationary problems and then for time-dependent problems. Issues related to stabilization and linearization are highlighted in the former case, while the interplay between storage, efficiency, and numerical accuracy of the forward and adjoint solutions is examined in the latter case.

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A PRIORI BASED MESH ADAPTATION FOR VISCOUS FLOW

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Key words: CFD, viscous flow, Large Eddy Simulation, mesh adaptation

Abstract. A priori estimates are applied to the anisotropic mesh adaptation for 2D viscous flows and 3D ones including Large Eddy Simulation.

1 METHODS

Two novelties were presented [1] in the recent ECCOMAS conference at Vienna. First an a priori analysis for diffusive flows allowing, through a goal-oriented criterion, the direct specification of mesh metric, *i.e.* mesh stretching and density, [3]. Second the extension of this method to the reduction of approximation error in LES formulations [2]. In contrast to the very preliminary numerical experiments presented at ECCOMAS, we plan to discuss a sequence of tests showing the interest of both methods.

2 AN EXAMPLE

The proposed mesh adaptation method is applied to the computation of the flow around an offshore platform with a very complex geometry. This flow was accurately computed and compared with experiments in a specialized conference [4]. For the present mesh adaptive calculation, we take into account a large enough time interval and compute the adjoint on this interval. The resulting mesh adaptation criterion can be concentrated on

the generation of a single mesh, since the vortices concentrate on a region of wake which is well identified by the algorithm. See illustration.

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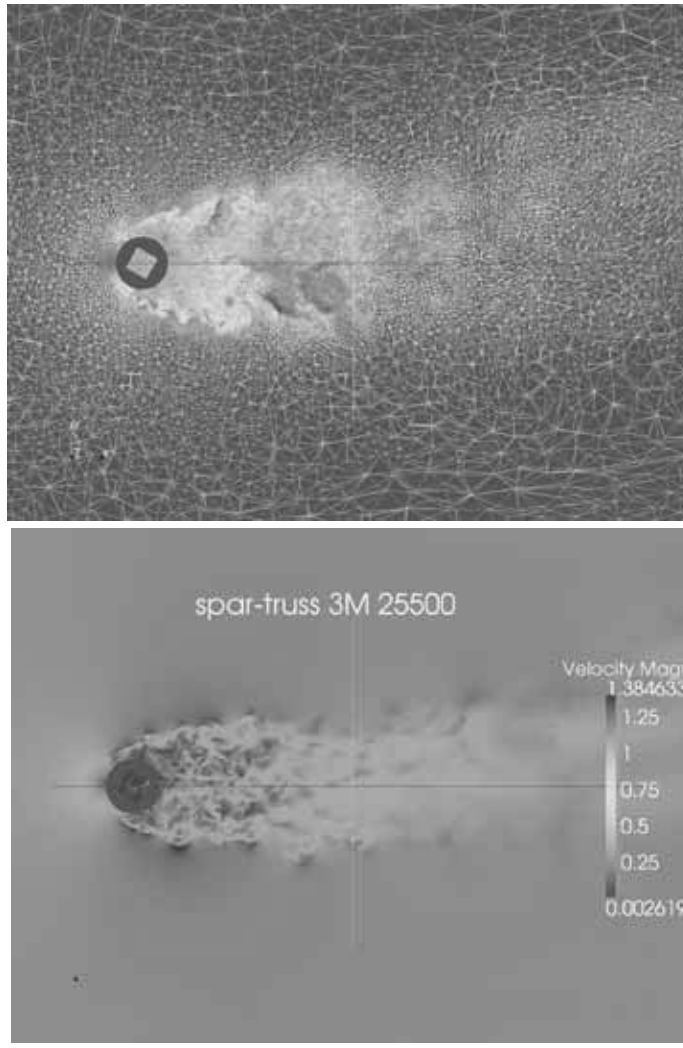

Figure 1: Mesh adaptive flow around an offshore platform: velocity module at two different times, the first one with mesh wireframe representation.

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HIERARCHICAL MODEL (HIMOD) REDUCTION FOR ADVECTION-DIFFUSION-REACTION PROBLEMS

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Key words: Hierarchical Model Reduction, Geometrical Multiscale

Abstract. The effective numerical description of challenging problems arising from engineering applications demands often the selection of an appropriate reduced - aka "surrogate" - model. The latter should result from a trade-off between reliability and computational affordability (see, e.g., [1, 8]). Different approaches can be pursued to set up the reduced model. In some cases, one can take advantage of specific features of the problem at hand for devising an effective *ad-hoc* model reduction. This is the case, for instance, of problems featuring a prevalent direction in the dynamics of interest, as in the modeling of the hemodynamics in arterial trees or of the hydrodynamics in a channel network. In this context, a possible approach is represented by the so-called *geometrical multiscale*, where dimensionally heterogeneous models are advocated for describing interactions at different scales: essentially, a lower dimensional (for instance, 1D) model is locally replaced by a higher dimensional (for instance, 3D) model to include local relevant transversal dynamics. This approach has been successfully applied both in hemodynamics (see, e.g., [3, 4]) and in river dynamics (see, e.g., [6, 5]).

As an alternative to the geometrical multiscale formulation, the so-called *hierarchical modeling* has been advocated in [2, 7]. The basic idea is to perform a classical finite element discretization along the mainstream direction of the problem at hand coupled with a modal decomposition for the transversal dynamics. The rationale behind this approach is that the transversal dynamics can be suitably captured by a few degrees of modal freedom. In addition, the dimenson of the modal discretization can be suitably adapted along the main direction, according to the local features of the transversal component of

the solution. This allows to improve hierarchically and adaptively the descripton of the local transversal dynamics, still in the context of a "psychologically" 1D solver.

Comparison and coupling with the geometrical multiscale approach, effective criteria for the selection of the hierarchical modal basis relying upon a principal component analysis (and alternative to the ones introduced in [2, 7]), applications to real 3D problems (such as the circulatory system) are steps to be tackled in the development of an effective HiMod approach in engineering applications.

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ADMOS 2013
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GENERATING ASSEMBLY MODELS FOR ADAPTIVE SIMULATIONS

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Key words: assembly, CAD models, idealization, mesh generation, functional information, a posteriori error estimator.

Abstract. Companies, especially in the aircraft and automotive industries are increasingly interested in setting up numerical simulations throughout a product development process. Because of the inherent complexity of their products, simulations are not only targeting isolated components but there is now a strong interest at studying the behavior of one or more subsystems of these products [1, 2]. The corresponding requirement is the setting of rather complex FE models that cannot be currently handled within the time scale prescribed by an industrial product development project.

The purpose of the proposed contribution is to describe how FE simulation models can be derived from assembly CAD models and how adaptive simulations can take place with these large scale models. Consequently, the contribution focuses on the major steps of simulation model preparation and its interactions with an adaptive simulation process. The target addressed falls into the scope of the national research project, ROMMA [3], and, if all the connections between the steps are not completed yet, the paper will report the current progress in each of them.

In a first place, studying the content and structure of an assembly model, as available in a Product Data Management System (PDMS), reveals that product assemblies or Digital Mock-Ups (DMUs) reduce to a set of components located in 3D space without geometric relationships between them. Complementarily, simulation models for assemblies strongly need geometric interfaces between components to be able to set up boundary conditions

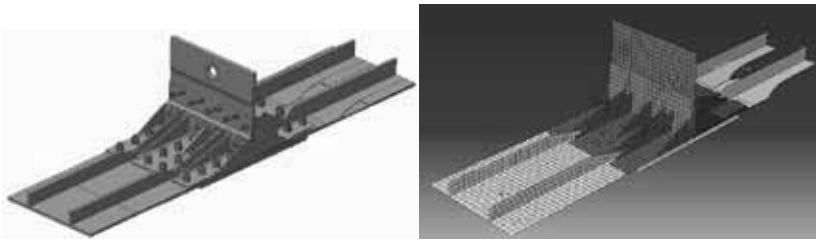
between them and/or meshing constraints, e.g. conformal mesh requirements.

Another observation derived from this analysis is the prominence of component functions as a means for specifying component simplifications/idealizations. This leads to a first step of the assembly processing scheme:

- Identification of geometric interfaces between components;
- Assignment of functional designations to components. Currently, functional information is automatically added to some categories of components using a qualitative reasoning process.

As a result, components are structured geometrically, i.e. key geometric interfaces are located on the boundary of each component and in its neighborhood, as well as from a functional standpoint, i.e. functional designations of components fit into a taxonomy and set constraints over technological data describing the interfaces involved in their definitions [4].

Because assembly models can lead to highly complex simulation models when it focuses on car and/or aircraft models, idealizations of components are key issues of simulation model preparation since dimensional reductions is a means to generate efficient simulation models. To this end component segmentation has been set up to analyze component morphology and produce robust idealization algorithms (see Figure 1). These idealization algorithms take also into account meshing constraints, i.e. locations of stiffeners interact with the shape and size of FEs and choosing ‘internal’ or ‘external’ stiffener positions rather than mid-surface can improve the FE mesh quality.



(a) (b)

Figure 1: (a) CAD model of an assembly, (b) model demonstrating the results obtained after component segmentations, an idealization process and a mesh generation. For illustration purposes some components have been idealized but not meshed, others have been idealized and meshed.

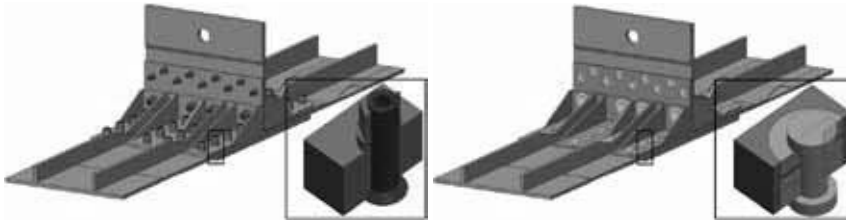
This result is a first step to connect with large scale simulation models as needed for COFAST software [5] to address simulation objectives at a rather global level.

The iterative scheme that is used in COFAST, is derived from the LATIN method. The main principle is to separate the equations in order to avoid solving simultaneously a global and a

nonlinear problem. The procedure searches for solutions that alternatively satisfy the global linear equations (kinematic admissibility and equilibrium on a substructure) and then, the local equations (interface equations). This leads to a decoupling of the problem. Because very few iterations of the LATIN method generate a solution over the whole time interval, the initialization overacts on the whole time interval. The solution obtained with this procedure ends up with a very low computation cost and can be parallelized to obtain a very good approximation of the solution.

Functional information becomes also important to set up simulation models dedicated to local analyses. Figure 2 illustrates how functional information can be used to simplify bolts and derive control areas around these bolts that are used to precisely monitor the mesh generation process so that meshing strategies can be efficiently set up when processing complex assemblies.

Functional information derived from the DMU is of qualitative type, e.g. cylindrical fittings are not quantified but classified as ‘tight fit’ or ‘loose fit’. However, this information acts as a template that can be used when setting up the simulation parameters required at interfaces between components. Because components interfaces are clearly identified and can be categorized from a mechanical point of view, the simulation model preparation is strengthened: the number and type of parameters needed at various interfaces can be unambiguously identified, thus avoiding inconsistencies that could arise when setting up complex simulation models.



(a) (b)

Figure 2: (a) CAD model of an assembly after the identification of functional designations of components (colors indicate the differences of functional designations), (b) model demonstrating the use of functional designations to simplify bolts and set up control volumes around them to adapt the model to the simulation objectives.

Additionally, the precise location of interfaces becomes helpful for setting up input for a posteriori error estimators. Indeed, the estimator used here is based on the constitutive error relation concept. A pillar of the method is to construct admissible fields. The knowledge of interfaces between substructures is then of primary importance. Nevertheless, in order to simplify a generic construction has been built when some data are missing [6]. When available, the precise location of the interfaces and more generally all the knowledge about the mechanical loading can be integrated in the generic method developed and improves the

quality of the computed error estimation. The first results obtained in the framework of linear elasticity have to be extended to the framework of contact with and without friction. The final objective is to obtain a tool that make possible to design a robust simulation of assemblies through an adaptive process.

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ADAPTIVE MODELLING AND MESHING FOR TIME DEPENDENT PROBLEMS BASED ON TIME AVERAGES

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Key words: a posteriori estimator, adaptive meshing and modelling

Abstract. We present a duality based a posteriori error estimator for the computation of functionals averaged in time for nonlinear time dependent problems. Such functionals are typically relevant for periodic or quasi-periodic solutions in time. Applications arise, e.g., in systems of convection-diffusion-reaction equations including a large amount of chemical reactions. In order to reduce the numerical complexity, we use simultaneously locally refined meshes and adaptive (chemical) models. Such strategies come along the question of how to control the discretization error and the model error.

These error parts are expressed in terms of output functionals. Hence, considerations of adjoint problems measuring the sensitivity of the functional output are needed. In contrast to the classical dual-weighted residual (DWR) method, we favor a fixed mesh and model strategy in time. Taking advantage of the (quasi-)periodic behaviour, only a stationary dual problem has to be solved. This implies that the computation of an evolutionary adjoint problem is circumvented. Storing the primal solution at every timestep is also not necessary. Only averaging in time is needed.

This a posteriori estimation technique is applied, e.g., to a system of convection-diffusion-reaction equations. The perfomance is checked by evaluating and comparing the estimated and exact erros for the mesh and the used model.

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STRUCTURAL OPTIMISATION AS A MOVING BOUNDARY PROBLEM USING LEVEL SET FUNCTIONS

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Key words: Topology optimisation, Tow-steered fibre composites, Level set functions, Aerostructural Optimisation

This paper will present two structural optimisation formulations which use level set functions representing the moving boundaries. The first of these is topology optimisation. The level set function based approach to topology optimisation has gained much popularity in the recent years due to its numerical stabilities and clear boundary representation of the solution. One advantage of the level set representation is its inherent capability to handle topological changes such as merging and splitting boundaries. We have developed a stable hole nucleation algorithm which makes the level set formulation completely suitable for topology optimisation. We demonstrate that our level set topology optimisation, both in 2D and 3D, have good convergence properties and less dependent on the initial design. We apply this to typical structural optimisation problems as well as coupled aero-structural problems. As coupled multidisciplinary optimisation problems have multiple optima, we find that the solutions 3D level set topology optimisation produce can be quite different from the solutions from the previous element-based approaches and simplified 2D solutions, suggesting interesting alternatives. The second structural optimisation using level set functions in composite fibre angle optimisation. We are the first to take this approach in this domain and the paper will introduce and show the feasibility. The advantages of the level set approach is better convergence properties compared to the existing functional approaches and we can improve the continuity of fibres compared to the discrete element approaches, particularly in a complex loading scenario. The paper will introduce the methodologies with emphasis on how the level set functions are utilised in the optimisation formulation. It will then show some numerical results for both types of problems and benchmarked against the existing known solutions, thus demonstrating how level set functions work in the context of structural optimisation.

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ROBUST ERROR ESTIMATES IN WEAK NORMS WITH APPLICATION TO IMPLICIT LARGE EDDY SIMULATION

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Key words: Computability, Stabilized FEM, Burgers' equation, Navier-Stokes' equation, Stability, A posteriori error estimates, A priori error estimates

Abstract. In this talk we will discuss a posteriori and a priori error estimates of filtered quantities for solutions to some equations of fluid mechanics. For the computation of the solution we use low order finite element methods using either linear or nonlinear stabilization. In reference [1], we introduced a class of weak norms corresponding to taking a weighted H^1-norm of a filtered solution. For these weak norms we proved error estimates for the Burgers' equation whose error constants depend only on the regularity of the initial data. In particular the estimates are independent of the Reynolds number, the Sobolev norm of the exact solution at time $t > 0$, or nonlinear effects such as shock formation. It follows that we obtain a complete assessment of the computability of the solution given the initial data. After a detailed description of the analysis in the case of the Burgers' equation we widen the scope and discuss two dimensional incompressible turbulence and passive transport with rough data within the same paradigm.

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ERROR CONTROL FOR NONCONFORMING FINITE ELEMENT METHODS FOR THE AFFINE OBSTACLE PROBLEM

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Key words: obstacle problem, Crouzeix Raviard finite element, a posteriori, a priori

Abstract. In a simple obstacle problems with affine obstacle and the weak regularity assumption of Lebesgue integrable Lagrange multiplier in $L^2(\Omega)$, the Crouzeix-Raviart nonconforming finite element methods allows for some best-approximation result for the gradients plus terms which explicitly converge linearly as the maximal mesh-size approaches zero. For instance in the case of singular solutions when the later contributions are less dominant, this allows for a comparison result that states that the energy norm of the nonconforming finite element solution is essentially smaller than that of the conforming one. The proofs are based on particular conforming companions plus standard arguments from convex analysis and variational inequalities such as the complementary conditions.
The a posteriori error control follows the general approach of D.Braess and designs a new discrete Lagrange multipliers which allow the computation of a guaranteed upper error bound. The practical performance in numerical examples and the question of efficiency concludes the paper.

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VASCULAR RECONSTRUCTION MODELLING OF LUMEN-ADAPTED ARTERIES WITH STIFFENED GRAFTS

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Key words: Shape Optimization, Genetic Algorithms, Biomedical Engineering, ANN Applications.

Abstract. Optimization of prosthetic graft configuration with regard to blood dynamics is the major target of this research. Hemodynamic simulations of idealized arterial bypass systems are acquired using a finite element arterial blood simulator exhibiting the hemodynamic flow changes due to compliance differences of a stiff graft and an elastic arterial wall. An artificial neural network simulating hemodynamic specific conditions is developed in order to reduce computational time. Optimal graft configurations are searched using a multi-objective genetic algorithm. An optimal set of solutions are presented and analyzed.

1 INTRODUCTION

Vascular grafts are special tubes that serve as replacements for damaged blood vessels. When suitable autologous veins are unavailable, prosthetic graft materials are used for peripheral arterial revascularisations. Compliance and calibre mismatch between native vessel and graft contributes towards poor long term patency [1].

The ideal vascular bypass graft would replicate the mechanical properties of native artery perfectly to maximize patency. Research study of dynamic arterial wall properties of large arteries such as the carotid and femoral arteries is becoming more common. Using non-invasive techniques the maximum and minimum arterial diameters and the intima-media thickness (IMT) at the point of maximum diameter and minimum diameter have been determined over the cardiac cycle. Moreover, the arterial diameter and IMT values can be used together with the blood pressure measurements to calculate several standard arterial stiffness indices [2].

Computational approaches have been used simulating blood flow through idealized bypass models [3, 4, 5]. They exhibit particular patterns characterized by the presence of recirculation zones and secondary flows in certain regions. The problem is related with both shape design and flow control that are involved in the simulation of the bypass system. Improving blood flow dynamics in the graft system is an important element for the long-term success of bypass surgeries.

In this project a developed multi-objective genetic algorithm [3] is considered in order to

reach optimal graft geometries for idealized arterial bypass systems of fully occluded host arteries. Genetic algorithms require a large number of computer simulations. So, an artificial neural network (ANN) is developed to efficiently simulate blood flow for specific graft geometries. Input and target data have been acquired using a finite element arterial blood simulator previously developed and tested considering fully unsteady incompressible Navier-Stokes equations and a three-dimensional geometry [6, 7].

2 RESULTS

The minimum carotid artery diameter occurs during the low-pressure end-diastolic cardiac phase and the maximum carotid artery diameter during the peak systolic phase and the IMT has an opposite behavior [2]. On the other hand, the prosthetic graft is stiff and the hemodynamic flow changes due to compliance differences across an anastomosis cause increased shear stress to damage endothelial cells and also reduced shear stress leading to areas of relative stagnation and increasing interaction between platelets and vessel wall. The aim of geometry design is to minimize these disruptive flow characteristics. The optimization process manages to achieve geometries presenting wall shear stress values with the expected variability for the blood behavior in the systemic arterial tree.

Acknowledgments

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RECENT ADVANCES IN THE CONTROL OF PGD-BASED APPROXIMATIONS

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Abstract. During the last few years, and due to the increasing number of multi-parameter simulation models, model reduction techniques have been the object of a growing interest in research and industry. In particular, an appealing technique based on separation of variables within a spectral resolution approach was recently introduced and successfully used in many applications of Computational Mechanics [1,2]. It is called *Proper Generalized Decomposition* (PGD), and can be seen as a POD extension. Contrary to the POD, the PGD approximation does not require any knowledge on the solution; it operates in an iterative strategy in which basis functions (or modes) are computed on the fly, by solving simple problems that can be seen as pseudo-eigenvalue problems. However, even though the PGD is usually very effective, a major question is to derive verification tools in order to control the quality of the approximate PGD solution.

After first works that developed error indicators in the PGD context [3], a verification approach was introduced to build guaranteed PGD-reduced models for linear elliptic or parabolic problems depending on parameters [4,5]. This approach is based on the concept of constitutive relation error and provides for strict bounds on both global error and error on outputs of interest. It also enables to assess contributions of various error sources (space and time discretizations, truncation of the PGD decomposition, etc.), which can help driving adaptive strategies.

In this work, we present the new advances which have been performed in the PGD-verification method. These advances particularly enable to deal with problems with lots of parameters, or new problems on which verification tools had not been tested until now (shape optimization for instance). Furthermore, they aim at setting up a non-intrusive procedure (in particular for the solution of the adjoint problem) in order to address implementation issues. Therefore, virtual charts associated with quantities of interest and computed from PGD models can now benefit fully from the verification method to satisfy a prescribed accuracy.

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ADAPTIVE MESHLESS ANALYSIS OF THIN SHELLS WITH THE AID OF THE INTERIOR PENALTY METHOD

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Abstract. Meshless approximations provide a great resource in the analysis of structures as the desired continuity in the approximated fields can be achieved. This feature is well suited for thin structures like shells, as stresses can be obtained as smoothly as desired. However, the non-interpolatory characteristic of such approximants makes the imposition of essential boundary and interface conditions not straightforward. For instance, in the classical Element-Free Galerkin Method (EFG), Lagrange multipliers are used to enforce such conditions. Recently, an alternative has been revisited: the Interior Penalty Method, usually referred to as Nietsche's Method, which identifies the Lagrange multiplier with the flux at the essential or interface boundary and introduces a penalty parameter, which warrants the convergence rate of the approximation. In the elasticity case, the reaction tractions are the same as the stress normal to the boundary. The present work aims at developing the study of this method in the linear elastic analysis of shells, firstly for the imposition of boundary displacements and latter for multi-region problems. In the former case, its advantage over Lagrange Multipliers is that no additional degrees of freedom are introduced and there is no need to introduce a new approximation space (which would have to obey an inf-sup condition), in the latter, refinement over one portion of the domain can be performed without affecting other regions, even maintaining their stiffness matrices, and different regions can be discretized with different approximants, *e.g.*, finite elements.

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DEVELOPMENT OF A 3D NAVIER-STOKES DG SOLVER FOR ADAPTIVE SCHEME AND MODELLING

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Keywords. Discontinuous Galerkin method, hybrid mesh, turbulent flow, High-order discretization methods

Abstract. Over the years, the development of new and increasingly powerful CFD simulation tools has helped manufacturers in the aerospace industry gain a greater understanding of the operating performance of their products. This has allowed them to progress through the design life cycle in a more timely and cost-effective manner by supplementing or replacing experimental testing with CFD computations.
The industrial demand for CFD predictions at an ever-increasing level of detail is the driving force for the development of highly accurate simulation techniques able to predict not only overall flow features, but also local values of the quantities of interest. This will allow engineers to expand the range of flow conditions to which CFD can be applied.
Nevertheless, most of the industrial CFD codes used today are based on second-order methods, which appear not to be sufficiently accurate to reach these goals. With the aim of overcoming the limitations of second-order approaches, Onera has launched the development of a DG solver called Aghora [1], [2]. The main goal is to develop a new demonstrator able to integrate efficient high-order schemes based on Discontinuous Galerkin methods using hybrid type meshes (tetrahedral, hexahedra, prisms and pyramids) for the simulation of turbulent flows using different levels of modelling, i.e. RANS [2], LES, hybrid RANS/LES and DNS. Adaptive techniques based on local HPM methods (H for grid, P for accuracy of shape function, M for model) will be used in order to represent accurately the flow physics.
However, these methods require the solution of very large discrete systems. This leads to long execution times and high memory requirements. Consequently, in order to tackle such challenges, the project focuses on the implementation of efficient algorithms for modern multi-core architectures with highly-scalable parallel strategies. The paper will present the status of the modal DG schemes implemented in Aghora as well as representative test cases illustrating the adaptability capacity of DG methods.
In order to illustrate the interest of DG approach with high order polynomial degrees, a convergence analysis in terms of number of Degrees of Freedom (DOFs) is presented hereafter. The calculations are performed with the compressible Navier-Stokes equations for the simulation of a manufactured solution of a Poiseuille flow (M=0.1). Fig. 1 shows the evolution of the L^2 norm of the error vs. the characteristic size of the elements h, represented here by the Degrees of Freedom. The slopes obtained by the computations, compared to the theoretical slopes,

demonstrate the effective accuracy of the implemented Navier-Stokes DG scheme in Aghora.

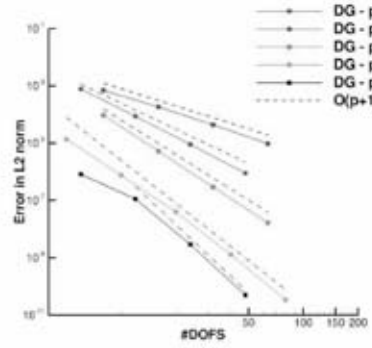

Figure 1: Convergence analysis in DoFs – Manufactured solutions for Navier-Stokes equations Aghora (laminar flow) - L2-norm on the error between numerical and exact solutions

Mesh convergence analysis (*h*) and polynomial degree convergence analysis (*p*) for turbulent flow computations will be presented. Fig. 2 illustrates the solution of a transonic flow around the Onera M6 wing for a DGP1 computation performed with the Kω Wilcox model.

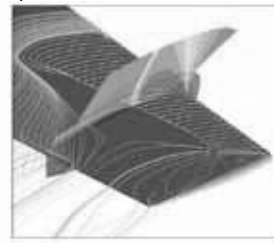

Figure 2: Turbulent flow around the Onera M6 wing – DGP1 computation with a RANS/Kω model

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ANISOTROPIC A-PRIORI ERROR ESTIMATES ON SURFACES

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Key words: anisotropic meshes, a-priori error estimators, finite elements

Abstract.

A lot of practical problems are related to the resolution of Partial Differential Equations (PDEs) defined on surfaces embedded in a three dimensional space. In such cases the classical differential operators have to be suitably modified to recover tangential information (see [1]); likewise, the derivation of error estimators is usually not a trivial task, essentially due to the fact that these estimators should include the error due to the finite element approximation as well as to the fitting of the computational domain (see [3]).

Moving from the theory proved in [2], we propose an *anisotropic a-priori error estimator* to control the L^2-norm of the interpolation error associated with linear finite elements defined on surfaces. This new error estimator consists of two different contributions:

- an *almost best-approximation term*, typical of a finite element discretization;
- a *geometric error term*, related to the discretization of the surface.

Moving from to this estimator, we settle a metric-based anisotropic mesh adaptation procedure which essentially employs local operations (node smoothing, edge collapsing, edge splitting, edge swapping) to adapt the mesh. Since an anisotropic estimator takes into account the directional features of the solution at hand, we obtain adapted meshes whose elements are suitably oriented to match the intrinsic directionality of the function defined on the surface, and of the surface itself.

As expected the employment of anisotropic meshes leads to a remarkable improvement of the mesh adaptation procedure in terms of computational costs.

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ON GLOBAL ERROR ESTIMATION AND CONTROL OF FINITE DIFFERENCE SOLUTIONS FOR PARABOLIC EQUATIONS

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Abstract. In this talk we will report on some joint activities with Jan Verwer (CWI) regarding efficiency and reliability questions for finite difference approximations of parabolic problems. First, systems of ODEs are considered. We have implemented classical global error estimation based on the first variational equation, and global error control, for which we have used the property of tolerance proportionality. We have found, using the Runge-Kutta-Rosenbrock method ROS3P as example integrator, that the classical approach is remarkably reliable. For finite difference approximations of parabolic PDEs, the ODE approach is combined with estimates for the spatial truncation errors based on Richardson extrapolation. Numerical examples are used to illustrate the reliability of the estimation and control strategies.

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ADMOS 2013
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MASSIVELY PARALLEL COMPUTATION ON ANISOTROPIC MESHES

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Keywords. massively parallel, anisotropic mesh adaptation, multigrid, finite element simulation

Abstract. In this paper, we present the work performed to enable massively parallel computations over anisotropic meshes and preserve a good efficiency, to take advantage of two main ways to speed-up an application or to improve the precision of the calculation. Firstly, today supercomputers provide access to a very large number of cores (several thousands), but the applications need to be adapted to fully benefit of such a large amount of power and memory. Such calculations can lead to the use of meshes of billion(s) of nodes. Another direction to improve finite element simulation consists in using anisotropic meshes that allow us to refine the mesh only in the direction of interest. In this way, the CPU cost to improve the precision of our simulations is reduced by increasing the number of nodes only in the direction needed and not in an isotropic way. This makes a huge difference, especially in 3d calculations: in the best case, we can improve by a factor two the accuracy using only 2 times much nodes rather than 8 times.

The first step has been to improve the mesher to enable it to generate very large distributed unstructured anisotropic meshes on thousands of cores. The second one concerned the implementation of a massively parallel multigrid solver to allow us to solve large linear systems generated by Finite Element formulations used to solve the Stokes/Navier Stokes equations. All these developments enabled our software, CimLib [1], to solve a 10 billion of unknowns system using 8192 cores in less than 200 seconds.

We first present an original parallelisation strategy for mesh adaptation [2]. It is based on an independent subdomain remeshing under the constraint of blocked interfaces. Furthermore, a new partition of the mesh is done in order to move the interfaces. Then, these two steps are iterated until we obtain a good mesh quality everywhere. The fact of using the original mesher in a parallel context rather than explicit parallelization provides easier anisotropic mesh adaptation to anisotropic mesh easier. Some examples with large distributed anisotropic meshes will be shown in 2d, as well as in 3d. In this work, we also describe the optimisation made to obtain a good parallel performance by reducing the complexity of the algorithm to a linear one only in the part where the mesher relaying needs to work and not on the whole mesh. This has been done by introducing a “permute-cut-and-paste” procedure: the ”bad quality” submeshes are extracted and then remeshed and pasted back to the complete mesh.

Then, we describe a parallel multigrid implementation for solving very large systems of equations. Even if the efficiency of our iterative parallel solver (GMRES,CR) with complex

parallel preconditionner ILU(k) inside the PETSc library [3] is good and close to the ideal Speed-Up , the non linear complexity of such algorithms fails to solve systems of billions of unknowns. Therefore, a multigrid method is needed. PETSc provides some facilities to implement multigrid algorithms, but for unstructured meshes the user still has to provide at each level the smoother operator, as well as the restriction/injection operators between each level. Building the smoother consists of the assembly step of the classical resolution and did not need any new developments, but building the restriction/injection operator for two unstructured distributed meshes revealed much more difficult. The sequential algorithm implemented was a simple one: for each node “n” of a mesh “A”, find the element of then mesh “B” containing “n” and compute its barycentric coordinates; for finding the element, an octree algorithm is used to speed-up de process. For the parallel version, the difficulty consisted in the fact that the node and the element may not be on the same core. An additional problem is due to the volume of data exchange: thanks to the mesh adaptation strategy chosen, most of the mapping of the two partitions is quite good and only a small percentage of nodes need to be communicated to other cores. Even with small exchange, using several thousands of cores was not straight forward : negligeable things on a small amount of cores can lead to a « blottleneck » on thousands of cores. Several optimisations will be presented and analysed over a large amount of cores.
Finally, parallel performance analysis is done with a massively parallel computer cores. Performances show a very good scalability of our library, including mesh adaptation and linear solver resolution. Multigrid implementation has
optimized the CPU time, as well as memory consuming of the supercomputer used during the numerical simulations. The use of the parallel visualisation software ParaView [4] allowed data processing directly on a end-user site [5].

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A FRAMEWORK FOR ROBUST A POSTERIORI ERROR CONTROL IN UNSTEADY NONLINEAR ADVECTION-DIFFUSION PROBLEMS

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Key words: Unsteady nonlinear advection-diffusion problem, a posteriori estimate, dual norm, flux reconstruction, flux equilibration, unified framework, robustness, discontinuous Galerkin method

Abstract. We derive a framework for a posteriori error estimates in unsteady, nonlinear, possibly degenerate, advection-diffusion problems. Our estimators are based on a space-time equilibrated flux reconstruction and are locally computable. They are derived for the error measured in a space-time mesh-dependent dual norm stemming from the problem and meshes at hand augmented by a jump seminorm measuring possible nonconformities in space. Owing to this choice, a guaranteed and globally efficient upper bound is achieved, as well as robustness with respect to nonlinearities, advection dominance, domain size, final time, and absolute and relative size of space and time steps. Local-in-time and in-space efficiency is also shown for a localized upper bound of the error measure. In order to apply the framework to a given numerical method, two simple conditions, local space-time mass conservation and an approximation property of the reconstructed fluxes, need to be verified. We show how to do this for the interior-penalty discontinuous Galerkin method in space and the Crank–Nicolson scheme in time. Numerical experiments illustrate the theory. More details on the analysis and results can be found in [1].

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NS-IBM: A PARALLEL INCOMPRESSIBLE NAVIER-STOKES SOLVER ON UNSTRUCTURED CARTESIAN MESH WITH AUTOMATIC MESH REFINEMENT

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A common feature of the various groups of the team "mécanique et environnement" of the Institute of Fluid Mechanics and Solid Strasbourg is the numerical modeling of various flows in complex geometries: turbulent flows, free surface flows, fluid-structure interaction, flows in airways. For this purpose, we use very different solvers, either free solvers or commercial solvers or solvers developed at IMFS developed. This raises, among others, the problem of continuity of knowledge.

Aware that a Navier-Stokes can not claim universality and potential to deal with any possible issues, we have developed a flexible and versatile tool for solving incompressible Navier-Stokes equations on Cartesian unstructured meshes. While the heart of a Navier-Stokes solver can be based on a relatively small selection of proven methods, the geometry processing for codes claiming geometric flexibility represents up to 90% of the investment in terms of development effort. The numerical method proposed is based on a finite volume conservative discretization and a unstructured and non-conforming grid designed to circumvent the problem of mesh generation by the use of automatic mesh refinement. The immersed boundary method is used handle the geometry.

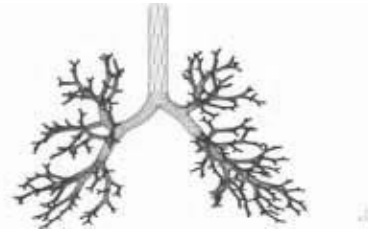

Figure 1Geometry of human airways

The solver is fully parallelized with MPI and so far it has been extensively validated on the test cases of the driven cavity, the cylinder and the square cylinder before it application on the simulation of flow in human airways. So far the AMR is only available as a pre-processing tool. In this conference we will present the concept of this solver, its validation and its application to the simulation of unsteady flows in a Human airways model under realistic breathing conditions.

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ADMOS 2013
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p-adaption for compressible flows

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Abstract

We present a p-adaptive method which takes advantage of the ability of a discontinuity sensor used to quantify the difference between the actual solution (p) and the projected reduced one ($p-1$) in order to vary the polynomial resolution in an element. The value of the sensor in an element is defined as:

$$S_e = \frac{||\rho_e^p - \rho_e^{p-1}||_{L_2}}{||\rho_e^p||_{L_2}}$$

where ρ_e^p and ρ_e^{p-1} are the average solutions of degree p and $p-1$ respectively on the same element. The polynomial degree is decreased when a discontinuity is present in order to avoid oscillations and increased when a high gradient is identified to improve the accuracy. This procedure allows the simulation to adapt to the flowfield, increasing the accuracy of the solution only where needed and, as a consequence, reducing the computational cost required for solving the problem.

Initially, a converged linear solution is obtained after which the sensor in each element is calculated. Based on the determined sensor value and the pre-defined sensor thresholds, the degree of the polynomial approximation in each element is increased, reduced or maintained and a new converged solution is obtained. The sensor distribution is divided into four zones:

$$p_e = \begin{cases} p_e - 1 & \text{if } s_e > s_{ds} \\ p_e + 1 & \text{if } s_{sm} < s_e < s_{ds} \\ p_e & \text{if } s_{fl} < s_e < s_{sm} \\ p_e - 1 & \text{if } s_e < s_{fl} \end{cases}$$

where s_{ds}, s_{sm} and s_{fl} are the threshold values to identify discontinuities, smooth and flat solutions respectively. This procedure is carried out iteratively.

The performance of the p-adaptive method is illustrated for the solution of the subsonic flow past a cylinder. In the figure below, the p-distribution around the cylinder is given after applying the p-adaptive procedure three times. High accuracy is required in the regions near the wall and in the wake. This example shows that it is possible to choose an appropriate polynomial degree in each element and yet achieve the same accuracy that can be obtained with a high polynomial degree everywhere but using less computational resources. The automatic procedure reaches a stable p-distribution with $p_{min} = 1$ and $p_{max} = 4$. The accuracy of the solution measured through the entropy error on the wall is of the same magnitude of the accuracy obtained with a $p = 4$ solution everywhere ($||\epsilon(p_{max}) - \epsilon(1 \leq p \leq p_{max})||_{L_2} < 0.01$) where ϵ is the L_2 norm of the difference

between the exact and the computed solution.

The efficiency of the p-adaptive procedure comes from the reduction in the number of operations required to solve the equations, but also the initial condition of each $1 \leq p \leq p_{max}$ simulation is a converged solution obtained with a lower degree $(1 \leq p \leq p_{max} - 1)$. However, the smaller CFL time restriction associated with p_{max} has to be imposed over all the domain, thus reducing the time step also in the regions with lower polynomial order. A possible improvement could be the application of a domain decomposition technique or variable timestepping to deal with different values of Δt through the domain.

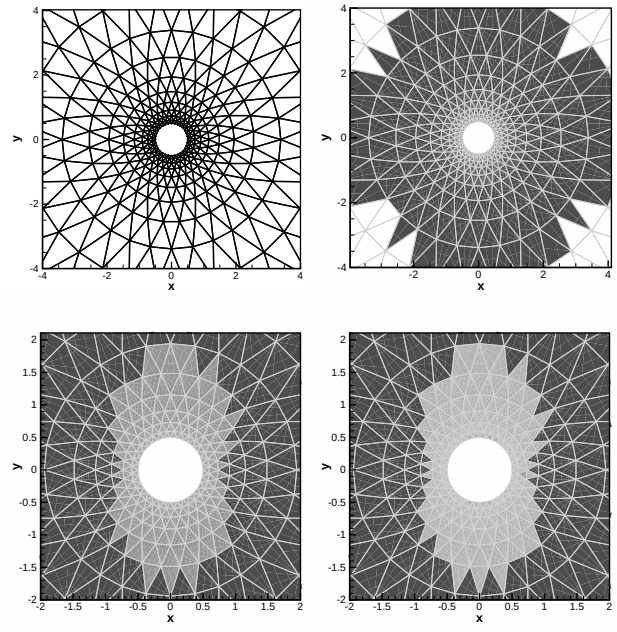

Figure 1: Polynomial degree distribution after applying the automatic p-adaption three times on a subsonic cylinder (a) p = 1 (white) (b) $1 \leq p \leq 2$ (red) (c) $1 \leq p \leq 3$ (green) (d) $1 \leq p \leq 4$ (blue).

MULTIOBJECTIVE AND MULTIPOINT OPTIMIZATION OF A HEAVY CLASS HELICOPTER ENGINE INSTALLATION USING EVOLUTIONARY ALGORITHMS

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Key words: Model Validation, CFD Coupled Solvers, Optimization Algorithms, Optimization Strategies, Industrial Application, Computing Methods.

Abstract. Aerodynamic design and optimization of the engine installation is a pivotal part of the helicopter design process. The engineers seek for an optimum configuration which maximizes the global efficiency of the aircraft resulting in lower fuel consumption. An adaptive, problem-independent and reliable optimization methodology would be particularly valuable in assisting the design process. In such a context, the application of advanced evolutionary algorithms coupled with CFD solvers for the accurate flow solution of validated numerical models represents a very powerful tool for parametric design and optimization of engine installation components. Within the JTI Clean Sky FP7 project "HeavyCopter" the consortium constituted by the University of Padova (UNIPD) and the spin-off company HIT09 developed an automatic optimization loop, based on the home made genetic algorithm GDEA, applicable to engine installation design as well as to general aircraft components optimization problems. This paper illustrates the application of the GDEA-based optimization loop at a forward and a hover reference flight conditions. The parametric modifications on the geometries are compliant with the architectural constraints of the engine bay. The algorithm pursues the minimization of the total pressure losses at the inlets, while keeping the flow distortion at the lowest through a functional penalization; the back-pressure is reduced at the exhausts in order to increase the power output of the engine, also preserving the entrainment ratio. The results highlight significant improved performance margins on all the components.

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A FULLY COUPLED FINITE VOLUME SOLVER FOR THE SOLUTION OF INCOMPRESSIBLE FLOWS ON LOCALLY REFINED NON-MATCHING BLOCK-STRUCTURED GRIDS

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Key words: computational fluid dynamics, finite volume method, pressure-based coupled solver, block-structured grid, non-matching block interface

Abstract. A fully coupled solver for the solution of steady laminar incompressible flow problems on locally refined non-matching block-structured grids that promises improved convergence properties is presented. For this a coupled velocity-pressure algorithm developed by Darwish [1] that solves the momentum and pressure equations simultaneously is extended correspondingly. The spatial finite-volume discretisation applied is of second-order accuracy. All blocks are implicitly coupled and the method is fully conservative. The newly developed method is verified via comparisons with manufactured solutions. Its performance is evaluated by systematic comparisons with standard segregated pressure-correction solution techniques for representative test cases.

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NON INTRUSIVE STOCHASTIC SIMULATIONS USING A GOAL ORIENTED ADAPTIVE STRATEGY.

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Key words: Reduced basis, Adaptivity, Stochastic modeling, Goal-oriented error assessment

Abstract. The paper presents a goal-oriented strategy in the framework of stochastic non-intrusive Monte Carlo finite element simulations. The methods consists in a successive enrichment of a reduced basis. This enrichment is performed on the fly, during the Monte Carlo process. The error made by the representation on the reduced basis is assessed introducing a dual problem associated to the quantity of interest. The efficiency of the proposed approach is illustrated in numerical examples. In particular, an extension of the work developed in [1] is introduced. It consists in introducing a reduced basis for solving the dual problem in an efficient way. Different algorithms are tested for the successive enrichment of the dual reduced basis.

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MULTI-BLOCK DECOMPOSITION USING CROSS-FIELDS.

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Key words: Multi-block decomposition, Quadrilateral Mesh, Cross-Field, Mesh Singularities.

ABSTRACT

The multi-block meshing strategy involves decomposing complex domains into a collection of simpler sub-regions to which structured meshes can be applied, thereby producing high quality block-structured meshes. However, the absence of effective automatic decomposition algorithms reduces the practicality of the method. In this paper a method is described for automatically generating multi-block decompositions of surfaces suitable for generating boundary aligned block-structured quadrilateral meshes with a small number of singularities far from boundaries.

The method uses a cross-field describing the local directionality of a square quadrilateral mesh, which is solved for on an existing triangular mesh. Crosses aligned with boundary components are initialised at boundary nodes. The cross-field is propagated into the interior at a constant rate with respect to distance using a smoothing method aimed at minimising its local distortion. Mesh singularities necessarily occur due to the particular nature of the local boundary alignment constraints or significant total Gaussian curvature. It is shown that they tend to appear in the cross-field solution at discrete positions near the medial axis. They are characterised by non-zero circulation of the cross-field around the edges of triangle elements. The final multi-block decomposition is generated from the cross-field simply by tracing the critical streamlines connected to singularities and boundary corners. Examples are included that demonstrate the process and showcase the final multi-block decompositions of planar and curved open surfaces, of arbitrary genus, with complex boundary edge features. The use of scratches is also explored as a means of applying additional direction constraints to produce block-structured meshes suitable for capturing important simulation solution features, such as shock waves and wakes in CFD analyses.

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A POSTERIORI ERROR ESTIMATES FOR A NEUMANN-NEUMANN DOMAIN DECOMPOSITION ALGORITHM APPLIED TO CONTACT PROBLEMS

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Key words: Error estimation, domain decomposition algorithm, contact problem, discretization error, algebraic error

Abstract. Contact problems are frequent in structural analysis. They are characterized by inequality constraints such as non-interpenetration conditions, sign condition on the normal constraints, and an active contact, an area that is a priori unknown. Several approaches exist for solving the non linear equations issued from the finite element discretization of frictionless contact problems. In this work, we consider a natural Neuman-Neumann domain decomposition algorithm, in which each iterative step consists of a Dirichlet problem for the one body, a contact problem for the other one and two Neumann problems to coordinate contact stresses. Two main approximation errors are introduced by this algorithm: a discretization error due to the finite element method (FEM) and an algebraic error due to the Neuman-Neuman domain decomposition algorithm (NNDD).

The objective of this paper is to present an a posteriori global error estimator for a frictionless contact problem, solved by a NNDD algorithm and two errors indicators which allow to estimate the part of the error due to the spatial discretization and the part of the error due to the domain decomposition algorithm. We show how to extend the error measure in the constitutive relation developed by the authors for contact problems solved by a Neumann-Dirichlet domain decomposition algorithm and how to modify the construction of the admissible fields. The proposed errors estimators and indicators are studied on several 2D-examples and the behavior of the NNDD algorithm is compared with the behavior of a Neumann-Dirchlet domain decomposition algorithm

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AIRFOIL OPTIMIZATION WITH TRANSITION CURVE AS OBJECTIVE FUNCTION

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Key words: Airfoil, Optimization, Low Reynolds, Aerodynamic Optimization, Transition Curve, Long Endurance UAV.

Abstract. In all conventional subsonic aircraft with medium/high aspect ratio wings (>6) the major single contribution to the overall aerodynamic performance of the vehicle comes from the wing airfoil and therefore its careful design is paramount. In the case of the fast growing market of UAV applications, the need for cost reduction is driving the designs to smaller scale and lower airspeeds. This brings the low Reynolds (60,000<Re<500,000) airfoil aerodynamic problem, where the boundary layer laminar separation bubble and transition in the upper surface influences decisively the drag polar merit [1]. Most formal approaches in the design of airfoils try to change the airfoil geometry in order to directly minimize the drag coefficient for a given flight condition or to match a given pressure distribution known to be favourable for a given application. The upper surface transition ramp manipulation is an example of such a methodology. Often, besides the resulting drag polar, the corresponding transition curve on the upper surface is shown as a representation of the effect of a prescribed pressure recovery/transition ramp. The present work describes the design optimization of a high lift airfoil where the objective function is that curve defined by the lift coefficient variation with the boundary layer transition position along the upper surface of the airfoil. An aerodynamic shape optimization program using XFOIL [2] as the solver, a viscous two-dimensional panel method formulation code, and a sequential quadratic programming optimization routine, solves a minimization problem to determine the optimal airfoil geometry which minimizes the difference between its transition curve and the specified objective curve while subject to geometric constraints and constant product of Reynolds number with the square root of lift coefficient for a given interval of lift coefficient values. The airfoil design variables are b-spline control points which define the airfoil camber line and the airfoil thickness distribution. A case study is presented for an airfoil design suitable for a long endurance UAV demonstrating the capability of the approach in producing an optimized design. Comparisons with other objective functions are also shown.

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STOCHASTIC MODEL REDUCTION APPLIED TO INVERSE PROBLEMS

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Key words: Inverse analysis, model reduction, stochastic optimization

Abstract. This article describes the use of Gaussian Processes in model reduction techniques with application to inverse problems. Mainly, the work is focused on the proper construction of the model approximation, namely on training process based on minimal number of learning samples, by making use of automatic samples selection through computed standard deviation of model prediction. An example of application of stochastic surrogate model for the paperboard characterization through biaxial tensile test and DIC measurements is also presented.

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HIGH-ORDER MESH GENERATION ON CAD GEOMETRIES

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Key words: high-order quality; high-order mesh generation; mesh optimization; curved elements; parameterized surfaces;

Abstract. During the last decade special effort has been focus on the development of high-orders methods. However, its application to industrial problems has been hampered by the need to generate high-order curved discretizations. In this work, we present a technique to extend Jacobian-based distortion (quality) measures for linear and planar triangles to high-order isoparametric elements of any interpolation degree on CAD parameterized surfaces. The resulting distortion (quality) measures are expressed in terms of the parametric coordinates of the nodes. These extended distortion (quality) measures can be used to check the quality and validity of a high-order surface mesh. Moreover, we apply them to develope a simultaneously smoothing and untangling optimization procedure that generates high-order surface meshes. The minimization is performed in terms of the parametric coordinates of the nodes. Thus, the nodes always lie on the surface. Finally, we present several examples to illustrate the application of the proposed technique.

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ON THE REDUCTION OF SOLID DYNAMICS EQUATIONS AND THEIR REAL-TIME DIRECT INTEGRATION

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Abstract. In this work we propose a particular form of the solid dynamics equations in a multidimensional framework. This particular viewpoint of the traditional dynamics equations is then discretized and solved by PGD approximations very efficiently.
As a result, the method here proposed provides with a meta-model or surface response of the system subjected to any type of force (taking values in a given interval) and for any initial boundary conditions. Since the time interval in which the integration is performed can be virtually any, and any integration scheme can be used, the proposed method, combined with an on-line/off-line strategy, provides with a sort of "black box" that computes the response of the system for apparently very large time intervals with great accuracy and under real time requirements.
Several aspects will be studied, such as the parameterization of the space of initial conditions, efficiency issues and others, together with examples showing the potential of the proposed technique.
Special attention will be paid to the issue of choosing the appropriate time step, the number of modes, strategies for optimal balance between accuracy and speed of simulation, etc.

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PARALLEL ADAPTIVE MESH ALGORITHMS FOR MULTICORE ARCHITECTURES

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Key words: parallel, adaptive mesh algorithms, multicore, MPI, OpenMP, NUMA

Abstract. Problems that require dynamic adaptation of an unstructured mesh are particularly challenging for multicore architectures. This work tackles concurrency control, memory management and locality in the context of adaptive mesh finite element simulations. We present experimental analysis of a range of implementation alternatives, and we demonstrate that good performance and parallel speedup are achievable. We study both OpenMP intra-node parallelisation and MPI internode parallel execution, with particular attention to memory hierarchy and NUMA issues.

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A RECOVERY-BASED ADAPTIVE MESH REFINEMENT ALGORITHM WITH APPLICATION TO GEOMATERIALS

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Key words: Adaptive Mesh Refinement, Geomaterials

Abstract. It has been recently highlighted that Adaptive Mesh Refinement (AMR) algorithms have not been fully exploited for applications in geomechanics [1]. This paper illustrates a simple AMR algorithm and demonstrates its performance by modelling standard soil test. The algorithm has been implemented for 6-noded triangular elements within the geotechnical finite element package PLAXIS 2D.

Localization is frequently observed in geomaterials, often as a precursor to failure. This phenomenon occurs in many situations ranging from biaxial tests to embankments and retaining walls. As loading on a body of soil increases, there comes a point when the strain field switches from being homogeneous in character to being inhomogeneous. High strains become concentrated in narrow zones known as shear bands. Either side of these bands, the material behaves almost as if it were a rigid body. To model such problems numerically is challenging. AMR presents itself as a natural solution because it provides an automated way of locating smaller elements where the high gradients are, and coarser elements elsewhere.

The algorithm described here is a recovery-based method (also referred to as "smoothing"). Nodal values are recovered from integration point values using Superconvergent Patch Recovery (SPR) [2]. The nodal values form a smoothed solution with which the finite element solution can be compared. An error in the finite element solution is then calculated based on this difference. Often the error estimator is based on incremental energy, but here, it is based on the second invariant of the incremental deviatoric strain [3]

as this would seem better suited to the localization problems studied here.

Instead of regenerating the mesh, elements whose error is larger than the target error are subdivided. The refinement algorithm combines regular refinement (splitting a triangle into 4 by joining the midpoints of its edges) [4] with longest edge refinement (Rivara's method, which limits the mesh degradation) [5]. Elements which are marked for refinement are regularly refined. At this stage the mesh is non-conforming, so neighbours of the refined elements must also be refined in order to have a conforming mesh. For this, Rivara's longest edge refinement is employed.

The combination of an error estimator well suited to detect localization and a simple remeshing scheme based on subdivision is shown to result in a stable and robust algorithm.

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ADMOS 2013
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INEXACT-HESSIAN-VECTOR PRODUCTS FOR EFFICIENT REDUCED-SPACE PDE-CONSTRAINED OPTIMIZATION

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Key words: Adaptive Modeling, Simulation, PDE-constrained optimization

Abstract. Partial differential equation (PDE) constrained optimization problems can be posed in the full-space or the reduced-space. In full-space formulations the PDE state variables — e.g. pressure and velocity for incompressible flows — are included as optimization variables, and the PDE becomes an explicit constraint in the optimization. In contrast, reduced-space formulations treat the state variables as implicit functions of the design variables: for a given set of design variables the PDE is solved for the states.

In practice, engineers often prefer reduced-space formulations. Reduced-space methods lend themselves to modularity, so implementation is typically easier than full-space methods. Unfortunately, conventional reduced-space optimization algorithms exhibit poor algorithmic scaling. For example, the computational cost of quasi-Newton methods is often proportional to the number of design variables. This scaling limits the number of design variables that can be considered.

Motivated by the above observations, we consider reduced-space inexact-Newton-Krylov (INK) algorithms, which offer the potential for design-dimension-independent algorithmic scaling. One of the challenges with reduced-space INK methods for PDE-constrained optimization is the efficient computation of Hessian-vector products needed by the Krylov solver. In particular, it is believed that these products must computed with high accuracy to avoid convergence difficulties. This accuracy requirement can render reduced-space INK methods orders of magnitude more expensive than full-space methods. In this paper, we argue that the Hessian-vector products can be computed inexactly provided an appropriate Krylov solver is adopted. Numerical examples demonstrate that the resulting reduced-space INK algorithms are competitive with their full-space counterparts.

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ADMOS 2013
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ERROR ESTIMATION AND ADAPTIVITY FOR TURBULENT FLOW

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Key words: Adaptive finite element method, transient problem, turbulence

Abstract. We present recent advances on a posteriori error estimation and adaptivity for turbulent flow, including deforming domains, fluid-structure interaction and high performance computing implementation in the open source software Unicorn [1]. Fluid-structure interaction is formulated in a Unified Continuum framework [2], and turbulent fluid flow is modeled by G2 implicit large eddy simulation with residual based stabilization modeling the effect of subgrid scales, and with skin friction boundary conditions modeling turbulent boundary layers. Examples are presented, including applications to aerodynamics, aeroacoustics and biomedicine.

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EFFECT OF PRESTRESSED EMBOSSMENTS UNDER VARIOUS TYPES OF LOADING USING FEM ANALYSIS

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ABSTRACT

Composite slabs of trapezoidal steel sheeting and concrete are widely used for ceiling structures in all types of buildings. Prestressed embossments can serve as a meaning to ensure the composite action without need of other load bearing reinforcement. Design of the composite slab according to valid codes is governed by semi-empirical methods using bending tests to obtain unique parameters for each type of sheeting. Smaller and less expensive shear slip-block tests are considered as a meaning to obtain shear characteristics of the sheeting, which could be used for design of the sheeting.

In our laboratory bending tests with different load arrangements and shear test were performed. The key role in load bearing capacity of the slab has the shear connection between steel sheeting and concrete.

The FE (Finite Element) modelling of the connection must deal with a complicated geometry of the embossments and several possible failure mechanisms. Three types of numerical models are being created using Atena software. 2D and 3D models of shear test serves to describe the failure mechanism of embossments. Bending model of one rib over the whole span serves to include effects curvature due to bending. Influence of elevated temperature on shear bearing capacity is observed as well. The models are being set, calibrated and compared regarding data from the experiments performed in our laboratory.

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VI International Conference on Adaptive Modeling and Simulation
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IMPROVING NUMERICAL EFFICIENCY WITH MODEL REDUCTION AND HIGH-ORDER ADAPTIVE DISCONTINUOUS GALERKIN

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Abstract.
Despite the impressive progress attained in the last decades by simulation-based engineering sciences, decision-making in engineering design, optimization and control, remains sub-optimal in many fields. Aerospace industry is probably one area where these limitations are more obvious.
On one hand, in a multitude of real engineering design problems a large number of scenarios must be considered and carefully analyzed. This task is very expensive both in specialized man-hours to prepare and analyze data and from a computational point of view. The space of design parameters is, in these cases, too large for an exhaustive exploration. In general, only a small sample of the parametric space is studied. Consequently, these models must be complemented with security coefficients conceived to cover the rest of the parametric space and to include unknown information, the inevitable uncertainty. Thus, in practice, designs remain suboptimal because of the computational complexity related to very rich descriptions of external actions, geometry, materials, processes, etc. In fact, even for cutting edge engineering, real practice imposes methodologies devised more than 30 years ago.
On the other hand, two contradictory goals are nowadays present in every challenging simulation based engineering problem: real-time and high fidelity. In order to speed-up engineering design or to assist decision-making strategies in engineering processes, faster simulations are required. Moreover, in many cases, there is the added restriction: such decision-making tools should run in light computing devices to increase portability, on-site evaluation, or democratize accessibility. Real-time is easier to attain with coarse models or meta-models involving few number of parameters. These requirements usually are

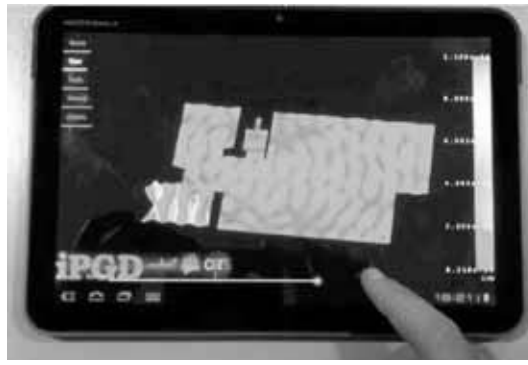
contradictory with high-fidelity simulations. Moreover, users are more demanding and prescribe error bounds on quantities of interest to minimize uncertainty in models and simulations.

These apparently incompatible goals can be integrated by means of a *computational vademecum*. A high-fidelity error-controlled off-line computation produces a solution of the model under consideration for all the possible design scenarios. Then, an on-line post-process, able to run on light computational devices if necessary, is used for fast decision-making purposes.

The Proper Generalized Decomposition (PGD), which relies in the assumption of separated approximations of the solution, has demonstrated its capabilities in dealing with high-dimensional problems. The multidimensional capabilities of this approach opens new possibilities to solve, for instance, problems where material or external parameters are set as additional extra-coordinates of the model. In this framework a general solution is obtained encompassing every solution for any possible value of the parameters, thus, a computational vademecum is produced. Under this rationale, parametric design, optimization of complex problems, uncertainty quantification, simulation-based control, and real-time simulation are seen as a post-process once the off-line strategy has produced the vademecum.

To illustrate the advantages of such an approach a simple shape optimization example will be shown before discussing a practical engineering problem governed by the Helmholtz equation with variable coefficients in an unbounded domain. This problem models harbor wave agitation, which is a primary engineering design challenge. Two major issues are discussed:

1. *Efficient and accurate computations*. This implies a large number of simulation challenges, which include, among others, reproducing the exact geometry to capture the small features that are influential, efficient adaptive approximations, precise high-gradients (shock-capturing) approximations, etc.
2. *Large number of external forcing conditions*. A general solution for the agitation in the harbor is obtained with the incident wavelength and its direction as extra coordinates covering an exhaustive evaluation of all possible scenarios and enabling on-line computations on tablets.



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ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

GEOMETRICALLY EXACT KIRCHHOFF-LOVE SHELL MODEL: THEORY AND MESHLESS IMPLEMENTATION

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Abstract. A geometrically exact shell model based on the Kirchhoff-Love theory, where shear deformation is not accounted for, has been developed in the present contribution. Energetically conjugated cross sectional stresses (first Piola-Kirchhoff tensor) and strains (deformation gradient) are defined. Elastic constitutive equations are consistently derived from fully three-dimensional finite strain constitutive models. A genuine plane-stress condition is enforced by vanishing the true mid-surface normal stress. Since only the bending deformation is included in this model no special technique has to be taken into account in order to avoid shear-locking.

Since the variational basis of the formulation requires the use of C1 approximations, the generation of compatible finite elements is not trivial in the present case. In order to overcome this inconvenience, meshless approximations are used. The first-order Generalized Moving-Least Squares Approximation has been proposed. Although it increases the number of degrees-of-freedom per node, its performance and quality of results are clearly superior to the conventional Moving-Least Squares Approximation in this specific class of problems.

Since the approximation does not possess the Kronecker-delta property, the essential boundary conditions are enforced using a hybrid-displacement version of the shell formulation, by means Lagrange multipliers. The corner reactions which naturally arise from the boundary integrals are carefully treated. This issue requires introduction of extra pointwise Lagrange multipliers. Its significant influence on the accuracy of results is demonstrated in some linear examples.

Imposition of the kinematic boundary conditions along the line also requires extra discussion. The proposed theory has no explicit expression for the boundary rotation angle arising on such boundaries and, moreover, this specific quantity may lead to nonsymmetric tangent matrix. Stitching domains along the line by means of Lagrange multipliers makes it possible to apply the proposed theory not only to smooth continuous shells but also to the folded ones.

Initially curved shells are regarded as a stress-free deformed state from a chosen plane reference configuration. The mapping between both configurations allows the exact consideration of the initial configuration.

The complete linearization of the weak form is presented. For hyperelastic materials,

conservative loadings and most cases of the kinematic boundary conditions the generalized stiffness matrix is symmetric even in points far from the generalized equilibrium positions. Nonconservative loads and some specific essential boundary conditions (as was mentioned above) lead to a nonsymmetric contribution to the resultant tangent stiffness. The latter is derived for several load types.

Results of numerical examples for both linear and nonlinear cases are presented, demonstrating the robustness and efficiency of the approach.

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ADMOS 2013
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FULLY SPACE-TIME METRIC BASED ANISOTROPIC MESH ADAPTATION FOR UNSTEADY PROBLEMS

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Key words: Anisotropic Mesh Adaptation, Adaptive Time-Stepping, 'Seek and Conquer' technique, Incompressible Flows, High Reynolds number, Variational MultiScale Method.

Abstract. This talk focuses on the development of a new fully space-time adaptive meshing algorithm applied to unsteady problems. We start by introducing the anisotropic mesh adaptation. The latter is developed using a posteriori estimates relying on the length distribution tensor approach and the associated edge based error analysis. Then we extend the mesh adaptation technique to contain adaptive time advancing based on a newly developed time error estimator that intends to homogenize the global error over space and time. The main feature of this work is the development of a seek and conquer method that provides optimal space and time meshes that hold for several simulation time subintervals. The advantage of the proposed method relies in its conceptual and computational simplicity as it only requires from the user a number of nodes according to which the mesh and the time-steps are automatically adapted. The objective of this talk is to show that the combination of time and space anisotropic adaptations with highly stretched elements can be used to accurately reproduce high Reynolds number flows within reasonable computational and storage costs. In particular, it will be shown in the numerical experiments that boundary layers, flow detachments and all vortices are well captured automatically by the mesh. The time-step is controlled by the interpolation error and preserves the accuracy of the mesh adapted solution. A Variational MultiScale (VMS) method is employed for the discretization of the Navier-Stokes equations. Numerical solutions of some 2D and 3D time-dependent benchmark problems demonstrate the accuracy and efficiency of the proposed space-time error estimator.

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ADMOS 2013
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A POSTERIORI ERROR ESTIMATION OF TARGET CONTROL PROBLEMS: WEAK FORMULATION OF INEQUALITY CONSTRAINTS

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Key words: optimal control, dynamic system, a posteriori error estimation

Abstract. We shall in this contribution consider optimal control problems concerning the steering of motion of a mechanical system from an initial state to a target state (target or trajectory control). The motion of the system depends on forces acting as controls and is represented by a set of ordinary differential equations with load terms. By considering the equations of motion and the relevant kinematic and kinetic limitations, a constrained optimization problem can be formulated where the control forces are sought to minimize a chosen objective function, such as the energy consumption.

A discretization of finite element type in time is introduced, whereby approximations for the state (coordinates and velocities) and the control (external forces) variables are introduced. The optimality conditions are expressed in weak form, in particular, the inequality constraints are enforced weakly, whereby to what extent the inequality constraints are satisfied depend on the chosen discretization. The subject of the present work is to determine the error in the approximate solution compared to the exact solution, in particular with respect to how well the discrete solution satisfies inequality constraints and target conditions.

To this end, we employ a posteriori error estimates based on the pertinent dual problem (from linearization of the weak form) with some modification, whereby discretization errors in both state and control variables can be estimated in terms of chosen goal quantities. The sources of errors can be traced to specific regions of the state and control time-meshes, which can be used in an adaptive mesh-refinement procedure since the control and state variables are discretized separately.

Earlier work on a posteriori error estimation for optimal control problems have been based on the "Heidelberg" approach[1, 3], whereas the present contribution will use our previous work in error control for parameter identification problems based on a tangent form of the dual problem [2]. Numerical examples indicate that a discretization error in the control variable arises in order to "compensate" for discretization errors in the solution of the equations of motion.

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ONLINE GREEDY REDUCED BASIS CONSTRUCTION USING DICTIONARIES

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Key words: Greedy algorithms, reduced basis methods, model order reduction, dictionary

Abstract. As numerical simulations find more and more use in real-world scenarios and industrial applications, demands concerning efficiency and reliability increase as well. Especially scenarios that call for real-time simulations or multi-query evaluations of partial differential equations (PDEs) often require means of model order reduction. Examples for such scenarios are optimal control and optimization settings.

The Reduced Basis (RB) method [7] provides model order reduction for a special class of PDEs, so-called parameterized partial differential equations (PPDEs), (in the weak and discretized form) given as

$$B_h(u_h(\boldsymbol{\mu}), v_h; \boldsymbol{\mu}) = L_h(v_h; \boldsymbol{\mu}) \quad \forall v_h \in X_h, \tag{1}$$

for $u_h(\boldsymbol{\mu}) \in X_h$, a parameter vector $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ and a suitable given discrete function space X_h. Here, $B_h : X_h \times X_h \times \mathcal{P} \to \mathbb{R}$ denotes a given parameterized bilinear form and $L_h : X_h \times \mathcal{P} \to \mathbb{R}$ denotes a given parameterized linear form. The RB method provides model order reduction for this class of PDEs by splitting all computations in two parts: The first part is a possibly time-consuming so-called *offline phase* that comprises all computations involving the grid width of the discretization. The second part is a usually very rapid *online phase* that performs computations only on a reduced system.

While the RB method has been applied successfully to elliptic [7], parabolic [5] and hyperbolic [4] equations and systems, efforts had to be made to apply them to problems with strong sensitivity with respect to the parameter $\boldsymbol{\mu}$. These efforts comprise the hp-method [3] where the parameter space $\mathcal{P}$ is adaptively split and multiple reduced bases are built. While this approach is very efficient during the online phase, it suffers from very high demands concerning runtime and storage during the offline phase.

In our contribution, we will introduce a new approach to the aforementioned problem that holds some similarity with the local greedy method introduced in [6]. Our method

constructs a huge "dictionary" of potential basis vectors during the offline phase. During the online phase, a small, parameter-dependent basis is constructed using a Greedy technique. By exploiting a posteriori error estimation for the basis construction during the online phase, we obtain optimal bases regarding basis size. We present different possible algorithms both for offline dictionary and online basis construction and present theoretical and numerical complexity studies. Furthermore, we present numerical investigations of our approach regarding final basis size, approximation quality and online runtime and a comparison to standard RB methods.

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QUANTIFYING THE COMPUTABILITY OF THE LORENZ SYSTEM USING A POSTERIORI ANALYSIS

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Abstract. It is well known that the computation of accurate trajectories of the Lorenz system is a difficult problem. Computed solutions are very sensitive to the discretization error determined by the time step size and polynomial order of the method, as well as round-off errors.

In this work, we show how round-off errors limit the computability of the Lorenz system and quantify exactly the length of intervals over which solutions can be computed, expressed in terms of the floating point precision. Using adjoint-based a posteriori error analysis techniques, we estimate the stability of computations with respect to initial data, discretization, and round-off errors, respectively.

The analysis is verified by computing accurate solution on the time interval [0, 1000] using a very high order (order 200) finite element method and very high floating point precision (400 digits).

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DAMAGE DETECTION THROUGH WAVELET TRANSFORM AND INVERSE ANALYSIS

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Key words: Wavelet Transformation, Inverse Analysis, Damage Detection

Abstract. Methods of damage detection are expected to provide information whether damage exists or not. This work is concerned with methods to identify damage based on measurement of structural response to the actual actions or actions specially planned and applied to the existing defected structure. If the response of the existing structure is compared to the response of its computer model which contain parameters characterizing the expected defects. Different kind of responses can be monitored, namely displacements, velocities or accelerations, to construct the discrepancy function. Through the minimization of the differences between measurable quantities: (a) computed by the numerical model, and, (b) recorded on the existing damaged structure, the information on the defects can be assessed. Recently alternative approaches have been developed, in which the time-consuming optimization procedures can be avoided. In these approaches data processing techniques are applied only to the response signal of the existing defective structure. This group of techniques includes special methods of artificial intelligence or stochastic programming combined to signal processing techniques, e.g. Wavelet Transform (WT), in continuous form (CWT) or discrete (DWT).

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ADMOS 2013
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A VARIATIONAL MULTISCALE APPROACH FOR ERROR ESTIMATION IN ADAPTIVE ISOGEOMETRIC ANALYSIS

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Key words: Isogeometric analysis, NURBS, A posteriori error estimation, Fluid dynamics, Variational multiscale method, Adapted methods.

Abstract. In this work, we present an explicit a-posteriori error estimator in isogeometric analysis for fluid dynamics problem like advection-diffusion equations. The technique is based on the theortical framework of the variational multiscale (VMS) method [1] and recently derived explicit formula of the fine-scale Green's function [2]. This technique is adequate for the methods with a local error distribution, such as stabilized methods, where the element local problem captures most of the error and the proposed error intrinsic parameter is an approximation to the solution of the dual problem. The proposed technique can be implemented straightforwardly in existing codes and is computationally efficient. We consider different test examples to show the robustness and effectivitness of this technique as a posteriori error estimator in isogeometric analysis.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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A posteriori error estimation in adaptive isogeometric analysis

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Key words: Isogeometric analysis, LR B-splines, posteriori error estimators, adaptive methods.

ABSTRACT

Reliability and efficiency are two major challenges in simulation based engineering. These two challenges may be addressed by error estimation combined with adaptive refinements. A lot of research has been performed on error estimation and adaptive mesh refinement. However, adaptive methods are not yet an industrial tool, partly because the need for a link to traditional CAD-system makes this difficult in industrial practice. Here, the use of an isogeometric analysis framework introduced by Professor Thomas J. R. Hughes (UT at Austin) and coworkers [1] may facilitate more widespread adoption of this technology in industry, as adaptive mesh refinement does not require any further communication with the CAD system.

A posteriori error estimation in numerical approximation of partial differential equations aims at:

- give an upper bound on the error of numerical solution, if possible give a guaranteed upper bound;
- estimate the error locally and assure that this represents a lower bound for the actual error, up to a multiplicative constant (i.e. efficiency);
- assure that the ratio of the estimated error and actual error goes to one, i.e., asymptotic exactness.

Three main techniques of a posteriori estimates in the finite element method have evolved during the last decades; *(i)* Explicit residual-based estimators *(ii)* Implicit residual based estimators and *(iii)* Recovery based estimators, see Ainsworth and Oden [2] . The purpose of this project is to extend these posteriori techniques in adaptive isogeometric analysis framework for elliptic problems. We also discussed the above three properties for our developed posteriori error estimators. The adaptive refinement is achieved using local refinement strategies developed in Johannessen *et al*. [3]. The developed a posteriori based adaptive refinement methodology will be tested on some classical benchmark elliptic problems.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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VERIFICATION AND VALIDATION FOR THE LARGE EDDY SIMULATION OF INCOMPRESSIBLE TURBULENT FLOWS WITH FENICS

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Abstract. We describe a framework for verification and validation in the frame of the development of turbulence models for the Large Eddy Simulation of incompressible flows, by means of residual-based subgrid stabilisation.
The main components consist of a posteriori error estimation of the numerical error, uncertainty quantification of data and modeling errors, and systematic verification of the software implementation in FEniCS (www.fenicsproject.org) by manufactured solutions.
We introduce the different components, and present the combined framework in a number of examples .

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ADMOS 2013
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REDUCED ORDER MULTISCALE FINITE ELEMENT METHODS BASED ON COMPONENT MODE SYNTHESIS

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Key words: Multiscale method, model reduction, a posterior error estimate

Abstract. We present a reduced order finite element method based on the variational multiscale method together with a component mode synthesis representation for the fine scale part of the solution. We derive an a posteriori error estimate in the energy norm for the discrete error in the approximation which measures the error associated with model reduction in the fine scale.

1 INTRODUCTION

In this contribution we briefly describe a recent multiscale finite element method, introduced in [6], which builds on using a reduced order model for the fine scale in a variational multiscale method, see [2] and the later developments [5].

Model reduction methods are commonly used to decrease the computational cost associated with simulations involving repeated use of large scale finite element models of for instance a complicated structure. The objective in model reduction is to find a low dimensional subspace of the finite element function space that still captures the structural behavior sufficiently well. A classical model reduction method is component mode synthesis (CMS), see [3].

In CMS the computational domain is split into subdomains and a reduced basis associated with the subdomain is constructed by solving localized constrained eigenvalue problems associated with the subdomains together with modes that represent the displacements of the interface between the subdomains, as in the Craig-Bampton method [1].

Here we construct a multiscale finite element method where the coarse scale is represented by piecewise linear continuous elements on a coarse mesh and the fine scale is defined by a CMS related approach on a refined mesh, using the coarse mesh elements as subdomains in the CMS method. The coupling modes are computed for each pair of

neighboring elements and couple the response in the subdomains. Thus the fine scale is finally represented as a direct sum of functions with support in each element and functions associated with each edge supported in the two elements neighboring the edge. Adaptive reduction is accomplished by choosing a basis in each such subspace consisting of a truncated sequence of eigenmodes. The eigenmodes are numerically computed and capture fine scale effects.

We derive an a posteriori error estimate for the multiscale finite element method that can be used to automatically tune the number of subscale modes in an adaptive algorithm. For further details we refer to [6] and the previous work on a posteriori error estimates for component mode synthesis [4].

2 LINEAR ELASTICITY

The equations of linear elasticity take the form: find displacements $\boldsymbol{u}$ such that

$$-\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}) + \tau \boldsymbol{u} = \boldsymbol{f}, \qquad \boldsymbol{x} \in \Omega, \tag{1a}$$

$$\boldsymbol{\sigma}(\boldsymbol{u}) = 2\mu\boldsymbol{\varepsilon}(\boldsymbol{u}) + \lambda(\nabla \cdot \boldsymbol{u})\boldsymbol{I}, \quad \boldsymbol{x} \in \Omega, \tag{1b}$$

$$\boldsymbol{u} = \boldsymbol{0}, \qquad \boldsymbol{x} \in \Gamma_D, \tag{1c}$$

$$\boldsymbol{n} \cdot \boldsymbol{\sigma}(\boldsymbol{u}) = \boldsymbol{g}_N, \qquad \boldsymbol{x} \in \Gamma_N, \tag{1d}$$

where $\tau \geq 0$ is a real parameter, $\boldsymbol{f}$ is a body force, $\boldsymbol{g}_N$ is a traction force, $\boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$ is the linear strain tensor, $\boldsymbol{\sigma}$ the stress tensor, $\boldsymbol{I}$ is the $d \times d$ identity matrix, and λ and μ are the Lamé parameters given by $\lambda = E\nu[(1+\nu)(1-2\nu)]^{-1}$ and $\mu = E[2(1+\nu)]^{-1}$, where E and ν is Young's modulus and Poisson's ratio respectively. The coefficients can have multiscale behavior, i.e. exhibit variation on a very fine scale or on multiple scales.

The corresponding variational form of (1) reads: find $\boldsymbol{u} \in V = \{\boldsymbol{v} \in [H^1(\Omega)]^d : \boldsymbol{v}|_{\Gamma_D} = \boldsymbol{0}\}$ such that

$$A(\boldsymbol{u}, \boldsymbol{v}) = b(\boldsymbol{v}), \quad \forall \boldsymbol{v} \in V, \tag{2}$$

where $A(\cdot, \cdot)$ is the bilinear form

$$A(\boldsymbol{v}, \boldsymbol{w}) = a(\boldsymbol{v}, \boldsymbol{w}) + \tau(\boldsymbol{v}, \boldsymbol{w}) \tag{3}$$

with

$$a(\boldsymbol{v}, \boldsymbol{v}) = 2(\mu\boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{\varepsilon}(\boldsymbol{w})) + (\kappa\nabla \cdot \boldsymbol{v}, \nabla \cdot \boldsymbol{w}), \tag{4}$$

and $b(\cdot)$ is the linear form

$$b(\boldsymbol{v}) = (\boldsymbol{f}, \boldsymbol{v}) + (\boldsymbol{g}_N, \boldsymbol{v})_{\Gamma_N}. \tag{5}$$

3 MULTISCALE METHOD

Let $\mathcal{T}^H$ be a coarse mesh on Ω consisting of shape regular triangles ($d = 2$) or tetrahedra ($d = 3$) and let $\mathcal{T}^h$ be a fine mesh obtained by a sequence of uniform refinements of $\mathcal{T}^H$. Let $V^H \subset V^h$ be the corresponding spaces of continuous piecewise linear element.

We then have the following splitting

$$V^h = V^H \oplus \left(\bigoplus_{E \in \mathcal{E}^H} V_E^h \right) \oplus \left(\bigoplus_{T \in \mathcal{T}^H} V_T^h \right) \tag{6}$$

Here $V_T^h \subset V^h$ is the space of functions with support in element $T \in \mathcal{T}^H$, $\mathcal{E}^H$ is the set of edges in the coarse mesh $\mathcal{T}^H$, and if the edge E is shared by elements T_1 and T_2 in $\mathcal{T}^H$ then the edge space V_E^h is defined by

$$V_E^h = \{ v \in V^h \, : \, \text{supp}(v) \subset T_1 \cup T_2, a(v, w) = 0 \; \forall w \in V_{T_1}^h \oplus V_{T_2}^h \} \tag{7}$$

To construct a basis in these subspaces we solve the following eigenvalue problems.

Basis in V_T^h: Find $(\boldsymbol{Z}, \Lambda) \in V_T^h \times \mathbb{R}^+$, such that

$$a(\boldsymbol{Z}, \boldsymbol{v}) = \Lambda(\boldsymbol{Z}, \boldsymbol{v}), \quad \forall \boldsymbol{v} \in V_T^h \tag{8}$$

Using modal truncation we obtain a reduced subspace $V_T^{h,m_T} \subset V_T^h$, defined by

$$V_T^{h,m_T} = \text{span}\{\boldsymbol{Z}_i\}_{i=1}^{m_T}, \tag{9}$$

where $m_T \ll \dim(V_T^h)$.

Basis in V_E^h: Find $(\boldsymbol{Z}, \Lambda) \in V_E^h \times \mathbb{R}^+$, such that

$$a(\boldsymbol{Z}, \boldsymbol{v}) = \Lambda(\boldsymbol{Z}, \boldsymbol{v}), \quad \forall \boldsymbol{v} \in V_E^h \tag{10}$$

Using modal truncation we obtain a reduced subspace $V_E^{h,m_E} \subset V_E^h$, defined by

$$V_E^{h,m_E} = \text{span}\{\boldsymbol{Z}_i\}_{i=1}^{m_E}, \tag{11}$$

where $m_E \ll \dim(V_E^h)$.

Finally, we arrive at the reduced order space

$$V^{h,\boldsymbol{m}} = V^H \oplus \left(\bigoplus_{E \in \mathcal{E}^H} V_E^{h,m_E} \right) \oplus \left(\bigoplus_{T \in \mathcal{T}^H} V_T^{h,m_T} \right) \tag{12}$$

where $\boldsymbol{m} = (\cup_{E \in \mathcal{E}^H} m_E) \cup (\cup_{T \in \mathcal{T}^H} m_T)$ is the multiindex containing the indices m_E and m_T for alla edges and elements.

The multiscale method is then simply obtained by using this reduced order space in the standard variational formulation: find $v \in V^{h,\boldsymbol{m}}$ such that

$$A(\boldsymbol{U}^{\boldsymbol{m}}, \boldsymbol{v}) = b(\boldsymbol{v}), \quad \forall \boldsymbol{v} \in V^{h,\boldsymbol{m}}, \tag{13}$$

4 A POSTERIORI ERROR ESTIMATE

Let $|||\cdot|||$ denote the energy norm, $|||v|||^2 = A(v,v)$ and let $\boldsymbol{U}^h$ denote the standard finite element solution in V^h. Then we have the following a posteriori error estimate

$$|||\boldsymbol{U}^h - \boldsymbol{U}^{\boldsymbol{m}}||| \leq \left(\sum_{E \in \mathcal{E}} \frac{\|\boldsymbol{R}_E(\boldsymbol{U})\|^2}{\Lambda_{E,m_E+1}} + \sum_{T \in \mathcal{T}} \frac{\|\boldsymbol{R}_T(\boldsymbol{U})\|^2}{\Lambda_{T,m_T+1}} \right)^{1/2}. \tag{14}$$

Here the subspace residual $\boldsymbol{R}_I(\boldsymbol{w}) \in V_I^h$, $I \in \mathcal{E}^H \cup \mathcal{T}^H$, is defined by

$$(\boldsymbol{R}_I(\boldsymbol{w}), \boldsymbol{v}) = b(\boldsymbol{v}) - A(\boldsymbol{w}, \boldsymbol{v}), \quad \forall \boldsymbol{v} \in V_I^h, \quad I \in \mathcal{E}^H \cup \mathcal{T}^H \tag{15}$$

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

GOAL-ORIENTED ERROR CONTROL FOR THE QUASI CONTINUUM METHOD

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Key words: Goal-oriented adaptivity, atomistic-to-continuum, Quasi-Continuum

Abstract. In order to consider virtual materials (not physically manufactured) or in order to predict complex behavior on one length scale where the physics is better understood on a lower scale, homogenization (or coarse-graining) can be a useful tool. Considering atomistic systems, homogenization can be used to derive continuum properties whereby the need for empirical continuum models i avoided. When there is a large separation of scales, i.e. when the length scales of the sought continuum solution by far exceeds the atomistic length scale, computational homogenization can be adopted, see e.g. [1]. Using this approach, the continuum stress-strain response can be obtained implicitly by considering a representative volume element (RVE), also called representative lattice unit in the case of a homogenization of a discrete lattice. However, when considering atomistic systems, it is well known that defects play an important role. When investigating the influence from single (or a few) defects, very large RVE's need be considered.

In the case of scale-mixing, i.e. when the continuum scale and the atomistic scale needs be resolved concurrently in the spatial domain, one popular method is the Quasi-Continuum (QC) method, cf. [2, 3]. It allows for coarse graining of atomistic response in terms of interpolation on a "finite-element-type" mesh. The QC method is an approximation of the atomistic problem, rather than a homogenization technique.

In this contribution we establish the RVE for carrying out atomistic-to-continuum homogenization of a molecular statics problem. In particular, we are interested in computing the representative response for different imperfections in a lattice. To this end, we wish to consider relatively large lattices on the atomistic scale. In order to facilitate such an analysis, we proceed along the lines of, e.g., [4] and device a goal-oriented adaptive QC procedure for solving the atomistic problem on the RVE. Within the goal-oriented framework it becomes natural to consider the macro scale (continuum) stress as the goal-quantity that is solved for.

The QC method is introduced in two steps. First, we consider the restriction of atom displacement in terms of the representative atoms as a model reduction, i.e., we describe the positions of all atoms in terms of discrete weights and the placements of certain so-called representative atoms. Based on this approximation, while accounting for the exact summation of all the bond-energies, we are able to compute goal-oriented error estimators in a straight-forward fashion based on an adjoint (dual) problem pertaining to the chosen output of interest. This computable error estimator pertains to a discretization error in the finite element method. The second step in the QC method is that of quadrature. For large QC elements, i.e. for a large amount of atoms whose placements are governed by the same representative atoms, the bond energy and its derivatives are typically computed using an appropriate discrete quadrature. We show how this approximation generates a quadrature error (in addition to the discretization error) in the framework for error estimation presented above. The combined error is estimated approximately based on the same dual problem in conjunction with a hierarchical strategy for approximating the residual.

As a model problem, we consider a mono-layer of graphene. The homogenization of the macro-scale membrane forces, including initial relaxation, is considered for defective graphene lattices. The 0 Kelvin condition is considered by omitting lattice vibration and the Carbon-Carbon energy bonds are modeled via the Tersoff-Brenner potential, cf. [5], which involves next-nearest neighbor couplings. In particular, we study the accuracy and robustness of the proposed error estimator and the pertinent adaptive algorithm.

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AN IMPRINTING ALGORITHM TO INSERT GEOMETRIC DETAILS INTO HEXAHEDRAL MESHES

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Key words: Parametric studies in Numerical Simulation, Hexahedral Meshes, Adaptive model, Sheet operations, Mesh Imprint

Abstract. In numerous computational engineering applications, such as automobile crash simulations, structural mechanics, neutronics or fluid-structure interactions, hexahedral meshes may be preferred over tetrahedral meshes. Unhappily, the generation of hexahedral meshes is known as a time-consuming stage in the simulation process. Indeed, unlike the generation of tetrahedral meshes, there does not exist any algorithm allowing to automatically generate an hexahedral mesh for any geometric domain. Semi-automatic approaches with a lot of user interactions are then often necessary.

The classical process for designing and optimizing a geometric shape requires parametric studies where the shape is modified and/or enriched by adding geometric details one per one. We have then to "adapt" the initial mesh and not to regenerate it for each new detail taken into account.

In order to perform such studies with hexahedral meshes, we propose an imprinting method allowing us to automatically add geometric details into an existing mesh. This addition is done using geometric projections, sheets (layers of hexahedral elements) insertions and combinatorial algorithms while preserving the hexahedral mesh structure as best as possible. This algorithm can be seen as an extended overlay-grid approach where the grid is replaced by any type of unstructured hexahedral mesh.

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ADMOS 2013
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IMPROVEMENT IN PERFORMANCE PARAMETERS BY SHAPE OPTIMIZATION OF A CONICAL FLOW AROUND DIFFUSER

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Key words: Optimization, Conical Flow Around Diffuser, 3D Flow, Performance Parameter, Turbulence Model

Abstract. Diffusers are mounted downstream of turbine runners, converting the remaining kinetic energy into pressure by decelerating the flow which leads to an increasing efficiency in turn. The flow rate of the medium passing through the turbine is influenced by the diffusers geometry, so geometrical restrictions must be observed to avoid adverse flow phenomena. Those ones even affect the operation negatively and cause pressure fluctuations that might crack the construction, if resistance tolerances are exceeded.
Therefore, this paper aims to develop a fully automated shape design optimization of a 3D conical flow around diffuser with fixed main dimensions surrounded by turbulent incompressible flow. The optimization process is based on *OpenFOAM-1.6-ext* in combination with a metamodel assisted evolutionary algorithm (*MAEA*) [1, 2], implemented in the optimizer *EASY* [3].

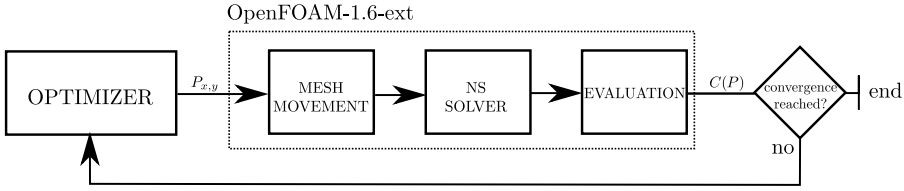

Figure 1: Simplified optimization process: After passing the costfunction obtained by the computation back to the optimizer, new x, y coordinates of all control points P are forwarded to the mesh deformation solver

For the parametrized boundary mesh movement a mesh motion solver based on Laplacian smoothing is applied. A variable diffusivity is prescribed during deformation to keep

the distortions in the boundary region low. The simplified optimization process is given in Fig **??**.

Focusing on typical inflow conditions obtained at the runner outlet of a hydrokinetic turbine, flow behavior in the diffuser are carried out and integral performance parameters of the diffuser are evaluated in order to draw conclusions about the diffusers efficiency. During optimization, typical cost functions are considered, describing the corresponding operation of the diffuser. Since the investigated diffuser is mounted in a free surface flow, the hydrostatic pressure is taken into account as well. The inner and outer contours of the conical flow around diffuser wall are each independently parameterized with a smooth *Bézier*-Spline of 4^{th}-order. The effect of a shock diffuser mounted downstream on the flow behavior and performance parameters as well are carried out. On the one hand, its contour is parametrized with a polynomial of 2^{nd}-order initiating a discontinuous transition, as can be seen in Fig. **??**(bottom). On the other hand, the contour is defined by a *Bézier*-Spline of 4^{th}-order causing smooth contour shapes, see Fig. **??**(top). In order to capture the fairly strong curved swirling flow, a modified k-ω-SST model with streamline-curvature correction [4] is applied, which is validated by comparison with data from [5]. By varying the Reynolds- and the Swirl-Number at the diffuser inlet, different wall shapes are obtained as a function of the specific flow quantities. Results are additionally compared with commercial code.

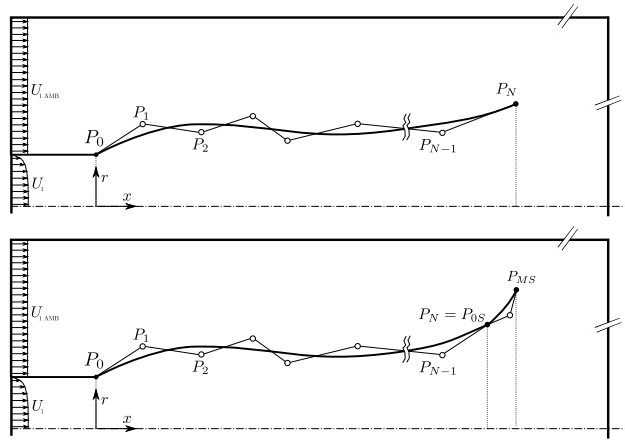

Figure 2: Interior Diffuser boundary with a *Bézier*-Spline Parametrization of N-order (top) or with an additional *Bézier*-Spline Parametrization of M-order for considering an installed shock diffuser (bottom); (dashed) evaluation plane

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A SIMPLE RECOVERY BASED ERROR ESTIMATOR FOR THE GFEM INCLUDING BLENDING

R. LINS, S. PROENÇA

Abstract. The generalized finite element method (GFEM) allows setting good conditions of local approximations by means of enrichments functions with special features. One major advantage of this method is the mesh independence for crack simulations. Moreover, the strong gradients typical of linear elastic fracture mechanics problems can be faced by customized enrichments. In spite of the good performance presented by the method on several numerical simulations it is very important to assess error estimates from the obtained results. In this context, a new a posteriori error estimator for the generalized finite element method is hereby considered aiming mainly to guarantee the more accurate and reliable stress distribution. A secondary aim is to employ the error estimates as indicator in hp-adaptive strategies. The proposed estimator is then based on the superconvergent patch recovery (SPR) technique, a widely used technique for evaluating recovered stress fields from the conventional finite element solutions. The GFEM-SPR procedure explores the clouds and partition of unity concepts to obtain recovered stress fields from interpolation polynomials. Such functions are identified using the singular value decomposition (SVD) strategy over superconvergent point values defined in each cloud in coincidence with the quadrature integration points. A particular issue that appears when enrichment is imposed over a localized region of the solid domain is related to the so called blending elements. Such elements blend nodes with and without enrichment, however presenting lack of partition of unity property and, hence, also losing the reprodutibility feature. Thus, the accuracy and convergence ratio of the GFEM can be affected. In this paper a modification in the standard GFEM proposed in literature to properly account for blending elements is adopted and the error estimator is also improved. Some benchmarks problems discretized by two-dimensional triangular and quadrilateral element meshes are presented in order to assess the efficiency and computational performance of the procedure hereby proposed. The energy norms of the recovered solutions, as well the effectivity index of the estimator are presented by comparing numerical and analytic solutions when available.

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FROM SEGMENTED MEDICAL IMAGES TO SURFACE AND VOLUME MESHES, USING EXISTING TOOLS AND ALGORITHMS

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Key words: Surface and Volume Meshing, Segmented Images, Finite Element Method.

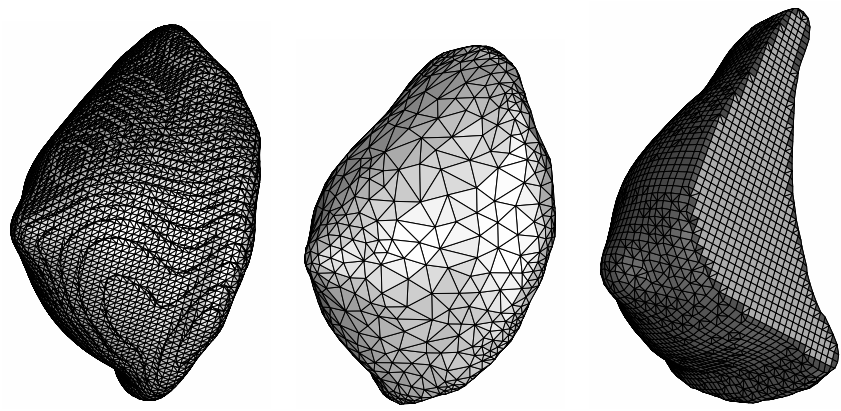
Abstract. In a medical context, one of the most used techniques to produce an initial mesh (starting from segmented medical images) is the Marching Cubes (MC) introduced by Lorensen and Cline in [1]. Unfortunately, the MC presents several issues in the meshing context. These problems can be summarized in three types: topological (presence of holes), of quality (sharp triangles) and accuracy in the representation of the target domain (the staircase effect). Even though there are several solutions to overcome topological and quality issues, the staircase effect remains as a challenging problem.

In the other hand, the Computational Geometry Algorithms Library (CGAL) [2], has implemented the *Poisson Surface Reconstruction* algorithm introduced in [3], which is capable of producing accurate and high quality triangulations based on a point set and its normal directions.

This paper shows how surface meshes can be produced using both, MC and CGAL. Moreover, once a high quality surface mesh is produced, this work also shows how volume meshes can be produced. In particular, tetrahedral and mixed–element meshing techniques are presented to produce a simulation with the Finite Element Method.

Most of the presented tools are open source or easy to implement meshing algorithms, hence, this work presents a complete process to produce surface and volume meshes, starting from segmented medical images, with accessible tools.

In order to illustrate the above, Figure 1 shows the resulting meshes for MC (Figure 1(a)), a surface mesh using CGAL (Figure 1(b)), and a volume mesh using a mixed–element technique (Figure 1(c)) for the breast.



(a) (b) (c)

Figure 1: Meshing the breast: (a) Marching Cubes, (b) Surface mesh using CGAL and (c) Volume mesh (with a cut to see internal elements) using mixed–elements.

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ADAPTIVE LIMIT ANALYSIS USING DEVIATORIC FIELDS

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Key words: Limit Analysis, Finite Elements, Error Estimation, Adaptive Remeshing

Abstract. Accurate estimates of limit loads for difficult stability problems in geotechnical engineering can rarely be obtained from a single finite element limit analysis without using an excessive number of elements. Therefore, efficient adaptive strategies which maximize the solution accuracy using minimum number of elements in the mesh are of great interest. The key to obtaining accurate solutions lies in accurately capturing the areas of plasticity within the problem domain, as their pattern and intensity characterize the solution. Several approaches have been practiced so far including those based on plastic multipliers, strain and power dissipation fields employed as control variables. All these schemes work quite well for cohesive or cohesive-frictional materials, but for purely frictional soils their performance stalls as e.g. plastic multipliers have substantially high values for all zero stress points on the surface of soil domain, therefore cannot indicate reliably plastic areas. Similar conclusion can be made about performance of schemes based on power dissipation or strain rates. This study explores the possibility of using the internal dissipation calculated from deviatoric stresses and strain rates as suitable control field for purely frictional materials. The performance observed for considered set of problematic for other adaptive schemes geotechnical examples is very promising. Moreover, the proposed approach works very well also for cohesive and cohesive frictional materials, suggesting its use as general engine for adaptive mesh refinement.

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FE ADAPTIVE ANALYSIS OF MULTI-REGIONS MODELS

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Key words: 3D Adaptive Analysis, Finite Element Method, Mesh Generation, Multi-regions.

Abstract. This work presents a methodology for adaptive generation of 3D finite element meshes using geometric modeling with multi-regions and parametric surfaces, considering a geometric model described by curves, surfaces, and volumes. The adaptive strategy adopted in this methodology is based on independent refinements of these entities. From an initial model, new sizes of elements obtained from numerical error analysis and from geometric restrictions are stored in a global background structure, a recursive spatial composition represented by an octree. Based on this background structure, the model curves are initially refined using a binary partition algorithm. The discretization of curves is then used as input for the refinement of adjacent surfaces. The surface discretization also employs the background octree-based refinement, which is coupled to an advancing front technique for the generation of an unstructured triangulation. Surface meshes are finally used as input for the refinement of adjacent volumetric domains. In all stages of the adaptive strategy, the refinement of curves, surface meshes, and solid meshes is based on estimated numerical errors associated with the mesh of the previous step in the adaptive process. In addition, curve and surface refinement takes into account curvature information. An example is presented in order to validate the methodology proposed in this work.

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ON THE KINEMATIC STABILITY OF HYBRID EQUILIBRIUM TETRAHEDRAL MODELS

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Key words: Equilibrium models, tetrahedral elements, kinematic stability.

Summary. *This paper is concerned with establishing the nature of the kinematic instabilities that arise in tetrahedral hybrid equilibrium models when the elements are formulated with polynomial approximation functions of a general degree. The instabilities are due to the spurious kinematic (or zero energy) modes, and these modes are first derived for a single element. The paper continues by identifying those spurious modes that can be propagated from one element to another via an interface. It is shown that at least three such modes exist for all degrees.*

1 INTRODUCTION

Hybrid equilibrium elements have been used to generate dual analyses for error estimation of conforming models[1]. Dual analyses may involve reanalysis of a complete mesh, or may involve local analyses of star patches[2]. In any event it becomes important to know whether spurious kinematic modes associated with hybrid equilibrium models may exist, and if so, whether they will affect the dual analyses. These questions have been studied for plate elements[3-5]. In this paper, we investigate the form taken by spurious kinematic modes for a single tetrahedral element of general polynomial degree, and consider the propagation of these modes between a pair of adjacent elements of the same degree. The results of this investigation should help to determine the general kinematic stability of patches of tetrahedral elements[6,7], thereby setting the basis for robust implementations of these approaches. The definition of spurious modes associated with an edge and an interface of an element exploit an orthogonal basis of polynomials for a triangular face[8] that are expressed in terms of area coordinates. These enable the spurious modes to be generated in a hierarchical fashion which takes advantage of cyclic symmetry.

2 GENERAL FEATURES OF SPURIOUS KINEMATIC MODES OF TETRAHEDRA

Spurious kinematic modes refer to boundary displacements that have the nature of pseudo-mechanisms and cause no internal stress. They do zero work with admissible boundary tractions, which are those that equilibrate with internal stress fields. Displacements of a face of a tetrahedron are described by complete polynomials of degree *d*, and this implies that the dimensions of the spaces of displacements and rigid body modes for an element are defined in Equation (1). Internal stress fields are described by polynomials of the same degree, and complete within the constraints set by equilibrating with zero body forces. In this case the dimensions of the stress and hyperstatic stress spaces are given by[9] Equation (2).

$$n_v = 4\times3\times0.5(d+1)(d+2);\ n_{rbm} = 6 \tag{1}$$

$$n_s = 0.5(d+1)(d+2)(d+6);\ n_{hyp} = 0.2(d-3)(d-2)(d+2) \text{ for } d > 2 \tag{2}$$

and then the number of independent spurious kinematic modes is given by Equation (3).

$$n_{skm} = (n_v - n_{rbm}) - (n_s - n_{hyp}) = 6(d+1) \text{ for } d > 2\,. \tag{3}$$

When $d \leq 2$, the element is isostatic and then:

$$n_{skm} = 0.5(d+1)(d+2)(6-d) - n_{rbm}\,. \tag{4}$$

Tractions applied to the boundary are considered as belonging to a space dual to that of displacements. Admisible tractions are those that equilibrate with an internal stress field, and the necessary and sufficient conditions for admissibility correspond to the need for complementary shear stresses along an edge of a tetrahedral element. With reference to Figure 1, the complementary shear stress condition along edge 3-4 has the form in Equation (5).

$$\sin\varphi\cdot\tau_{1n} - \cos\varphi\cdot\sigma_1 + \sin\varphi\cdot\tau_{2n} + \cos\varphi\cdot\sigma_2 = 0\,, \tag{5}$$

where φ is the dihedral angle between faces adjacent to the edge. For traction fields of degree $d \geq 2$, $(d+1)$ independent conditions associated with each edge lead to the homogeneous admissibility conditions on generalised element tractions represented by vector $\boldsymbol{g}$, i.e. $\boldsymbol{A}^T\boldsymbol{g} = \boldsymbol{0}$ where the dimensions of $\boldsymbol{A}$ are $n_v \times n_{skm}$. The spurious kinematic modes are then defined in terms of the dual basis for displacements by the columns of $\boldsymbol{A}$.

3 SPURIOUS KINEMATIC MODES FOR A TETRAHEDRAL ELEMENT OF GENERAL DEGREE

A convenient basis for polynomial displacement or traction functions over a triangular face is derived from the functions in the *Digital Library of Mathematical Functions* [8]. These $n = 0.5(d+1)(d+2)$ functions have the properties of orthogonality and the benefit of a hierarchical structure. When expressed in terms of area coordinates L_i they can be organised in a vector $\boldsymbol{h}$ to give Legendre polynomials along a particular edge, which leads to a very simple form of $\boldsymbol{A}$ when it is restricted to the two faces adjacent to that edge. This form, with dimensions $(4n\times(d+1))$, is defined by $\bar{A}$ in Equation (6), e.g. for the edge where $L_1 = 0$.

$$\bar{\boldsymbol{A}} = \begin{bmatrix} \sin\varphi \cdot \Delta_1^{-1} \boldsymbol{H}\boldsymbol{J} \\ -\cos\varphi \cdot \Delta_1^{-1} \boldsymbol{H}\boldsymbol{J} \\ \hline \sin\varphi \cdot \Delta_2^{-1} \boldsymbol{H} \\ \cos\varphi \cdot \Delta_2^{-1} \boldsymbol{H} \end{bmatrix} \tag{6}$$

where Δ_1 and Δ_2 are the areas of faces 1 and 2 in Figure 1, $\boldsymbol{J} = \boldsymbol{I}_{(d+1)}$ with even numbered diagonal coefficients = -1, and the $n\times(d+1)$ matrix $\boldsymbol{H}$ and the n dimensional vector $\boldsymbol{h}$ are defined in Equation (7).

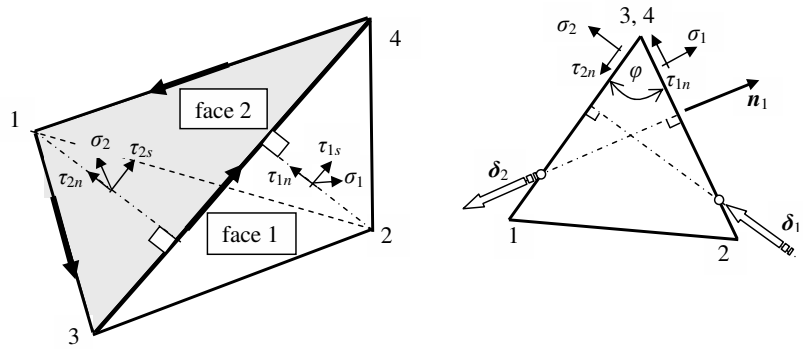

Figure 1: Traction components on a tetrahedron relative to edge connecting vertices 3 and 4. The right hand view is projected from vertex 3 to vertex 4.

$$\boldsymbol{H} = \left[\begin{array}{ccccc} 2 & 0 & 0 & \cdots & 0 \\ \hline 4 & 0 & 0 & \cdots & 0 \\ 0 & 12 & 0 & \cdots & 0 \\ \hline 6 & 0 & 0 & \cdots & 0 \\ 0 & 18 & 0 & \cdots & 0 \\ 0 & 0 & 30 & 0 & \cdots \\ \hline 8 & 0 & 0 & 0 & \cdots \\ 0 & 24 & 0 & 0 & \cdots \\ 0 & 0 & 40 & 0 & \cdots \\ 0 & 0 & 0 & 56 & \cdots \\ \hline \ddots & \ddots & \ddots & \ddots & \ddots \end{array}\right] \quad \text{when } \boldsymbol{h} = \left\{\begin{array}{c} 1 \\ \hline 1-3L_1 \\ -L_2+L_3 \\ \hline 1+2L_1\left(-4+5L_1\right) \\ \left(-1+5L_1\right)\left(L_2-L_3\right) \\ L_2^2-4L_2L_3+L_3^2 \\ \hline 1-5L_1\left(3+L_1\left(-9+7L_1\right)\right) \\ \left(1+3L_1\left(-4+7L_1\right)\right)\left(-L_2+L_3\right) \\ \left(1-7L_1\right)\left(L_2^2-4L_2L_3+L_3^2\right) \\ -\left(L_2-L_3\right)\left(L_2^2-8L_2L_3+L_3^2\right) \\ \hline \vdots \end{array}\right\} \tag{7}$$

Similar bases of $\boldsymbol{h}$ for other edges of the face are obtained using cyclic symmetry. Then the m^{th} column of $\boldsymbol{H}$ defines a signature function k_{2e}^m for face 2 corresponding to edge e as a combination of the basis functions in $\boldsymbol{h}$. The total displacement vector of a point in face 2 due to the spurious kinematic modes associated with its three edges, oriented as in Figure 1, is

given by Equation (8), where $\boldsymbol{n}_e$ is the unit outward normal vector to the other face adjacent to edge e, and a_e^m is the amplitude of the mth spurious mode associated with edge e.

$$\boldsymbol{\delta}_2 = \left(-\frac{1}{\Delta_2} \sum_m \sum_e k_{2e}^m \cdot a_e^m \right) . \boldsymbol{n}_e \tag{8}$$

4 PROPAGATION OF "MALIGNANT" SPURIOUS MODES BETWEEN TETRAHEDRAL ELEMENTS.

Propagation of spurious kinematic modes can occur between a pair of elements A and B when they result in compatible displacements at the interface. The displacements are resolved into in-plane and normal components as indicated in Figure 2 at a point P. For each signature function k_{je}^m displacements are evaluated at a set of n grid points with a common set of rigid body constraints. This leads to the displacement Equation (9) for element A.

$$\boldsymbol{u} = \boldsymbol{E}^{\boldsymbol{A}} \cdot \boldsymbol{a}^{\boldsymbol{A}} \quad \text{and} \quad w = \boldsymbol{C}^{\boldsymbol{A}} \cdot \boldsymbol{a}^{\boldsymbol{A}} \tag{9}$$

where $\boldsymbol{E}^{\boldsymbol{A}}$ and $\boldsymbol{C}^{\boldsymbol{A}}$ contain displacement components corresponding to spurious modes of unit amplitude, and have dimensions $(2n\times3(d+1))$ and $(n\times3(d+1))$ respectively. The amplitudes of the spurious modes are collected in the vector $\boldsymbol{a}^{\boldsymbol{A}}$. The matrices can be expressed as in Equation (10), where the diagonal matrices are defined in terms of the Kronecker products in Equation (11) and φ_e^A denotes the dihedral angle at edge e of element A.

$$\boldsymbol{E}^{\boldsymbol{A}} = \left[\boldsymbol{E}_1 \mid \boldsymbol{E}_2 \mid \boldsymbol{E}_3\right] \boldsymbol{D}_{\boldsymbol{s}}^{\boldsymbol{A}} = \boldsymbol{E} \cdot \boldsymbol{D}_{\boldsymbol{s}}^{\boldsymbol{A}}, \text{ and } \boldsymbol{C}^{\boldsymbol{A}} = \left[\boldsymbol{C}_1 \mid \boldsymbol{C}_2 \mid \boldsymbol{C}_3\right] \boldsymbol{D}_{\boldsymbol{c}}^{\boldsymbol{A}} = \boldsymbol{C} \cdot \boldsymbol{D}_{\boldsymbol{c}}^{\boldsymbol{A}} \tag{10}$$

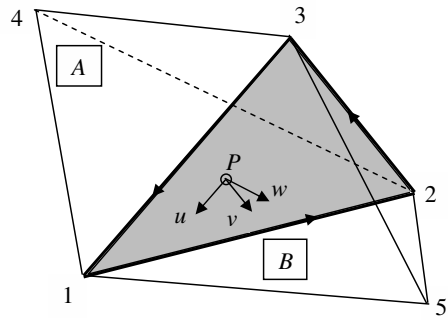

Figure 2: Interface between elements A and B.

Matrices $\boldsymbol{E}$ and $\boldsymbol{C}$ are partitioned in Equation (10) to match the coefficients from edges 1 to 3. Since these matrices are only dependent on the signature functions, which are expressed in terms of area coordinates, they are independent of the shape of the interface or the dihedral angles.

$$\boldsymbol{D}_s^A = \frac{1}{2\Delta}\begin{bmatrix} \sin\varphi_1^A & 0 & 0 \\ 0 & \sin\varphi_2^A & 0 \\ 0 & 0 & \sin\varphi_3^A \end{bmatrix} \otimes \boldsymbol{I}_{d+1} \quad \text{and} \quad \boldsymbol{D}_c^A = \frac{1}{2\Delta}\begin{bmatrix} \cos\varphi_1^A & 0 & 0 \\ 0 & \cos\varphi_2^A & 0 \\ 0 & 0 & \cos\varphi_3^A \end{bmatrix} \otimes \boldsymbol{I}_{d+1}. \quad (11)$$

Compatibility conditions take the form in Equation (12), where the vector $\left\lfloor \boldsymbol{a}^A \mid \boldsymbol{a}^B \right\rfloor^T$ contains the amplitudes of the 6(d+1) spurious modes associated with the edges of the interface belonging to elements A and B. The diagonal matrices $\boldsymbol{D}_s^B$ and $\boldsymbol{D}_c^B$ for element B are similar to those for element A, but involve the dihedral angles φ_e^B.

$$\left[\begin{array}{c|c} \boldsymbol{E}\boldsymbol{D}_s^A & -\boldsymbol{E}\boldsymbol{D}_s^B \\ \hline \boldsymbol{C}\boldsymbol{D}_c^A & \boldsymbol{C}\boldsymbol{D}_c^B \end{array}\right]\left\{\begin{array}{c} \boldsymbol{a}^A \\ \hline \boldsymbol{a}^B \end{array}\right\} = \left\{\begin{array}{c} \boldsymbol{0} \\ \hline \boldsymbol{0} \end{array}\right\} \quad (12)$$

It is found that generally ($d \geq 2$) $\boldsymbol{E}$ has full column rank and so any spurious mode involves in-plane deformation of the interface, and compatibility requires $\boldsymbol{D}_s^A \cdot \boldsymbol{a}^A = \boldsymbol{D}_s^B \cdot \boldsymbol{a}^B$. Eliminating $\boldsymbol{a}^A$ from the second set of Equation (12), leads to Equation (13).

$$\boldsymbol{C}\left[\boldsymbol{D}_{\cot}^A + \boldsymbol{D}_{\cot}^B\right]\left[\boldsymbol{D}_s^B\right]\boldsymbol{a}^B = \boldsymbol{0} \quad (13)$$

where the suffix "cot" implies that cotφ_e replaces cosφ_e or sinφ_e in the diagonal matrices. The consequence of Equation (13) is that compatibility can be satisfied:

- when $\boldsymbol{C}$ is column rank deficient, and/or
- the geometrical configuration is degenerate in the sense that $\cot\varphi_e^A + \cot\varphi_e^B = 0$ for one or more dihedral angles, i.e. faces in adjacent elements are coplanar.

Numerical trials involving singular value decomposition reveal that, when $d > 3$, $\boldsymbol{C}$ has column rank 3d and hence 3 spurious kinematic modes can be propagated via the interface in the non-degenerate case. These modes are linearly related to independent solutions of the homogeneous equations $\boldsymbol{Ca} = \boldsymbol{0}$, and such solutions are given by the 3×3(d+1) matrix in Equation (14).

$$\boldsymbol{a}^T = \left[\begin{array}{cccccc|cccccc|cccccc} 0 & 1 & 0 & 1 & \cdots & & -1 & 0 & -1 & 0 & \cdots & & 1 & 0 & 1 & 0 & \cdots \\ 1 & 0 & 1 & 0 & \cdots & & 0 & 1 & 0 & 1 & \cdots & & -1 & 0 & -1 & 0 & \cdots \\ -1 & 0 & -1 & 0 & \cdots & & 1 & 0 & 1 & 0 & \cdots & & 0 & 1 & 0 & 1 & \cdots \end{array}\right]. \quad (14)$$

The corresponding spurious mode amplitudes for element A can then be defined in Equation (15).

$$\boldsymbol{a}^A = \frac{1}{\Delta^2}\left[\boldsymbol{D}_s^A\right]^{-1}\left[\boldsymbol{D}_{\cot}^A + \boldsymbol{D}_{\cot}^B\right]^{-1}\boldsymbol{a}. \quad (15)$$

This solution can also be expressed, using the Kronecker matrix product in Equation (16).

$$\boldsymbol{a}^{\boldsymbol{A}} = \begin{bmatrix} \dfrac{\sin\varphi_1^{\boldsymbol{B}}}{\sin\left(\varphi_1^{\boldsymbol{A}}+\varphi_1^{\boldsymbol{B}}\right)} & 0 & 0 \\ 0 & \dfrac{\sin\varphi_2^{\boldsymbol{B}}}{\sin\left(\varphi_2^{\boldsymbol{A}}+\varphi_2^{\boldsymbol{B}}\right)} & 0 \\ 0 & 0 & \dfrac{\sin\varphi_3^{\boldsymbol{B}}}{\sin\left(\varphi_3^{\boldsymbol{A}}+\varphi_3^{\boldsymbol{B}}\right)} \end{bmatrix} \otimes \boldsymbol{I}_{\boldsymbol{d}+1} \cdot \boldsymbol{a} \tag{16}$$

It is observed from the form of $\boldsymbol{a}^T$ that the three modes can be characterised by a single one, which generates two more independent ones by using cyclic symmetry. When the pair of elements are symmetrical about the interface, $\boldsymbol{D}_{\text{cot}}^{\boldsymbol{A}} = \boldsymbol{D}_{\text{cot}}^{\boldsymbol{B}}$ and in this case $\boldsymbol{CD}_{\boldsymbol{c}}^{\boldsymbol{A}} \cdot \boldsymbol{a}^{\boldsymbol{A}} = \boldsymbol{0}$ and consequently the interface remains plane. The characteristic mode for a pair of regular tetrahedra of degree 4 is illustrated by the in-plane displacements shown in Figure 3.

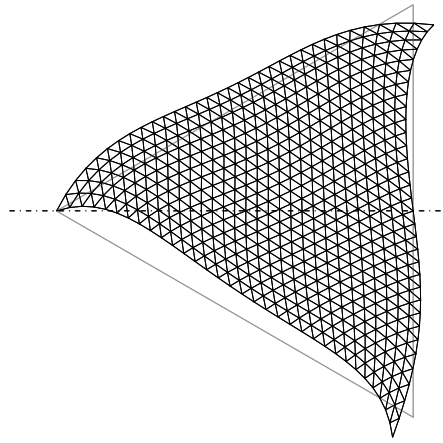

Figure 3: Characteristic spurious kinematic mode that can be propagated between a pair of regular tetrahedral elements of degree 4.

The number of malignant modes for non-degenerate cases increases for $d < 4$, and the complete set of numbers is presented in Table 1.

Table 1: Number of malignant modes for a general degree.

d	0	1	2	3	≥ 4
number of malignant modes	3	6	6	5	3

It should be noted that when:

d = 1, rank($\boldsymbol{E}$) = 3, and the 6 spurious modes associated with the interface of one of the elements can freely exist in a state of constant strain coupled with a rigid body displacement. Thus only 3 of the combined modes can be propagated to involve deformations.

d = 0, the 3 spurious modes associated with the interface of one of the elements can freely exist as rigid body translations. Thus all the modes can be freely propagated as rigid body modes.

5. CLOSURE

A pair of tetrahedral hybrid equilibrium elements always has the potential for at least three spurious kinematic modes to be propagated from one element to the other. This feature of 3D tetrahedral models is more complicated than the case with 2D models with triangular elements, where such propagation is normally blocked for degrees greater than two.
Thus establishing the existence of spurious kinematic modes in a pair of tetrahedral elements is just the first stage in understanding when and how these modes can propagate in a more general mesh. Whilst experience has shown[6] that assemblies of four tetrahedra into a single macro-element is free of spurious kinematic modes, it is intended to pursue further research to address the stability of more general configurations.

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CONSTRUCTION OF DYNAMICALLY ADAPTING COMPUTATIONAL GRIDS IN SYSTEMS OF DIFFERENTIAL EQUATIONS DESCRIBING THE NON-EQUILIBRIUM PROCESSES

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Abstract. The processes occurring in solid targets (metals, semiconductors) initiated by pulsed flows of condensed energy is described by two-temperature model (TTM). The simplest TTM model for metals consists of two, and for semiconductors of three non-linear parabolic equations. Ultrafast impact (pico-femtosecond pulse duration) predetermines the appearance of large solution gradients that require in numerical solution application of computational grids with dynamic adaptation. Transition to an arbitrary non-stationary system of coordinates, the velocity of which is unknown and depends on the desired solution is the basis of the construction of a dynamically adaptive grids. Velocity of the system of coordinates for the numerical discretization is used as a function that control the motion of grid nodes . Agreed change of movement of grid nodes with the solution is achieved by constructing of transformation function derived from the principle of quasi-stationarity.
Simulation of some specific regimes pulsed heating, melting and evaporation of metals (Al), and semiconductors (Si), that use grids with automatic distribution of nodes.

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ADMOS 2013
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MATHEMATICAL MODELING OF SPALLATION OF CONDENSED MATTER UNDER THE INFLUENCE OF CONCENTRATED ENERGY FLOW

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Abstract. The process of spallation a solid aluminum target under the influence of an ultrashort laser pulse is considered. Modeling was carried out using the method of dynamic adaptation with explicit front tracking. The pulse duration was 100 ps - 1 fs, fluence was selected from a range of 0.1 - 1 J/cm2. Tensile strength was determined using the molecular dynamics simulation. Modeling allowed to determine the thickness of the spallated layer, investigate the regimes in which spallation occurs in melt and solid. Also regimes where discovered where spallation occurs in solid in the absence of melting.

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VERY HIGH ORDER MESH ADAPTATION

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Key words: Anisotropic mesh adaptation

Abstract. This paper addresses the construction of anisotropic metrics from higher-order interpolation error in 2 dimensions [2, 3] for mesh adaptation. Our approach is based on homogeneous polynomials that model a local interpolation error. Optimal orientation and ratios are found by using the Sylvester decomposition [4]. Then we apply a global calculus of variation to get the optimal metric field minimizing the $\mathbf{L}^p$ norm of the interpolation error. We illustrate this approach on 3D numerical examples.

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ADMOS 2013
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TIME ADAPTIVITY AND ANISOTROPIC MESH ADAPTATION FOR CFD APPLICATIONS

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Key words: Space-time Adaptation, Anisotropic Meshes

Abstract. In this communication we present some recent results about time adaptivity with applications to fluid-dynamics. In particular, we are interested in phenomena characterized by temporal multiscale as well as strong spatial heterogeneities, e.g., heat flow problems, shallow water flows, hydrogeology, particle diffusion phenomena, etc. The proposed adaptation procedure relies on a theoretical tool, i.e., an a posteriori error estimator, driving the automatic choice of both the spatial and temporal meshes. The key point is to identify, in the error estimator, separate space and time contributions, as discussed, e.g., in [1, 2, 3]. Thus, on the one hand, we devise a sound criterion to update the time step, able to follow the evolution of the problem under investigation. On the other hand, we exploit an anisotropic adapted triangular grid. It is in fact well known that, by better orienting the mesh elements according to the main features of the solution, it is possible to maximize the solution accuracy for a fixed number of elements, rather than reduce the number of degrees of freedom for a fixed solution accuracy (see, e.g., [4, 5]). Application to purely diffusive problems was first provided in [6, 7]. Here we extend our approach to nonlinear problems, such as the shallow water system considered in [8, 9].

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GOAL-ORIENTED ERROR ESTIMATION FOR NONLINEAR PARABOLIC EQUATIONS BASED ON THE RECONSTRUCTION OF EQUILIBRATED FLUXES

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Key words: Adjoint problem, Discontinuous Galerkin Method, Asymptotically exact estimator

Abstract. We derive a goal-oriented estimate of the error in finite element approximations of nonlinear parabolic equations based on a representation that involves an equilibrated flux reconstruction in space variable of the solution to the primal and to the (linear) dual backward-in-time problem. The error estimate can be applied to any arbitrary finite element discretization of the primal problem that admits a flux reconstruction in space variable satisfying some local space-time conservation and approximation properties [1]. We assume that an implicit-in-time Euler-type scheme is employed for the primal problem. The adjoint problem is then approximated using the same type of discretization scheme in time and a discontinuous Galerkin (dG) finite element method in space on the same mesh as the one used for the primal problem. Owing to the local conservation property of the dG, reconstructed equilibrated fluxes associated with the dual problem [2] can be straightforwardly obtained for the calculation of the error estimates. In fact, the dG method naturally produces fully computable elementwise contributions to the error, which are accurate even on the original mesh since the support of the basis functions coincides with the elements, see [3]. In this talk, we prove, and confirm with numerical experiments, that the proposed error estimator is asymptotically exact.

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ADMOS 2013
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FULLY EQUILIBRATED STRESS RECOVERED FIELD FOR ERROR BOUNDING

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Key words: Error bounding, Error estimator, Recovery technique, Statically admisible

Abstract. In this communication, we present a stress recovery technique based on the Superconvergent Patch Recovery (SPR) technique, for linear elasticity problems, solved within the framework of the Finite Element Method (FEM). This work pretends to investigate the application of recovery techniques that provide statically admissible stress fields.

Several error estimator techniques that provide upper bounds in energy norm are available, most of them based in equilibrating residuals, which do not always provide good accuracy levels. Furthermore, engineers prefer to use recovery techniques, because they are robust, easy to implement and provide a higher accuracy. In all cases the difference between a kinematically admissible field, i.e. the raw FE solution, and a statically admissible stress field, i.e. our recovered solution, provides an upper bound of the true error. This result is relevant in order to obtain an overestimation of the exact error in energy norm, which guarantees a certain error level in our simulation.

Using a previously proposed approach we were only able to obtain nearly statically admissible stress fields, consequently, to ensure an upper bound some extra correction terms were added to the Zienkiewicz & Zhu (ZZ) error estimator. As these correction terms depend on the exact displacement error, only an approximation of the upper bound was obtained. By using these new results, the correction terms are not needed any more, and the ZZ error estimator naturally yields an upper bound of the energy error.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

CONFORMAL HEXAHEDRAL MESHES AND ADAPTIVE MESH REFINEMENT

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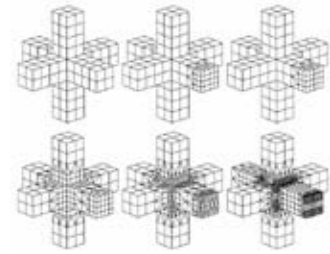
Abstract. In a numerical simulation using the finite element method, the mesh has to be fine enough to guarantee the accuracy of the solution. To achieve this goal, mesh adaptation offers an effective compromise, combining a fine mesh with a low computational cost. With the h-refinement method, some meshes are divided but difficulties occur at the interface between two zones with different levels of refinement, if a conformal mesh is required. That problem is solved either by specific finite elements in the junction or by a specific splitting of these meshes.
If the initial mesh is made of tetrahedra, the splitting of the meshes at the interface produces new tetrahedra. Since the early 90's, this method has been implemented in HOMARD, our software for mesh refinement [1]. But in some numeric simulations, the initial mesh is made of hexahedra because they are more efficient than the tetrahedra. In that case, the transition is not as simple as it is with the tetrahedra: the conformal connection cannot be made with others hexahedra. To solve this problem, we developed a new method: using tetrahedra and pyramids makes possible a conformal connection of the zones of different levels of refinement.
To perform the mesh refinement for conformal hexahedral meshes, first, the error indicator from the computed solution is used to produce a non-conformal mesh [2]. Then, every hexahedron that is at the interface is examined. Counting the number of cut edges, only four situations may occur: 1, 2, 3 or 4. Each of these 4 situations corresponds to a specific pattern for the refinement of the hexahedron.
This conformal refinement method was evaluated with some test cases that use specific finite elements in the transitional zone [3]. The evolution of the refined meshes along the iterations of the adaptation (see figure) ensures the diminution of the global error of the problem.
A test involving an industrial geometry will be presented at the conference.



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GOAL ORIENTED MESH ADAPTATION WITHOUT FINE GRID INTERPOLATION FOR FINITE-VOLUME CFD

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Abstract. In aeronautical CFD, engineers require accurate predictions of the forces and moments but they are less concerned with flow-field accuracy. Hence, the so-called "goal oriented" mesh adaptation strategies have been introduced to get satisfactory values of functional outputs at an acceptable cost, using local node displacement and insertion of new points rather than mesh refinement guided by uniform accuracy[2, 3, 4, 5, 6]. Most often, such methods involve the adjoint vector of the function of interest. Our purpose is to present goal oriented criteria of mesh quality and local mesh adaptation strategies in the framework of finite-volume schemes and a discrete adjoint vector method [1]. They are based on the total derivative of the goal with respect to (w.r.t.) mesh nodes. More precisely, a projection of the goal derivative, removing all components corresponding to geometrical changes in the solid walls or the support of the output [7]. The methods are assessed in the case of 2D and 3D Euler flow computations, with structured and unstructured meshes.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

NEW BOUNDING TECHNIQUES FOR GOAL-ORIENTED ERROR ESTIMATION IN FE SIMULATIONS

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Abstract. In the context of finite element (FE) model verification, research and engineering activities focus on the development of robust goal-oriented error estimation methods designed to achieve strict and high-quality error bounds associated to specific quantities of interest. A general method [1,2,3] consists in using extraction techniques as well as robust global error estimation methods, and leads to the global solution of an auxiliary problem, also known as dual or adjoint problem. The derivation of accurate local error bounds entails a fine resolution of this auxiliary problem. Nevertheless, the classical bounding technique may provide low-quality error bounds on specific quantities of interest, particularly when the global estimated errors related to both reference (primal) and adjoint (dual) problems are mainly concentrated in disjoint regions. The main source of overestimation presumably stems form the Cauchy-Schwarz inequality, especially when the zone of interest is located far from the predominant contributions of the global estimate associated to reference problem. This observation has spurred the development of new bounding techniques able to circumvent, or at least alleviate, this serious drawback by optimizing the sharpness and practical relevance of the classical computed bounds.

In this work, we propose and analyze two new improved bounding techniques based on non-classical and innovative tools, such as homotheticity properties [4]. These techniques are carefully tailored for the derivation of inequalities between appropriate quantities over two homothetic domains contained in the whole structure. Such relations are based on Saint Venant's principle and seem to be limited to solely linear problems. The classical and enhanced techniques are combined with an intrusive approach (local refinement techniques) or a non-intrusive one (handbook techniques [5]) to get a reliable solution of the adjoint problem. Handbook techniques consist in enriching the approximate solution of the adjoint problem locally by introducing precomputed or analytical known handbook functions through the partition of unity method (PUM). Numerical examples are provided with comparative results between conventional and alternative bounding techniques within the linear elasticity framework. Various linear quantities of interest (such as the local average of a stress component, the pointwise value of a displacement component or a stress intensity factor) are considered to illustrate the effectivity of the two proposed techniques.

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ADMOS 2013
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IDENTIFICATION OF ADMITTANCE COEFFICIENTS FROM IN-SITU MEASUREMENTS IN ACOUSTIC CAVITIES

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Abstract. In recent decades, sound intensity and quality is taking an increasingly important place in the design process of products like cars or aircrafts. Different types of absorbing materials have therefore been developed and used in such products to achieve this purpose. Acoustical calculations are quite heavy and industries generally have to use numerical tools to predict the influence of absorbing materials on the sound propagation inside cavities. In these ones, the acoustical properties of absorbing materials are described by the admittance (or impedance) coefficient, which is a simplification of the physical model. However, the limits of applicability of this model are not well known and the conditions in which its parameters are measured can differ significantly from the ones in which the materials are really used.
In this paper, a model updating technique process is used to identify the parameters required to describe admittance coefficients from sound pressure measurements inside a closed cavity. Updating techniques have been used for many years to improve numerical models, and consist in minimizing an error between the numerical solutions and a set of experimental results. The technique based on the Constitutive Relation Error (CRE), initially proposed by Ladevèze [1] for structural dynamics problems, is an indirect method in which the cost function, called the CRE, is based on an energy norm. The main advantages of this method are that the updated parameters keep a physical meaning, that it allows taking into account the measurement error and that it allows locally evaluating the modeling and measurement errors [2].
In this paper the CRE-based updating technique is applied to the acoustical problem ([3], [4]) in order to identify the admittance coefficients and the local estimators are developed. The method is applied on real 2D (Kundt's tube) and 3D (concrete box) experimental data.

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ACCURATE MODELLING OF STRAIN DISCONTINUITIES IN BEAMS USING AN XFEM APPROACH

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Key words: XFEM, Timoshenko beams, Euler-Bernoulli beams, assumed natural strain method, shear locking

Abstract. Thin piezoelectric transducers are widely used in applications such as active vibration control, wave generation in materials and structural health monitoring. The finite element modelling of piezoelectric transducers is well established; an overview of the existing models can be found in [1]. Current practice for the modelling of structures equipped with flat piezoelectric transducers requires the development of specific beam or plate elements which are usually not available in commercial codes. The most important criteria when using this technique is that the mesh must exactly match the boundary between the piezoelectric transducers and the host structure, which requires extensive remeshing when optimal transducers configurations are investigated.

The need for conforming meshes arises due to the following reasons: the occurrence of a strain jump across the interface between the piezoelectric transducer and the host structure, the continuity of the displacement field across the interface, and the presence of an electric field only in the piezoelectric material. To overcome meshing difficulties and capture local phenomenon, the extended finite element method (XFEM) for weak discontinuities was proposed for two-dimensional problems [2].

The aim of this paper is to study the possibility of using XFEM for the modelling of piezoelectric transducers attached to beam structures without the need for a conforming mesh. The first challenge is to locate the interface in the mesh. This can be done using explicit or implicit methods. In our case, we use the implicit level-set representation of the interface. The second challenge is to determine the right enrichment function. The main focus of this study is to propose enrichment functions to represent accurately the strain discontinuities in Euler-Bernoulli and Timoshenko beams. Further, we assess the performance of the enrichment functions on simple static cases with a special emphasis on the shear locking in the Timoshenko beam.

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ADMOS 2013
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ADAPTIVE TIME STEP CONTROL FOR THE GENERALISED-α METHOD

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Abstract. The most important requirements for the numerical solution of fluid and structure problems are accuracy and efficiency. Therefore adaptivity in space and time is advantageous [1]. For obtaining a stable numerical solution of fluid and structure problems implicit or linear-implicit methods should be used [4,5]. In this talk we concentrate on the generalised-α method for first order problems [3] and second order problems [2].

A good time integration method needs an error estimator for increasing efficiency. This error estimator suggests a new time step size to reach a given accuracy. If the time step size is too small a lot of unnecessary computational work has to be done. Otherwise, if the time step size is too large, the results become less accurate.

In this talk we analyse the generalised-α method and develop with the help of this analysis an adaptive method. Finally we apply this scheme on several test problems.

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FAST TIME IMPLICIT DISCRETIZATION FOR COMPRESSIBLE FLOW EQUATIONS VIA A DISCONTINUOUS GALERKIN METHOD

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Key words: discontinuous Galerkin method, implicit-time integration, compressible flows

Abstract. In this study, we investigate efficient time integration techniques for a high-order accurate discontinuous Galerkin method. The method is associated to a Jacobian-free Newton-Krylov algorithm. This method is known to resolve the problem of strong restriction on the time step due to the so-called Courant-Friedrichs-Levy condition for stability of the discontinuous Galerkin scheme associated to an explicit time discretization. However, the shortcoming of implicit time integration methods is the extremely high computational cost and memory requirement induced by the large number of degrees of freedom in practical applications. In the present work, we focus on efficient preconditioning techniques. In a first time, we will review and compare techniques in the context of Jacobian-free Newton-Krylov algorithm such as block-Jacobi, LU SGS and ILU(0) preconditioners. Then, we will exploit the possibility of using approximate Jacobians as preconditioning matrix to reduce the strong computational cost and memory requirement associated to a high-order discontinuous Galerkin method. Steady-state and time-dependent solutions of the compressible Euler equations in two and three space dimensions will be considered to assess the performances of the present method.

VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

A GUARANTEED ERROR BOUND SEPARATING ALGEBRAIC AND DISCRETIZATION CONTRIBUTIONS IN NON-OVERLAPPING DOMAIN DECOMPOSITION METHODS

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Key words: Algebraic error, Discretization error, Stopping criterion, Verification

Abstract. For the last decades, three trends have grown and reinforced each other: the fast growth of hardware computational capacities, the requirement of finer and larger finite element models for industrial simulations and the development of efficient computational strategies amongst which non-overlapping domain decomposition (DD) methods [2, 3, 4] are very popular since they have proved to be scalable in many applications. One main shortcoming in DD lies on the absence of verification of the discretized models in order to warranty the quality of numerical simulations (global or goal-oriented error estimators). In a recent work [1], we introduced a first error estimator in a non-overlapping domain decomposition framework and outlined its connection with two iterative non-overlapping domain decomposition solvers (FETI and BDD). It is fully parallel in the sense that it involves a simple preprocessing of interface tractions and the use of standard black-box sequential error estimators [5, 6, 8] independently on each subdomain. It yields a guaranteed upper bound on the error whatever the state (converged or not) of the iterative solver associated to the interface continuity. It has been numerically observed that our first DD-error estimator enables to recover the same efficiency factor as the standard sequential. However, its main drawback is its inability to separate the algebraic error (coming from the DD iterative solver) from the discretization error per subdomains.

In this talk, we present some of our recent work that aims at separating the algebraic error and the discretization error. We introduce a new guaranteed upper bound that enables to introduce such a separation. This leads to the definition of new convergence criteria of DD iterative solvers based on the estimation of the discretization error instead of purely algebraic criteria. Works in progress are related to (i) goal-oriented error estimator (ii) nonlinear problems.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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GOAL-ORIENTED ERROR ESTIMATOR FOR THE FRACTIONAL STEP θ TIME-STEPPING SCHEME

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Key words: error estimation, fractional step time-stepping, DWR

Abstract. In this contribution we present an adjoint based a posteriori error estimator for (nonlinear) parabolic problems discretized with the fractional step θ time-stepping scheme. This scheme combines several highly desired attributes: it is second order accurate, strongly A-stable and shows very little numerical dissipation. The drawback of this time-stepping scheme is its time-stepping character based on a finite difference approximation which makes it ill-suited for variational and in particular adjoint error estimation techniques.

We will propose a Petrov-Galerkin scheme, that is shown to be algebraically equivalent to the fractional step θ time-stepping scheme for linear problems and that can be regarded as an approximation of this scheme for general nonlinear problems.

The error estimator is split into two parts: the first is a traditional residual based estimator of the Galerkin scheme, the second measures the defect in Galerkin orthogonality given by the numerical quadrature error. Both estimator parts require the solution of an adjoint in time solution.

VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

EXPLICIT EXPRESSIONS OF DUAL LOADS FOR ACCURATE ERROR ESTIMATION AND BOUNDING IN GOAL ORIENTED ADAPTIVITY

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Key words: Quantities of Interest, Error estimator, Goal oriented adaptivity

Abstract. Recently, Goal Oriented Adaptivity (GOA) has been an active research area because of its advantages in terms of computational cost and accuracy. A widely used technique to perform a Goal Oriented (GO) analysis consists in solving two Finite Element (FE) problems: the primal one, which is the actual problem and the dual or adjoint one, which is an auxiliary problem depending on the Quantity of Interest (QoI) whose loads are used to extract the QoI.

Traditionally, under the FE framework, the force vector for the dual problem has been numerically evaluated using the FE discretization without knowing the explicit expressions of the loads for the dual problem. Our objective in this paper is to obtain the explicit expression for the extraction loads used in the dual problem for linear QoI in the context of linear elasticity, that is boundary forces, body loads and initial stresses and strains. In particular, we will evaluate the explicit loads for the dual problem when the QoI is the Generalized Stress Intensity Factor (GSIF) that characterizes the singularity in singular problems. In this case the extraction loads can be represented by a distribution of body forces and initial strains over a domain around the singularity.

A recovery procedure, which makes use of the explicit expressions of the applied loads to enforce the local satisfaction of the equilibrium equation for an accurate stress representation [2], has been used to obtain accurate estimations and bounds of the error in the QoI using a ZZ-type error estimator [1] as shown by the numerical tests.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

SHAPE SENSITIVITY ANALYSIS INCLUDING QUALITY CONTROL WITH CARTESIAN FINITE ELEMENT MESHES

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Key words: Cartesian Grid-FEM, NURBS, velocity field, shape sensitivity analysis

Abstract. The gradient-based optimization methods used for optimization of structural components require that the information of the gradients (sensitivity) of the magnitudes of interest is calculated with sufficient accuracy. The aim of this paper is to present a module for calculation of shape sensitivities with geometric representation by NURBS (Non-Uniform Rational B-Splines) for a program created to analyze 2-D linear elasticity problems, solved by FEM using cartesian grids independent of the geometry, CG-FEM.

First, it has been implemented the ability to define the geometry using NURBS, which have become in recent years in the most used geometric technology in the field of engineering design. In order to be able to represent exact geometries, a scheme based on matrix representation of this type of curve and proper integration is proposed. Moreover, the procedures for shape sensitivities calculation, for standard FEM, have been adapted to an environment based on cartesian meshes independent of geometry, which implies, for instance, a special treatment of the elements trimmed by the boundary and the implementation of new efficient methods of velocity field generation, which is a crucial step in this kind of analysis.

Secondly, an error estimator, as an extension of the error estimator in energy norm developed by Zienkiewicz and Zhu, has been proposed for its application to the estimation of the discretization error arising from shape sensitivity analysis in the context of cartesian grids.

The results will show how using NURBS curves involves significant decrease of geometrical error during FE calculation, and that the calculation module implemented is able to efficiently provide accurate results in sensitivity analysis thanks to the use of the CG-FEM technology.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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PROBABILITY AND VARIANCE-BASED STOCHASTIC DESIGN OPTIMIZATION OF A RADIAL COMPRESSOR CONCERNING FLUID-STRUCTURE INTERACTION

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Key words: robust design optimization, robustness evaluation, reliability analysis, fluid-structure interaction, surrogate models, adaptive design of experiment, importance sampling, directional sampling, cluster analysis

Abstract. Within the design development phases the Design for Six Sigma concept optimizes a design such that the products conform to Six Sigma quality. Which means that robustness and reliability are explicit optimization goals even with variations e.g. in manufacturing, design configuration and environment.

Since the engineering of radial compressors the improvement of specific physical behavior, especially the efficiency, is one of the key issues. In conventional engineering the design is improved by evaluating design response and making design changes based on experience, intuition or guess. Due to the introduction of virtual prototyping the radial compressor analysis have a very high degree of complexity and desired improvements are hard to reach with conventional trial and error procedure.

In the reliability-based robust design optimization, the optimization problem

$$\begin{aligned}
&f(d_1, d_2, \dots d_{n_d}) \rightarrow \min \\
&g_k(d_1, d_2, \dots d_{n_d}) = 0;\ k = 1, m_e \\
&h_l(d_1, d_2, \dots d_{n_d}) \geq 0;\ l = 1, m_u \\
&1 - \frac{P(\mathcal{F})}{P^t(\mathcal{F})} \geq 0;\ P(\mathcal{F}) = \int_{g_j(\mathbf{x}) \leq 0} \dots^{n_r} \dots \int f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \\
&\frac{\sigma_{L_j}}{\sigma_L^t} - 1 \geq 0;\ \sigma_{L_j} = \frac{g_j(X_i) - \bar{X}_j}{\sigma_{X_j}};\ j = 1, m_g \\
&d_i \in [d_l, d_u] \subset \mathbb{R}^{n_d};\ d_{l_i} \leq d_i \leq d_{u_i};\ d_i = E[X_i]
\end{aligned} \tag{1}$$

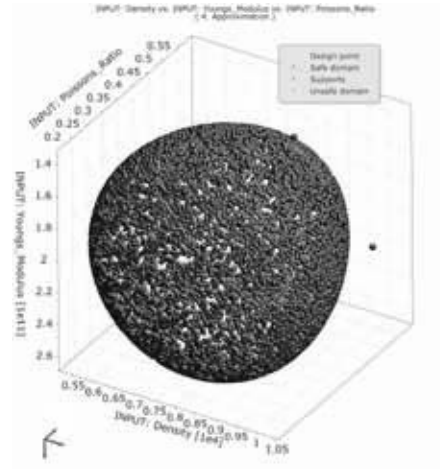

Figure 1: Eigenvalue analysis with ANSYS Workbench to calculate the state condition $g(\mathbf{X})$ for the reliability analysis.

Figure 2: The oscillatory phenomenon of the first eigen frequencies with the rotational velocity of the rotor results in a small non-closed failure domain in the space of the random material parameters.

can be enhanced by additional stochastic restrictions regarding the sigma levels σ_{L_j} ensuring that the probability of failure can not exceed the target probability, for example $P(\mathcal{F}) \leq 3.4 \cdot 10^{-6} = P^t(\mathcal{F})$. Problem (1) is solved as a combination of a deterministic optimization in the n_d-dimensional design space, whereby the design parameters $\mathbf{d} = E[\mathbf{X}]$ are the means of the n_r random influences $\mathbf{X}$ for every deterministic design with the joint probability density function of the basic random variables $f_{\mathbf{X}}(\mathbf{x})$ and m_g limit state functions $g_j(\mathbf{x}) \leq 0$.

This procedure leads in general to an inefficient double loop with a large number of design evaluations. The most general way for reducing the required number of design evaluations is the application of an iterative decoupled loop approach (see e.g. Chen et al., 2003). This effective approach can be enhancement by updating the constrains during the internal optimization using statistical moments in place of the exceedance probability. Essentially, by means of this transformation, the probability-based highly nonlinear and non-differentiable constrains may be more well conditioned for the optimization approach. In this paper an efficient iterative decoupled loop approach is provided for reducing the necessary number of design evaluations.

For an efficient reliability assessment, a new multi-domain adaptive design of experiment in combination with importance sampling and directional sampling is introduced to improve the accuracy and predictability of surrogate models, commonly used in applica-

tions with several limit state conditions (see Roos, 2011). Furthermore, the identification of the failure domains using the directional sampling procedure, the pre-estimation and the priori knowledge of the probability level is no longer required. Therefore the presented method is particularly suitable to solve reliability-based structural design optimization problems considering uncertainties with ever-changing failure probabilities of the nominal designs.

The applicability for real case applications is demonstrated exemplary for a radial compressor, used in power plants or aircraft engines. In the presented example the target of the optimization process is to maximize the efficiency of the turbine engine with respect to a limitation of the maximal v. Mises stress. Additional constrains are defined by resonance of any eigen frequency with the rotational velocity of the rotor (see Figures 1 and 2).

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

ON A TIME-SEQUENTIAL ADAPTIVE STRATEGY IN SPACE-TIME FOR FINITE STRAIN CONSOLIDATION PROBLEMS

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Key words: Goal-oriented adaptivity, time-sequential strategy

Abstract. The paper outlines a time-sequential space-time adaptive FE-strategy applied to finite strain coupled consolidation, which can be viewed as a prototype model of a class of nonlinear and time-dependent poro-mechanics problems. The natural variational setting for the consolidation problem allows for space-time FE using dG- or cG-methods in time depending on the expected character (quasistatic or dynamic). We discuss goal-oriented error computation and the combined space-time adaptivity while accounting for non-linearities in the model as well as the output functional.

One key ingredient in the proposed strategy is to introduce a hierarchical decomposition in space-time of the discrete function space(s) in which the approximate dual solution is sought. As a result, it is possible to decompose the estimated error from the discretization in space and time in a unified fashion within the same algorithm. This decomposition of error contributions allows for efficient adaptive mesh-refinement in space and time separately. Moreover, other sources of error (model and solution errors) can be identified.

Traditionally, controlling the global error in space-time problems involves storing the complete solution and, when adopting an adaptive algorithm, complete re-computation of the solution for each iteration of the space-time mesh. The main idea proposed in this contribution is to increase the computational efficiency of the adaptive scheme by avoiding recursive adaptations of the entire space-time mesh; rather, the space-mesh and the time-step defining each finite space-time slab are defined in a truly sequential fashion. The procedure involves the solution of an initial, approximate, dual solution on a coarse "background" space-time mesh which is kept fixed during the space-time re-meshing for the primal problem.

The overall performance of the proposed strategy is investigated using a few numerical examples.

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ADMOS 2013
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A VARIATIONAL FORMULATION OF DAMAGE FOR THERMO-VISCOELASTIC PROBLEMS IN LARGE STRAINS

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Key words: Variational formulation, Damage, Thermo-viscoelasticity, Large strains.

Abstract. A variational formulation of damage for thermomechanically coupled problems is proposed. Based on variational methods for dissipative materials developed in the last few years (especially since [1]), this formulation allows for the accurate simulation of a wide variety of damage models, encompassing the behavior of various classes of polymers, the target application of the present paper.

A full development of the proposed formulation is presented in the first section. From an energy-like scalar-valued functional, the balance equations of the problem are derived, including the coupling terms between the different physics. The treatment of thermal effects follows [2]. A distinction between an internal and an external temperature allows for a factorization that, contrary to more classic formulations, keeps a symmetric structure to the problem. In order to describe rate dependence phenomena, the deformation energy potential is constructed from a generalized Kelvin-Voigt/Maxwell rheological model. Eigenvalues of strains are used as independent variables so that large strains are properly treated, following [3]. Having established the ingredients for a variational formulation of thermo-viscoelasticity, we move on to include damage effects. After a brief description of the choices made in [4] for the modeling of low cycle metal fatigue, a general framework for the inclusion of different damage models is presented.

In the second section, different damage models are applied. Although the framework we present is sufficiently general to consider anisotropic models, only isotropic examples of damage are presented in this article. The simplest case, where a scalar damage variable acts only upon the elastic part of the deformations, is presented first. We then apply the damage variable to both elastic and viscous parts of the deformation, which yields a more complex behavior. The possibilities of developing even more complex damage models, with different

damage variables acting upon each rheological Maxwell branch, is also discussed – it should be noted, though, that such models bring about increasingly tougher challenges in parameter identification. Different damage evolution laws are tested to show the versatility of the formulation.

The third and final section consists of the validation of the proposed model for the simulation of some characteristic phenomena of polymer damage behavior. A final discussion of further possible applications of the formulation concludes the present article.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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METHODS AND TOOLS FOR PARALLEL ANISOTROPIC MESH ADAPTATION AND ANALYSIS

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Key words: Mesh adaptation, parallel adaptation, dynamic load balancing.

Abstract. It is well know that adaptive methods are the most effective means to obtain reliable solutions and control the amount of computation required. However, for many classes of problems the best adaptive method still require a level of computation that demands massively parallel computing. The evolving nature of adaptive simulations constantly changes the computational balance, thus requiring general structures and dynamic load balancing based on those structures. This paper will discuss recent advances on the development of methods and software components to execute and support the effective anisotropic mesh adaptation on massively parallel computers. One area to be discussed is parallel mesh adaptation on general unstructured anisotropic meshes considering various aspects of dynamic load balancing and parallel communication minimization. Another area to be considered is the development of general methods to support the execution, including dynamic load balancing, of adaptive computations.

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ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

ERROR ESTIMATION FOR THE CONVECTIVE CAHN – HILLIARD EQUATION

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Key words: Cahn–Hilliard equation, mixed finite element method, a-posteriori error analysis

Abstract. The Cahn–Hilliard phase-field (or diffuse-interface) model has a wide range of fluid applications where the interest is the modelling of phase segregation and evolution of multiphase flow systems. In order to capture the physics of these systems, diffuse-interface models presume a nonzero interface thickness between immiscible constituents, see [1]. The multiscale nature inherent in these models (interface thickness and domain size of interest) urges the use of space-adaptivity in discretization.

In this contribution we consider the a-posteriori error analysis of the convective Cahn–Hilliard [4] model for varying Péclet number and interface-thickness (diffusivity) parameter. The adaptive discretization strategy uses mixed finite elements, a stable time-stepping algorithm and residual-based a-posteriori error estimation [2, 5]. This analysis for the convective model forms a basic step in our research and will be helpful to the coupled Cahn–Hilliard/Navier–Stokes system [3] which is the desired model for future research.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

HEMODYNAMICS OF A STENOSED CAROTID BIFURCATION

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Key words: Carotid Artery Bifurcation; Stenosis; Imaging; 3D Reconstruction And Mesh Generation; Doppler Ultrasound.

Abstract. A methodology for patient-specific computational 3D reconstruction and structured hexahedral meshing of the carotid artery bifurcation with a stenosis is described. The purpose of this work is the use of anatomically realistic blood flow simulations by the finite element method derived from in vivo medical imaging to make patient specific studies of flow phenomena associated with the development of atherosclerosis disease. Blood flow is described by the incompressible Navier-Stokes equations and the simulation is carried out under pulsatile conditions. The study of a diseased carotid bifurcation illustrates the extremely complex hemodynamical behaviour along the cardiac cycle.

1 INTRODUCTION

Recent non-invasive medical imaging data acquisition made feasible to construct three dimensional models of blood vessels. Colour Doppler ultrasound is inexpensive, widely accessible, fast and safe, and provides real-time images of endovascular structure; also measuring techniques have improved to provide accurate information on the flow fields. Validated computational fluid dynamics models using data obtained by these currently available measurement techniques can be very valuable in the early detection of vessels at risk and prediction of future disease progression.

In this work flow characteristics in a patient-specific carotid bifurcation with a stenosis are investigated by using direct numerical simulation. Since the carotid is a superficial artery and it is quite suited for medical ultrasound imaging, a semi-automatic methodology for patient-specific reconstruction and structured meshing of the left carotid bifurcation is presented. As hexahedral meshes compared to tetrahedral/prismatic meshes converge better, and for the same accuracy of the result less computational time is required [1] a tool to generate suitable structured hexahedral meshes for vascular modelling frameworks from Doppler ultrasound images is considered.

Blood flow simulation models [2] using pulsatile inlet conditions based on in vivo color Doppler ultrasound measurements of blood velocity, allow to compare numerical results with experimental data collected in clinical practice. The three-dimensional, unsteady, incompressible Navier–Stokes equations are solved with the assumptions of rigid vessel walls and constant viscosity (Newtonian fluid).

The ultimate aim of this study is the reconstruction of geometry and flow environment from in-vivo patient data, particularly at the extra-cranial carotid arteries, using Doppler ultrasound data.

2 RESULTS AND DISCUSSION

The accuracy and efficiency of the blood simulation is validated comparing velocities given by numerical calculations with experimental data collected in clinical practice. Left carotid artery bifurcation geometry, blood flow velocities, as well as, the flow wave form defining one cardiac cycle were obtained. Numerical velocities at different cross-section locations are compared with Doppler ultrasound measurements. In order to elucidate the role of carotid hemodynamics on plaque vulnerability WSS distribution at various flow phases are studied.

This work addresses the hemodynamical environment of a diseased carotid bifurcation concluding to be extremely complex during systolic phase and significantly different from that of a healthy carotid bifurcation.

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ADMOS 2013
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NUMERICAL INTEGRATION OF WEAK FORM IN EMBEDDED INTERFACE METHODS

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Key words: Divergence theorem, embedded interface methods, integration over polyhedra, XFEM

Abstract. The numerical integration of weak form over the elements that are crossed by discontinuities in embedded interface methods is addressed in this work. Since these methods lead to complex shaped cut volumes, integration of weak form requires an efficient method for integration of polynomials over arbitrary polyhedra. Most widely, volume decomposition [1] or moment fitting methods [2] are used for such integrations. In this work, we present an efficient and robust method, based on the divergence theorem, for integration of polynomials over polyhedra. For a scalar function $\mathcal{F}$, using the divergence theorem, the integration over $\mathcal{R} \subset \mathbb{R}^3$ whose boundary is given by $\mathcal{S}$ can be written as,

$$\int_{\mathcal{R}} \mathcal{F} dV = \int_{\mathcal{S}} \mathcal{G} n_x \, dA; \quad where \quad \mathcal{G} = \int_{\kappa}^{\mathcal{S}} \mathcal{F} dx \tag{1}$$

where κ is an arbitrary reference point. $\mathcal{G}$ is evaluated by integrating $\mathcal{F}$ using one-dimensional Gauss quadrature, and then to compute the required integral, $\mathcal{G}$ is integrated using another set of Gauss quadratures defined on surfaces of the polyhedra. The method is extremely easy to implement, and we show through numerical examples that it is efficient as well.

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INNOVATION TOOL USING TAGUCHI-METHODS FOR DEVELOPMENT OF A NEW PRODUCT WITH OPTIMUM CONDITION

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Key words: Taguchi-methods, Tool, Optimum Condition, Innovation, Development, Trial

Abstract. As a development with short-term and lower cost is strongly required in 21st century. Therefore the innovation tool using Taguchi-methods [1], [2] for development of a new product with optimum condition was developed and evaluated. Flow-chart of the innovation tool using the Taguchi-methods is shown in Figure 1. The tool consists of two trials using the Taguchi-methods; these are "First trial for selection of the several important parameters" and "Second trial for decision of the optimum condition". In the First trial, all levers of all control factors should try for the final properties or the final functions. This trial is for picking out the important parameters and for throwing away the meaningless parameters. If difference of influence on the each level regarding a control factor in the effective figure of "the Sensitive" is very little, the control factor is judged to the meaningless parameter. And when SN ratio is very small, the level of the control factor is judged to low robustness. Only important parameters selected in the First trial are used in the Second trial. In this trial, each

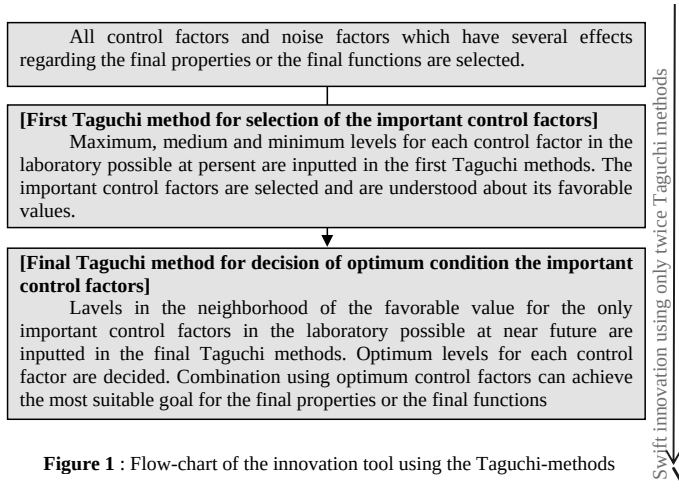

Figure 1 : Flow-chart of the innovation tool using the Taguchi-methods

important parameter is checked in more detail. If the important parameters require the larger or smaller level of a control factor for optimum condition, the new equipment for the larger or smaller level of the control factor is supplied in here. And if the important parameters require the level with high precision of the control factor for optimum condition, the new equipment with high precision is also then supplied in here. This second trial becomes the final trial, because optimum condition is decided in the second trial using innovation tool using Taguchi-methods with the best condition in the laboratory. This new method will be more proper than the conventional Taguchi-methods [3] or other methods [4],[5] for searching the optimum condition.

The optimum condition for polishing a minute die was investigated for evaluating this innovation tool in the experiment. Polishing tool and polishing procedure are shown in Figures 2 and 3, respectively[6]. This polishing tool consists of the pipe and the ball head with

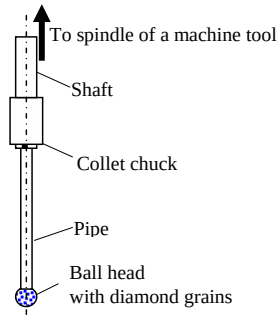

Figure 2: Schematic view of the polishing tool

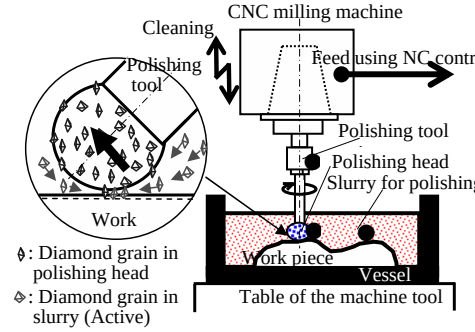

Figure 3: Schematic view of polishing (Principle)

Table 1: Best and worst conditions for the polishing

Polishing condition		Best condition	Worst condition
Spindle speed	min^{-1}	10000	9000
Feed speed	mm/min	0.5	0.7
Polishing pressure	MPa	140	100
Polishing pitch	mm	0.3	0.2

Polishing tool	Material of polishing head (Ball head)	Epoxy resin
	Diameter of polishing head (Ball head)	ϕ 1.0 mm
	Diamond grain in ball head (＃=Mesh size)	#2500
	Pipe	0.7 mm
Slurry	Base liquid	Water
	Diamond grain in slurry (＃=Mesh size)	#2500
	Rate of grain (slurry : diamond)	10 wt% (9:1)
	Ratio of PEO（Poly-ethylene-oxide）for water	2 wt%
Work piece		Carbide

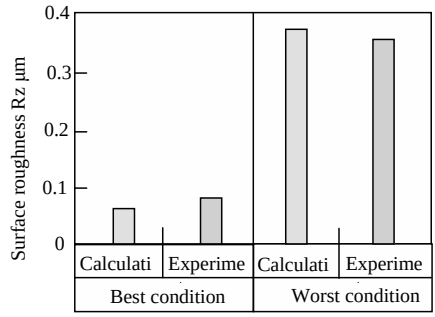

Figure 4 : Surface roughness of the polishing with best and worst conditions (By the innovation tool using Taguchi-methods)

diamond grains. Base material of the ball head is epoxy resin. Slurry consists of water, a polymer and diamond grains. The polishing tool is installed on the spindle of CNC milling machine, is rotating and moving in three dimensional directions by NC control. Several diamond grains in the polishing head and in the slurry can cut on the work piece. The polishing trace becomes very shallow because of soft ball head. However surface roughness of the work piece becomes very small because of shallow trace. After all, the polishing tool can polish to mirror-like surface. Particularly the ball head of the polishing tool has small diameter which is smaller than 1 mm. Therefore the polishing tool can polish a minute die.

The optimum condition for polishing tool is evaluated in the experiment. Polishing condition used in the experiment is shown in Table 1. Work piece material is carbide. Specifications of the polishing tool and the slurry are similar to the previous experiment. Best and worst conditions in the Second trial are included for the polishing conditions.

Surface roughness of the polishing with best and worst conditions is shown in Figure 4. The results of the experiment are similar to the calculated results by the innovation tool using Taguchi-methods. The optimum condition for polishing tool was decided by only twice trials. Therefore the innovation tool using the Taguchi-methods was useful for development with short-term and lower cost.

It is concluded from the result that (1) Innovation tool using the Taguchi-methods was useful for development with short-term and lower cost, and (2) This tool could quickly and exactly decide the optimum polishing condition.

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ANISOTROPIC ADAPTIVE FINITE ELEMENT MESHES FOR INCOMPRESSIBLE FLOWS

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Key words: anisotropic adaptive, level-set, embedded interface, embedded Dirichlet, incompressible flows

Abstract. Because of the increasingly complex geometries involved in flow problems of industrial relevance, numerical methods based on unstructured meshes have become popular in CFD. However, the corresponding meshing methods require a high-quality CAD description of the geometry, which is not part of the traditional workflow in fields like architecture or medicine. Many professionals also lack the expertise required to build appropriate meshes for flow problems. Nevertheless, recent progresses in meshing technology could overcome these barriers.

In this talk, we propose to use anisotropic adaption to generate a *nearly* body-fitted mesh. The mesh is locally refined depending on a level-set function that describes the geometry without resorting to a CAD model. Dirichlet boundary conditions can then be imposed in a strong manner by node collocation, just as with classical body-fitted meshes. Unlike other treatments of embedded geometries, this technique only requires a standard finite element formulation, without basis enrichement or Lagrange multipliers that alter its numerical properties.

In a first step, we apply this method to academic Poisson problems. We show that an appropriate level of local refinement around the geometry recovers the optimal grid convergence rate for the solution, whereas uniform refinement yields first-order convergence. Controlling the anisotropic character of the adaption further enables the error of the geometrical discretization to decrease at optimal rate, while there is no geometrical convergence with isotropic refinement. This affects particularly the computation of integral

quantities, such as lift and drag, in practical simulations. Anisotropic adaptive refinement also slows down the growth of the number of unknowns, which limits the computational overhead.

Then, we combine the embedded geometry treatment with iterative anisotropic adaption to the solution, for two incompressible flow problems involving respectively a cylinder and a NACA0012 airfoil. The methodology yields accurate flow solutions, despite very limited user interaction.

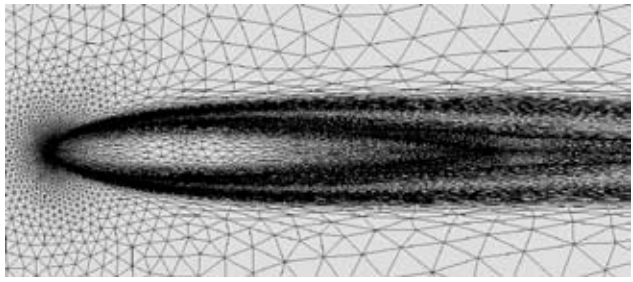

Figure 1: Anisotropic mesh adapted to the geometry and to the solution for the non-lifting incompressible flow around a NACA0012 airfoil at Reynolds number 5000.

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ADAPTIVE MODELING FOR PARTITIONED-DOMAIN CONCURRENT MULTISCALE CONTINUUM MODELS

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Key words: adaptive modeling, partitioned-domain concurrent multiscale modeling, a posteriori error estimates, shape derivatives

Abstract. In this contribution adaptive modeling strategies are considered for the control of modeling errors in so-called partitioned-domain concurrent multiscale models. In these models, the exact fine model is considered intractable to solve throughout the entire domain. It is therefore replaced by an approximate multiscale model where the fine model is only solved in a small subdomain, and a coarse model is employed in the remainder.

We review two approaches to adaptively improve the approximate model in a general framework assuming that the fine and coarse model are described by (local) continuum models separated by a sharp interface. In the classical approach [1] an a posteriori error estimate is computed, and the model is improved in those regions with the largest contributions to this estimate. In the recent shape-derivative approach [2] the interface between the fine and coarse model is perturbed so as to decrease a shape functional associated with the error. Several numerical experiments illustrate the strategies.

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Phase-field-driven model adaptivity

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October 4, 2012

Methods for coupling two compatible models have been developed during the last decade or so to simulate problems for which one may identify a small subregion where the assumptions of a *coarse-scale model* break down and whose physical behavior should rather be described by some *fine-scale* model. Examples of blending techniques to couple continuum models with non-local particle models can be found, for instance, in [1, 2]. The main motivation in using such approaches is that fine-scale models are usually too expensive to be employed in the entire domain Ω due to their small length- and time-scale features and their nonlinear behavior. Therefore, the idea is to use the fine model only in a subdomain $\omega \subset \Omega$, where it is deemed necessary, and the coarse-scale model in the remainder of Ω, except in a layer separating these two within which one imposes a gradual transition, via a so-called weighting or *blending function*, from the fine-scale to the coarse-scale model. More concretely, the blending function has value unity in the region of the fine-scale model, zero in the region of the coarse-scale model, and monotonically varies from unity to zero between these two regions.

Questions that naturally arise are how to quantify the errors incurred by substituting a hybrid model for the fine-scale model and how to choose the domain of the fine-scale model in an optimal way. Note that errors and optimality should be measured in terms of a quantity of interest $Q = Q(u)$, a functional of the solution u of the problem, that characterizes the goal of the simulations. Goal-oriented adaptivity provides a framework to estimate, and substantially control, these approximation errors. Finding the optimal configuration of the coupled problem can be achieved by considering the blending function as an unknown and determining its optimal shape. We develop here a phase-field formulation to solve for the blending function as the problem drives the solution either to the value one or to the value zero with a smooth, narrow transition in between. In addition, a phase-field model satisfies a gradient flow structure, for which an energy is minimized. By adding to the energy functional the error in the quantity of interest, one can thus determine the evolution of the blending function that drives down the error with respect to the goal.

The phase-field formulation for model blending adaptivity will be explored on a simple problem that couples a fourth-order partial differential equation model (the fine-scale model that incorporates non-local effects) with a second-order partial differential equation model (the coarse-scale model that ignores those non-local effects). In particular, we will present some mathematical properties of the formulation, provide some numerical results, and discuss the viability of the methodology.

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Error assessment for timeline-dependent quantities of interest in transient elastodynamics

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ABSTRACT

This work presents a new approach to assess the error in specific quantities of interest in the framework of linear elastodynamics. In particular, a new type of quantities of interest (referred as timeline-dependent quantities) is proposed. These quantities are scalar time-dependent outputs of the transient solution which are better suited to time-dependent problems than the standard scalar ones available in the literature [1]. The proposed methodology furnishes error estimates for both the standard scalar and the new timeline-dependent quantities of interest. The key ingredient is the modal-based approximation of the associated adjoint problems which allows efficiently computing and storing the adjoint solution.

The adjoint solution is readily post-processed to produce an enhanced solution, requiring only one spatial post-process for each vibration mode and using the time-harmonic hypothesis to recover the time dependence. The recovery procedure of the vibration modes is very simmilar to the one presented in [2]. The proposed goal-oriented error estimate consists in injecting this enhanced adjoint solution into the residual of the direct problem. The resulting estimate is very well suited for transient dynamic simulations because the enhanced adjoint solution is computed before starting the fordward time integration of the direct problem. Thus, the cost of the error estimate at each time step is much reduced.

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ON THE FEASIBILITY OF GOAL-ORIENTED ERROR ESTIMATION FOR SHIP HYDRODYNAMICS

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Abstract. The goal of this paper is to investigate the use of adjoint-based techniques of error estimation for the simulation of the flow around ships. These flows are characterised by turbulence at very high Reynolds numbers as well as complex geometries and flow topologies, which generally involve separation and reattachment zones on the aft part of the ship. For simulation in a finite-volume context, this means that grids with high aspect-ratio cells are used. Also, the flow is strongly nonlinear and is expected to be away from the asymptotic range of grid convergence for realistic grids.

Given this context, we will investigate whether goal-oriented error estimation is possible for such flows. The work is based on the ISIS-CFD unstructured finite-volume Navier-Stokes solver developed by ECN-CNRS, which has been optimised for the simulation of hydrodynamic flows and has a proven record of reliability and accuracy for such simulations [1,2]. The solver has a face-based discretisation of the fluxes and is therefore suitable for arbitrary unstructured grids. Pressure-velocity coupling is achieved through a segregated SIMPLE-like resolution procedure.

The paper indicates first how we see the concept of goal-oriented error estimation in a finite-volume context. Then the continuous adjoint solver developed for ISIS-CFD is described. While this solver reuses as much as possible the discretisation and resolution procedures of the primal solver, the existing flux discretisation cannot be used due to the non-conservative nature of the adjoint convective terms. We show how stability can be achieved through a combination of central and upwind discretisation for these terms. Finally, with minor modifications, the SIMPLE-like pressure-velocity coupling can be maintained.

Adjoint error estimation for finite volumes requires a high-order accurate evaluation of the local residuals. This is obtained by substituting the numerical solution in a finite-volume discretisation which uses least-square fitting of third-order polynomials for the reconstruction of the solution from the cell centres to the face centres and nodes, followed by quadrature integration of the fluxes over the faces. While this procedure is accurate, it is sensitive to the reduced stencils available at the domain boundaries. We demonstrate extrapolation to ghost cells behind the boundary, which reduces this problem.

Finally, the usefulness of the error estimation procedure is investigated for 2D airfoils and 3D ship geometries. It is shown that due to the nonlinearity of the flow and the presence of turbulence, the error estimates are not sufficiently accurate to be used as a correction term for the computed functionals. However, in many cases the estimation gives a good indication of the actual error. It may be possible to improve the estimation further by finding a better reconstruction of the local residuals.

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ADAPTIVE SPACE-TIME FINITE ELEMENT METHOD FOR A NONLINEAR EVOLUTIONARY MONOTONE PROBLEM FROM APPLIED SUPERCONDUCTIVITY

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Key words: adaptivity, error estimation, space-time, finite element method, Maxwell's equations, nonlinear parabolic PDE, superconductivity

Abstract. The steady improvement of the performances of high temperature superconductors (HTS) brings them within reach of new applications, such as HTS motors, transformers and fault current limiters. To optimize the design of these devices, one must be able to predict the magnetic and electric fields in complex 3-D geometries, but doing so efficiently and accurately is still a challenging task. Within the engineering community, phenomenological models relating the electric field and current density of HTS lead to a novel nonlinear evolutionary monotone PDE based on Maxwell's equations, which is effectively a generalization of the classical p-Laplacian problem. Unfortunately, these models possesses sharp moving fronts that lead to the use of prohibitively small time steps in numerical simulations, even in 2-D domains.

In this work, we propose a new numerical space-time method that allows for local space and time adaptivity without the restrictive global timestep constraint. We present an a posteriori error estimator for the computation of the AC loss, a key design parameter for HTS devices. Numerical results are presented in one and two space dimensions attesting to the efficiency of the numerical method.

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MOVING NODES ADAPTION COMBINED TO MESHLESS METHODS FOR SOLVING CFD OPTIMIZATION PROBLEMS

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Key words: Adaptive meshless method, Sub-clouds, Nash algorithms, Drag minimization, Multi-objective problem.

Abstract. In past decades, many adaptive mesh schemes have been developed and become important tools for designers to simultaneously increase accuracy of their computations and reduce the cost of numerical computations in many engineering problems. In most of the cases the adaptation is done by subdividing cells or elements into finer cells or elements. Maintaining mesh quality during optimization procedure is still a critical constraint to satisfy for accurate design. In the discretized approach using meshless methods, there are no cells or elements but only a cloud of points which flexibility is an advantage compared to the mesh topology constraint. This attractive property facilitates the coupling of meshless methods with adaptive techniques for inverse or optimization problems.

In this paper, an algebraic adaptive meshless scheme based on a weighted reference radius equi distribution is presented. Cloud nodes adaption combined to meshless methods are used to solve inverse and drag minimization Computational Fluid Dynamics (CFD) problems.

The adaptive meshless method coupled with advanced Evolutionary Algorithms (EAs) is considered as a first test case to rebuild via prescribed surface pressure target the shape of the circular arc bump or ogive operating at supersonic shocked flow regimes. The objective functions could be chosen as the distance between candidate and prescribed pressure coefficients minimized in L_2 norm and uniform level of errors minimized in L_2 norm.

Then, a second optimization problem solved with cloud nodes adaption, namely the drag minimization of a natural laminar flow airfoil (RAE5243) operating at a Mach number 0.68 and a fixed lift coefficient 0.82 with an active shock control bump is conducted by controlling a uniformly distributed level of errors in the computational domain minimized using a sub-clouds and Nash game strategy. The two minimized objective are the shock drag satisfying a fixed lift constraint and the distance of the level of errors to a desired accuracy minimized in a L_2 norm.

Numerical results demonstrate numerically that adaptive meshless methodology presented in this paper can provide efficiently optimization solutions with a desired accuracy in aerodynamics. Results will be compared with other adaption methods, namely the so called goal oriented method.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

ABOUT THE GENERATION OF UNSTRUCTURED MESH FAMILIES FOR GRID CONVERGENCE ASSESSMENT BY MIXED MESHES

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Key words: Grid Generation, Unstructured Meshes, Anisotropic Meshes, Mixed Meshes, CFD.

Abstract. This work describes properties of the mixed mesh approach that are especially suitable for generating families of meshes to assess the grid refinement convergence of CFD solvers. The paper outlines how a regular grid refinement is achieved throughout the domain. The distributions of characteristic grid quality metrics are compared and a grid convergence study is outlined for a commonly used case for outer aerodynamics, the Boeing CRM configuration of the 5th AIAA Drag Prediction Workshop.

1 INTRODUCTION

The assessment of the order of a simulation method is a crucial step during the verification and validation process of the simulation software. Even the best mathematically derived formulation has to prove the rate of convergence with increasing mesh resolution for designated applications.

For applications of CFD for aerodynamics of aircrafts a series of five workshops has been organized under the governance of the American Institute of Aeronautics and Astronautics (AIAA) [1]. A major focus of the comparisons of solvers for simulation accuracy was laid on the grid convergence, for which families of grids have been provided, both structured and unstructured ones. A major conclusion of all workshops has been the highly demanding generation of unstructured mesh families.

While for structured meshes the generation of self-similar grids with different but regularly refined grid resolutions is straight forward, for unstructured hybrid meshes this is a more complicated task. Due to the – in most cases – fully automatic generation a distinct control on local mesh resolution and there influence into other parts of the mesh is hard to control.

This paper outlines the usability of the mixed mesh approach for the purpose of generating families of meshes for grid convergence assessment. Block-unstructured mixed meshes provide structured meshes in the near field of the aerodynamic boy where viscous effects dominate and a high resolution normal to the wall is needed. In contrast to pure block-structured meshes, limitations of topologies are overcome by locally using unstructured mesh element types, mainly prismatic elements. For the outer field an a priori defined anisotropic

field triangulation is applied to allow for maximum flexibility and to minimize the effort of user input.

2 THE MIXED MESH FRAMEWORK

The meshing framework used is the formerly structured multi-block grid generation MegaCads developed at DLR [2]. In recent years unstructured capabilities have been introduced. Among these are a parabolic marching procedure to generate prismatic layers based on the same mathematical approach as used in the elliptic smoothing of structured blocks [3][4], the linking to a number of volume triangulation codes including the SIMMETRIX software [5] used within this work, and a memory efficient way to specify a priori a smooth anisotropic metric field for the triangulation smoothly adopting to the underlying structured and quasi-structured elements [6].

Figure 1 shows a view on the grid family around the Boeing Common Research Model (CRM) [7] depicting the meshing strategy by coloring the different types of grid elements. The boundary layer regions of the wing are meshed with structured mesh blocks. The implicit anisotropy of the structured meshes allows for much less grid points than in unstructured meshes while retaining a high grid density in circumferential direction. For the grid family the number of cells in each direction is multiplied by a factor of 1.5 for adjacent grid levels, while the cell sizes are reduced by the same magnitude. The portion of the fluid volume meshed by structured elements is not changed in order to obtain self-similar meshes

The wing tip and the fuselage are covered by prismatic elements, since for these objects usually the generation of a suitable block-structured topology is more challenging, sometimes impossible. The outer flow field is filled with tetrahedrons. The used method derives a smooth anisotropic metric field based on the anisotropy of the adjacent structured hexahedrons and quasi-structured prisms. This anisotropic metric field is inherently responsible to achieve the self-similarity and grid family properties in the unstructured domain of the meshed volume.

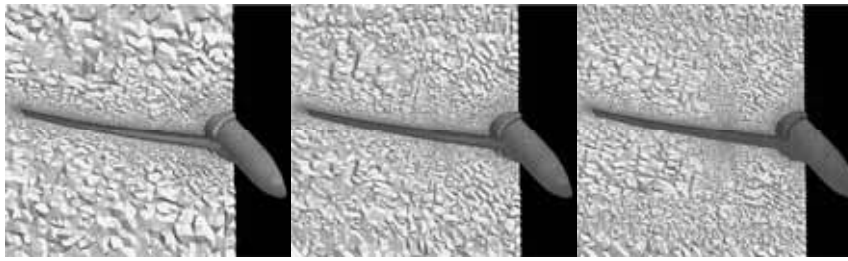

Figure 1: Family of grids around the Boeing CRM configuration, left to right: coarse – medium – fine; colors indicate cell type: red=hexahedrons, blue=prisms, green=tetrahedrons

3 GRID CONVERGENCE OF THE BOEING CRM CASE

3.1 Grid quality indicators

The selection of indicators for a priori grid quality assessment has to respect the type of solver later on used for the simulation. For finite element methods (FEM) most commonly used are indicators that look for the shape of single elements and detecting badly shaped cells like slivers, needles, and hats that inherently disrupt the numerical accuracy of the solution. For the targeted finite volume (FVM) flow solver these element based metrics are of less significance since for the flux computations needed the relationship of neighboring elements is at least as important. Knupp [8] introduced algebraic grid quality metrics based on the Jacobian of elements, which are the transformation matrices from computational into physical space. They are more representative, since the averaging of the cell based Jacobians for a common grid node provide an indication for the smoothness of the surrounding cells. In the following two of the metrics provided by Knupp's MESQUITE library are used to show the comparability of the generated grids in the sense of self-similarity for a family of grids. **Figure 2** shows the histogram of the variations of the "local size" quality metric for the three generated meshes around the Boeing CRM. A value of one indicates that all elements surrounding a grid node have the same size. The counts of grid nodes in the histogram are normalized by the number of overall grid points and are plotted on a logarithmic axis to more precisely inspect the behavior of the different grid levels at values of the lower quality metric values. The figure shows that the distributions of the "local size" quality metric is nearly identical for all three mesh levels indicating that the characteristics of the grid are not depending on the grid size in this respect. **Figure 3** shows a histogram for the vertex based condition number, which is an average of the condition numbers of the Jacobians of the elements surrounding a grid node. Since the targeted meshes are anisotropic high values of are expected since the value directly reflects the anisotropy of the grid. The histogram shows that the generated grids show similar distributions of anisotropy in the mesh and therefore the needed self-similarity.

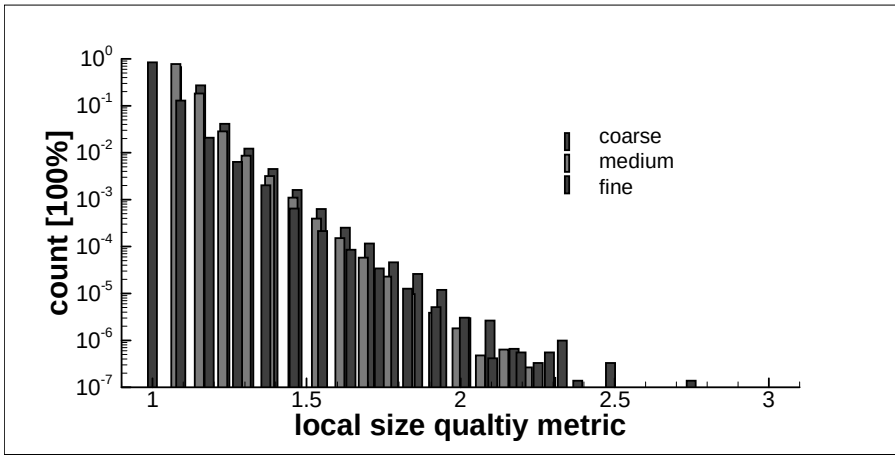

Figure 2: historgamms of local size variation of the cells around a grid node for three mesh levels of the grids around the Boeing CRM.

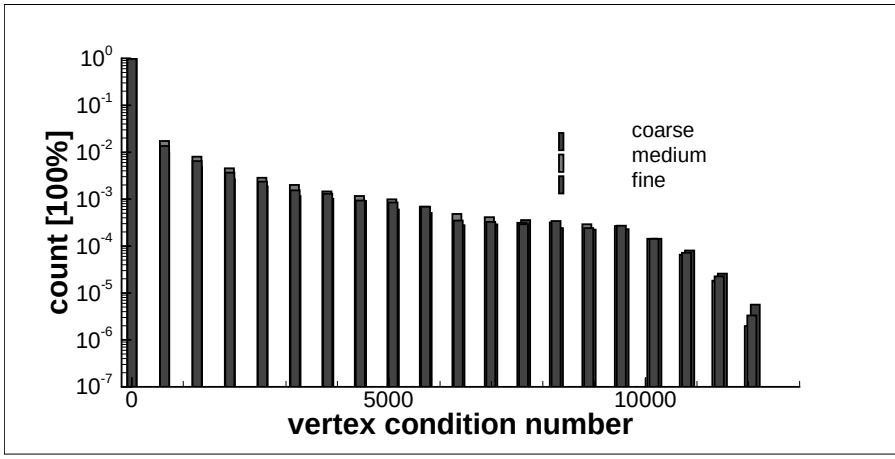

Figure 3: Histogram of the vertex based condition number variation for three mesh levels of the grids around the Boeing CRM.

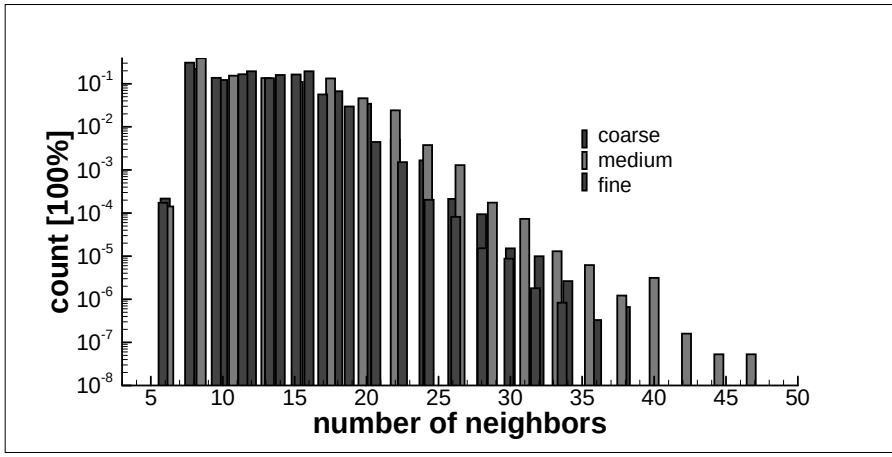

Figure 4: Histogram of the variation of the number of neighbors of a grid node for three mesh levels of the grids around the Boeing CRM.

Another important indicator of the suitability of a grid for CFD is the local number of neighbors to a grid node. Meshes often degrade the simulation quality by having local hot-spots of the neighboring node count. Especially hybrid meshes where the anistoroby of quasi-structrured cells is not respected can have up to 200 neighboring nodes and the flux computations are comprised by this. **Figure 4** shows the distribution of the number of neighboring nodes and – again – shows that the characteristics of the three mesh levels are very similar.

3.2 Grid convergence assessment

The final contribution will contain an assessment of the grid convergence of the second order finite volume CFD solver TAU. The assessment will be made based on overall aerodynamic characteristics and on the contributions of local parts to show the suitability of the mixed mesh approach for such studies in global and local effects.

4 CONCLUSIONS

The mixed meshing approach allows for the generation of mesh families for the assessment of grid convergence behavior of CFD solvers. The use of block-structured cells in near wall regions inherently possesses this capability. The derivation and usage of an adjacent smooth anisotropic metric field for the flow field triangulation promotes the self-similarity of the structured part of the mesh into the unstructured part.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

ADJOINT BASED A POSTERIORI ERROR ESTIMATES USING DATA COMPRESSION

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Key words: data compression, adjoint problem, error analysis, Navier-Stokes

Abstract. One of the major computational burdens in the application of adjoint techniques to time-dependent nonlinear problems is the need to store the full forward approximation to define the adjoint of the linearized forward problem and to evaluate the dual-weighted residual [1, 2]. An approach for mitigating the storage cost is checkpointing, whereby the forward solution is stored at a series of carefully selected time nodes. During an adjoint computations these checkpoints are used to reconstruct the forward solution, recomputing on each subinterval as needed. A notable implementation of the checkpointing scheme is the REVOLVE [3] algorithm. This method minimizes the number of recomputations of the forward solution at any timestep allowing for a fixed storage budget and fixed number of time steps. Recent versions of this algorithm permit a varying number of timesteps with bounded maximum number of recomputations, albeit with a slowly growing storage cost [4]. These approaches successfully reduce the storage cost when the exact solution to the forward problem is required. However, the cost of recomputing the forward solution may be to great of a burden for some applications.

We relax the assumption that the computed forward solution is needed to evaluate the adjoint when used in goal-oriented error estimation. We show that the accuracy of the forward solution has limited effect on the accuracy of the error estimate, and use this to develop a method for approximation of the forward solution that gives reasonably good error estimates. To this end, a number of data compression algorithms are proposed where the storage cost of the approximate foward solution is small compared to storing the exact forward solution. Yet the accuracy of the resulting error estimates are of good quality and no recomputations of the forward solution are required.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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ADAPTIVE TIME-STEPPING FOR CAHN-HILLIARD-TYPE EQUATIONS WITH APPLICATION TO DIFFUSE-INTERFACE TUMOR-GROWTH MODELS

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Key words: Adaptive time-stepping, Second-order time-accurate algorithms, Diffuse-interface tumor-growth model, Cahn-Hilliard equation

Abstract. Many tumor-growth phenomena can be considered as multiphase problems. Employing the continuum theory of mixtures, phase-field tumor-growth models can be derived with diffuse interfaces. The chosen form of the Helmholtz free-energy leads to equations of the Cahn-Hilliard type. Such nonlinear fourth-order partial-differential equations are time-dependent, and their solutions exhibit alternating fast and slow variations in time. It is therefore of prime importance to use adaptive time-stepping to efficiently simulate the entire dynamics of the system [1].
In this contribution, we consider a thermodynamically consistent four-species model of tumor growth in which the energy is non-increasing and total mass is conserved [2]. In order to inherit the two main characteristics of the system at the discrete level, we propose a gradient-stable time-stepping scheme with second-order accuracy. Mixed finite elements are used for spatial discretization. For this discretization, we discuss simple adaptive time-stepping strategies as well as a posteriori error estimates in time. Furthermore, we present illustrative numerical results.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
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EFFECTIVE APPLICATION OF THE EQUILIBRATED RESIDUAL METHOD IN ERROR ESTIMATION OF THE HP-APPROXIMATED 3D-BASED MODELS OF COMPLEX STRUCTURES

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Abstract. The paper recalls our previous theoretical results on [1] hierarchical modeling and adaptive analysis of complex structures (described with more than one mechanical model). Within such structures we apply 3D-based approach utilizing only three-dimensional degrees of freedom. The proposed estimation method [2] is based on the equilibrated residual one [3] and is applied to the assessment of the global, total and approximation errors. The global modeling error is obtained as a difference of the former two errors. The global modeling error estimate and the element contributions to it allow for the adaptive hierarchical modeling within first order shell, hierarchical shell and the corresponding transition (either shell-to-shell or solid to-shell) domains of complex structures. Both, the change of the mechanical model or q-adaptivity are possible, with q denoting the transverse order of approximation within hierarchical shell models. In the recalled approach also adaptive 2D, 3D or mixed (2D/3D) hp-approximations are possible in the shell, solid and transition zones of the complex structures, respectively, with h standing for the averaged element dimension and p denoting the longitudinal or three-dimensional order of approximation. The element contributions to the estimated global approximation error serve these two types of adaptivity.

In the above described context, it is very important to have the estimation method which can satisfy the specific needs of the complex structures 3D-based modeling and analysis and delivers sufficiently accurate estimated values of the global errors, and acceptable element contributions to them as well. In order to satisfy the mentioned needs we extend the existing algorithms of the equilibrated residual method [4, 5], applied so far to either three-dimensional elasticity [6] or conventional hierarchical shell models [7], onto the analysis of 3D-based first-order shell models [8, 9], 3D-based hierarchical shells and transition models as well. In particular we show unpublished technical details on how to apply this method to the 3D-based (constrained) shell model of the first order and the corresponding transition models as well. Such an application needs different equilibration procedure than the three-dimensional equilibration applied to 3D-elasticity (or hierarchical shells) and performed in the global directions. The adopted approach requires introduction of the local nodal directions and different treatment of the constrained and unconstrained ones.

In order to assess the quality of the equilibrated residual method we compare three versions of the method. The differences between these versions are visible while defining the element

local problems. Let us remember that the collection of solutions to such problems serves as a base for the assessment of the approximation of the exact global solution. In the first version we average the interelement stress fluxes, in the second one we perform linear (element vertex nodes)equilibration of these fluxes, while in the third one we constrain local problems at element vertices with global displacements. Then, for the most effective version (the third one), we perform unique parametric studies of the modeling, approximation and total error estimations. These studies include such important factors as: orders p and q, the element size h, the structure thickness, the applied mechanical model, the problem type, and mechanical complexity of the model. Our studies are completed with an analysis of the results. This analysis leads to practical hints concerning appropriate definitions of the local problems, so as to assure the most effective error estimation within complex structures.

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VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Pares (Eds)

ANALYSIS OF LINEARIZATION ERROR FOR GOAL-ORIENTED ADAPTIVITY OF NONLINEAR PROBLEMS

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Key words: Nonlinear primal problem, Linearization error, Refinement indicators

Abstract. We propose in this talk to address the issue and effect of linearization in the quality of the error estimates in quantities of interest for strongly nonlinear problems (see e.g. [1, 2]). It is well known that the error representation in this case can be decomposed into two contributions: 1) one contribution in the form of the product of the residual by the solution of a linearized adjoint problem that describes the discretization error and 2) the other contribution that combines all higher-order terms with respect to the error in the primal solution that describes the linearization error. In most works on goal-oriented error estimation, the linearization error contribution is usually neglected with respect to the discretization error. However, when the nonlinear effects are significant, one cannot assume any longer that the latter is dominant over the former. In fact, it becomes obvious in those cases that linearization errors should be also controlled. We will present here the construction of refinement indicators that combine both sources of errors in order to simultaneously control those in a balanced manner.

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AUTHOR INDEX

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Numerical Modeling and Simulation is increasingly used as a complement to Experimental Modeling and Analysis and as a design or certification tool in engineering applications. However, after more than thirty years of worldwide research efforts around Adaptive Modeling and Simulation, the problem of properly assessing and controlling the quality of the numerical solutions is still relevant, as the design of sophisticated engineering systems requires increasingly complex and coupled modeling, which leads to increasingly time-consuming computations. Adaptive approaches, which provide reliable and cost efficient modeling and coherent coupling of different scales and mechanisms in a unique model, are more strategic and indispensable than ever.