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Computational Engineering

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Abstract. The focus of this Computational Engineering Workshop was on the mathematical foundation of state-of-the-art and emerging finite element methods in engineering analysis. The 52 participants included mathematicians and engineers with shared interest on discontinuous Galerkin or Petrov-Galerkin methods and other generalized nonconforming or mixed finite element methods.

Mathematics Subject Classification (2010): 65K15, 65N15, 65N25, 65N30, 65N50, 65N55, 74B05, 74B20, 74G15, 74S05.

Introduction by the Organisers

This Computational Engineering Workshop at Oberwolfach focused on mathematical and numerical aspects of emerging methodologies in mixed and nonstandard finite element methods and their applications in computational engineering. This large class of numerical methods included adaptive methods, classical nonconforming methods, h-p finite element methods, discontinuous Galerkin methods, discontinuous Petrov-Galerkin methods, generalized finite element methods, mixed and hybrid methods, multiscale methods, virtual finite element methods, kinetic methods, mortar methods, mapped tent-pitching methods and the finite cell method.

Application areas included electromagnetics, solid mechanics, fluid dynamics and optimal control.

Thirty three talks were given during the main part of the workshop. A special Thursday evening "After Dinner Special" was also held, which highlighted the research of some of the younger participants.

The workshop continued the older tradition of fruitful interactions of applied mathematics and computational engineering at Oberwolfach with rewarding outcomes like the Priority Program 1748 “Reliable simulation techniques in solid mechanics. Development of non-standard discretization methods, mechanical and mathematical analysis” of the German Research Foundation.

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Workshop: Computational Engineering

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Abstracts

DPG Methods for Maxwell Equations

Jay Gopalakrishnan
(joint work with Carsten Carstensen, Leszek Demkowicz)

A DPG method for the time-harmonic Maxwell equations in an electrically sealed cavity Ω can be designed starting from a weak formulation in $\mathring{H}(\text{curl}, \Omega)$. Like other DPG methods, this method is also made easily implementable using a "broken" test space, i.e., space of functions with no continuity constraints across mesh element interfaces, derived from the standard "unbroken" space $\mathring{H}(\text{curl}, \Omega)$. Letting Ω_h denote the mesh partitioning of Ω, consisting of elements K with Lipschitz boundaries, the broken space is

$$H(\text{curl}, \Omega_h) = \prod_{K \in \Omega_h} H(\text{curl}, K).$$

We then present a variational formulation for the Maxwell equations using $H(\text{curl}, \Omega_h)$. As an illustration of a general principle [1] that allows one to conclude that

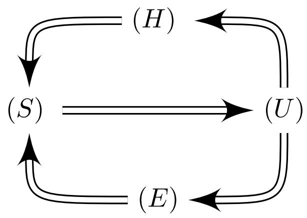
$$\left.\begin{matrix}\text{Stability of standard} \\ \text{"unbroken" formulation}\end{matrix}\right\} \implies \left\{\begin{matrix}\text{Stability of} \\ \text{"broken" formulation,}\end{matrix}\right. \tag{1}$$

in this talk, we present a full proof of the stability of a DPG formulation for Maxwell equations. An ingredient in the proof, that has applications beyond the DPG method, is an elementary proof of

$$\|n \times E\|_{H^{-1/2}(\text{div}, \partial K)} = \|n \times E\|_{[H^{-1/2}(\text{curl}, \partial K)]^*}$$

for any E in $H(\text{curl}, K)$. The proof uses a simple relationship between the norm of a minimal $H(\text{curl}, K)$-norm extension and the norm of the inverse of a Riesz map applied to $n \times E$.

The Maxwell cavity problem admits a plethora of weak forms, depending on which of its equations are treated weakly. Two standard formulations in $\mathring{H}(\text{curl}, \Omega)$ are the "electric form" (E) (obtained by eliminating the magnetic field) and the "magnetic form" (M) (obtained by eliminating the electric field). A less standard form is the "ultraweak form" (U) obtained by weakly imposing both the equations of the Maxwell system. The "strong form" (S) imposes both the equations strongly. We report our results that show that the stability of one formulation implies the stability of any other, via the following diagram of stability implications.



The proof of these implications, as well as application of the general principle (1) to problems other than Maxwell equations, can be found in [1].

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Rate optimality of adaptive algorithms with separate marking

Hella Rabus
(joint work with Carsten Carstensen)

Mixed finite element methods with flux errors in $H(\mathrm{div})$-norms and div-least-squares finite element methods require the separate marking strategy in obligatory adaptive mesh-refining. The refinement indicator $\sigma_\ell^2(K) = \eta_\ell^2(K) + \mu^2(K)$ of a finite element domain K in a triangulation $\mathcal{T}_\ell$ on the level ℓ consists of some residual-based error estimator η_ℓ with some reduction property under local mesh-refining and some data approximation error μ_ℓ. Separate marking (Safem) means either Dörfler marking if $\mu_\ell^2 \leq \kappa\eta_\ell^2$ or otherwise an optimal data approximation algorithm run with controlled accuracy as established in [CR11, Rab15] and reads as follows

for $\ell = 0, 1, \ldots$ **do**
  Compute $\eta_\ell(K)$, $\mu(K)$ for all $K \in \mathcal{T}_\ell$
  if $\mu_\ell^2 := \mu^2(\mathcal{T}_\ell) \leq \kappa\eta_\ell^2 \equiv \kappa\eta_\ell^2(\mathcal{T}_\ell)$ **then**
    $\mathcal{T}_{\ell+1} := \texttt{Dörfler\_marking}(\theta_A, \mathcal{T}_\ell, \eta_\ell^2)$
  else
    $\mathcal{T}_{\ell+1} := \mathcal{T}_\ell \oplus \texttt{approx}(\rho_B \mu_\ell^2, \mathcal{T}_0, \mu_\ell^2)$.

The enfolded set of axioms simplifies [CFPP14] for collective marking (with $\sigma^2 = \eta^2 + \mu^2$ for Case A and $\mu^2 \equiv 0$ for Case B), treats separate marking established for the first time in an abstract framework, generalizes [CP15] for least-squares schemes, and extends [CR11] to the mixed FEM with flux error control in $H(\mathrm{div})$.

The axioms (A1)–(A4) involve $\rho_2 < 1, \Lambda_k < \infty$, estimators σ, η, μ and and distances $0 \le \delta(\mathcal{T}, \hat{\mathcal{T}}) < \infty$ for all $\in \mathcal{T} \in \mathbb{T}$ and $\hat{\mathcal{T}} \in \mathbb{T}(\mathcal{T})$ and are sufficient for optimal asymptotic convergence rates. There exists $\mathcal{R} \subset \mathcal{T}$ such that $\mathcal{T} \setminus \hat{\mathcal{T}} \subseteq \mathcal{R} \wedge |\mathcal{R}| \le \Lambda_3 |\mathcal{T} \setminus \hat{\mathcal{T}}|$ and

$$\text{(A1)} \qquad |\eta(\hat{\mathcal{T}}, \mathcal{T} \cap \hat{\mathcal{T}}) - \eta(\mathcal{T}, \mathcal{T} \cap \hat{\mathcal{T}})| \le \Lambda_1 \delta(\mathcal{T}, \hat{\mathcal{T}}),$$

$$\text{(A2)} \qquad \eta(\hat{\mathcal{T}}, \hat{\mathcal{T}} \setminus \mathcal{T}) \le \rho_2 \eta(\mathcal{T}, \mathcal{T} \setminus \hat{\mathcal{T}}), + \Lambda_2 \delta(\mathcal{T}, \hat{\mathcal{T}})$$

$$\text{(A3)} \qquad \delta(\mathcal{T}, \hat{\mathcal{T}}) \le \Lambda_4 \left(\eta(\mathcal{T}, \mathcal{R}) + \mu(\mathcal{T}) \right) + \Lambda_5 \eta(\hat{\mathcal{T}}),$$

$$\text{(A4)} \qquad \sum_{k=\ell}^{\infty} \delta^2(\mathcal{T}_k, \mathcal{T}_{k+1}) \le \Lambda_6 \sigma_\ell^2 \quad \text{for all } \ell \in \mathbb{N}_0,$$

$\forall\, \mathrm{Tol} > 0$ $\mathcal{T}_{\mathrm{Tol}} = \texttt{data\_approx}(\mathrm{Tol}, \mathcal{T}_0, \mu^2) \in \mathbb{T}$ satisfies $\mu^2(\mathcal{T}_{\mathrm{Tol}}) \le \mathrm{Tol}$ and

$$\text{(B1)} \qquad |\mathcal{T}_{\mathrm{Tol}}| - |\mathcal{T}_0| \le \Lambda_7 \, \mathrm{Tol}^{-1/(2s)},$$

$$\text{(B2)} \qquad \mu^2(\hat{\mathcal{T}}) \le \Lambda_8 \mu^2(\mathcal{T}).$$

Theorem. SAFEM *with (A1)-(A4), (B1)-(B2) leads to optimal convergence rates for total estimator provided* $\theta_A < \theta_0 := 1/(1 + \Lambda_2^2 \Lambda_3)$ *and* $\kappa < \kappa_0 := (1 - \rho_A)/(\Lambda_6 - 1)$ *plus quasimononicity (e.g. for* $(\Lambda_1^2 + \Lambda_2^2)\Lambda_5^2 < 1$*) in the following sense*

$$\sup_{N \in \mathbb{N}_0} (1+N)^s \min_{\mathcal{T} \in \mathbb{T}(N)} \sigma(\mathcal{T}) \approx \sup_{\ell \in \mathbb{N}_0} (1 + |\mathcal{T}_\ell| - |\mathcal{T}_0|)^s \sigma_\ell.$$

Example. Besides from natural a posteriori error control with residuals in least squares functional, [CP15] establishes an a posteriori error estimator $\sigma_\ell^2(K) := \eta_\ell^2(K) + \mu^2(K)$ in $H(\mathrm{div}, \Omega)$ with $\mu^2(K) := \|f - \Pi_\ell f\|_{L^2(K)}^2$. Since μ does not satisfy an estimator reduction SAFEM has to be applied instead of collective marking. The proof of discrete reliability (A3) (for $k = 0$) still leaves the extra term

$$\begin{aligned} &\|p_{\ell+m} - p_\ell - \nabla(u_{\ell+m} - u_\ell)\|_{L^2(\Omega)}^2 + \|\mathrm{div}(p_{\ell+m} - p_\ell)\|_{L^2(\Omega)}^2 \\ &\lesssim \eta_\ell^2(\mathcal{T}_\ell \setminus \mathcal{T}_{\ell+m}) + \|(1 - \Pi_\ell)\,\mathrm{div}\, p_{\ell+m}\|_{L^2(\Omega)}^2, \end{aligned}$$

which is not covered in [CFPP14]. The presented set of generalized axioms coveres this special application [CR15].

Final Remark. The presented set of axioms guarantees rate optimality for AFEMs based on collective and separate marking and covers existing literature of rate optimality of adaptive FEM. Separate marking is necessary for least-squares FEM and mixed FEM with convergence rates in $H(\mathrm{div}, \Omega) \times L^2(\Omega)$.

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An HDG-DG IMEX Scheme for Shallow Water System on the Globe

Tan Bui-Thanh
(joint work with Shinhoo Kang, Frank Giraldo)

We extend our previous work [1] on upwind hybridized discontinuous Galerkin (HDG) to the nonlinear system of shallow water equations on the globe. The governing partial differential equations read

$$\frac{\partial \boldsymbol{q}}{\partial t} + \nabla \cdot \mathbf{F}(\boldsymbol{q}) = -\phi \nabla \phi_s - \frac{2\Omega z}{R^2}(\mathbf{r} \times \mathbf{U}) + \mu \mathbf{r}, \tag{1}$$

where $\boldsymbol{q}$ is the conservation variable composed of the geopotential height $\phi = gh$ and the velocity fields $\mathbf{U} := (u, v, w)$, i.e.,

$$\boldsymbol{q} := \left\{ \begin{array}{c} \phi \\ \phi u \\ \phi v \\ \phi w \end{array} \right\}, \quad \text{and the flux} \quad \mathbf{F}(\boldsymbol{q}) := \left[\begin{array}{ccc} \phi u & \phi v & \phi w \\ \phi u^2 + \frac{\phi^2}{2} & \phi v u & \phi w u \\ \phi u v & \phi v^2 + \frac{\phi^2}{2} & \phi w v \\ \phi u w & \phi v w & \phi w^2 + \frac{\phi^2}{2} \end{array} \right].$$

Here, $\phi_s = gh_s$ is the bathymetry, R the radius of the globe, Ω the angular frequency, $\mathbf{r} := (x, y, z)$, and μ the Lagrange multiplier which keeps the fluid particles remain on surface of the earth.

We choose to solve (1) using an operator splitting approach. In particular, we split the nonlinear flux as follows

$$\mathbf{F}(\boldsymbol{q}) = \underbrace{\mathbf{F}(\boldsymbol{q}) - \mathbf{F}_L(\boldsymbol{q})}_{\text{slow}} + \underbrace{\mathbf{F}_L(\boldsymbol{q})}_{\text{fast}}, \text{ with } \mathbf{F}_L(\boldsymbol{q}) := \left[\begin{array}{ccc} \phi u & \phi v & \phi w \\ \phi_b \phi & 0 & 0 \\ 0 & \phi_b \phi & 0 \\ 0 & 0 & \phi_b \phi \end{array} \right],$$

where ϕ_b is a reference geopotential height.

This approach facilitates a class of efficient implicit-explicit (IMEX) time stepping scheme. In particular, we employ an additive Runge-Kutta (ARK) method in which the nonlinear flux $\mathbf{F}(\boldsymbol{q}) - \mathbf{F}_L(\boldsymbol{q})$ associated with slow waves is treated with explicit time integration and the linear flux $\mathbf{F}_L(\boldsymbol{q})$ associated with fast waves is solved using implicit method. This allows the shallow water system to be forwared in time with large time step while keeping stability. To efficiently integrate the linear flux $\mathbf{F}_L(\boldsymbol{q})$, within an implicit time stepping scheme, we develop an

HDG spatial discretization by hybridizing the Lax-Friedrichs with unknown trace $\hat{\boldsymbol{q}} = \left[\hat{\phi}, \hat{u}, \hat{v}, \hat{w}\right]$:

$$\mathbf{n}\cdot\hat{\mathbf{F}}_L(\boldsymbol{q},\hat{\boldsymbol{q}}) = \left\{\begin{array}{c} n_x\phi_b u + n_y\phi_b v + n_z\phi_b w \\ n_x\phi_b\phi \\ n_y\phi_b\phi \\ n_z\phi_b\phi \end{array}\right\} + \sqrt{\phi_b}\left\{\begin{array}{c} \phi - \hat{\phi} \\ \phi_b u - \phi_b\hat{u} \\ \phi_b v - \phi_b\hat{v} \\ \phi_b w - \phi_b\hat{w} \end{array}\right\}$$

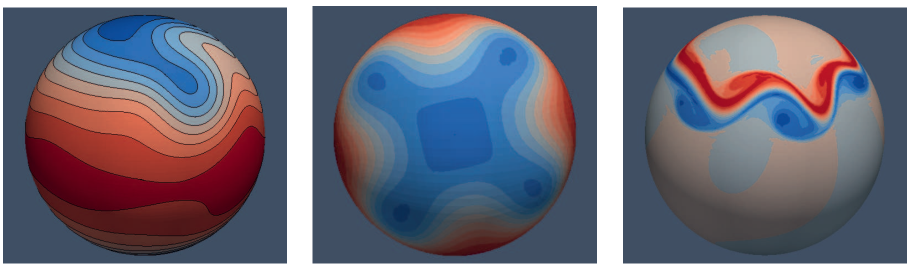
With this HDG flux we can show in [2] the resulting HDG is well-posed, stable, and convergent with solution order p and mesh size h.

Theorem. *Assume* $(\phi, \phi_b\mathbf{U}) \in [H^s(K)]^4, s \geq 3/2$ *for every element* K. *There exists a constant* c *that depends only on the angle condition of* K, s, *and on* ϕ_b *such that*

$$\mathsf{E}(t) \leq c\frac{h^{2\sigma-1}}{p^{2s-1}}t\max_{\theta\in[0,t]}\mathcal{E}^e(\theta), \tag{2}$$

with $\sigma = \min\{p+1, s\}$ *and*

$$\mathcal{E}^e(t) := \sum_K \|\phi(t)\|^2_{H^s(K)} + \|\phi_b\mathbf{U}(t)\|^2_{H^s(K)}.$$



(a) (b) (c)

FIGURE 1. Numerical results using HDG-DG IMEX method with second order ARK scheme for shallow water equations on the globe: a) Zonal flow over an isolated mountain; b) Rossby-Haurwitz wave; c) Barotropic instability.

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hp-adaptive Interior Penalty FEM for Elliptic Obstacle Problems DG for Laplace, C^0 for bi-Laplace

Ernst P. Stephan
(joint work with Lothar Banz)

Firstly, from [1] we consider a mixed formulation for an elliptic obstacle problem for a 2^{nd} order operator and present an hp-FE interior penalty discontinous Galerkin (IPDG) method. The primal variable is approximated by a linear combination of Gauss-Lobatto-Lagrange(GLL)-basis functions, whereas the discrete Lagrangian multiplier is a linear combination of biorthogonal basis functions. A residual based a posteriori error estimate is derived. For its construction the approximation error is split into a discretization error of a linear variational equality problem and additional consistency and obstacle condition terms.

Secondly, an hp-adaptive C^0-interior penalty method for the bi-Laplace obstacle problem is presented from [2]. Again we take a mixed formulation using GLL-basis functions for the primal variable and biorthogonal basis functions for the Lagrangian multiplier and present also a residual a posteriori error estimate. For both cases (2^{nd} and 4^{th} order obstacle problems) our numerical experiments clearly demonstrate the superior convergence of the hp-adaptive schemes compared with uniform and h-adaptive schemes.

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Theory of thin elastic shells: From the past to the present and towards the future

Antti H. Niemi

Thin shell analysis can nowadays be based directly on three-dimensional elasticity theory. Such an approach rules out the modelling errors arising from the simplifications of dimensionally reduced structural models but requires more degrees of freedom for the discrete model. Also, if simplified representations of the stress state such as the stress resultants are needed, they must be post-processed from the three-dimensional stress field and this can be non-trivial, see e.g. [3].

On the other hand, conventional finite element formulations employed in industrial finite element analysis have been developed mainly through so called "finite element modelling", where the kinematic assumptions are described directly in terms of the approximative mesh geometry in conjunction with different strain reduction techniques. This makes error analysis of such formulations cumbersome because the methods have first to be reformulated in context of a well-posed variational problem in a Sobolev space setting. The shell theories formulated in curvilinear coordinates provide such a setting so that they are still needed in numerical analysis. For instance, the degenerated solid approach employed in many quadrilateral shell elements has been interpreted in context of a specific shell model in [1] and numerically analysed e.g. in [2] and in the references therein.

However, this line of research is not limited to analysing existing formulations only, but can also be used to design new ones. In particular, special quadrilateral and triangular shell elements can be constructed that take into account geometric curvature locally on each element by using the interpolated normal vector. For instance, the formulations developed in [4, 5] have better convergence constants than the corresponding conventional shell elements.

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Remarks on the hypercircle method

Rolf Stenberg

(joint work with Torsten Malm, Mika Juntunen)

The classical hypercircle theorem states: Suppose that we have a statically and kinematically admissible stress fields. Then the distance in energy norm from the exact stress to the average of the statically and kinematically fields equals half the distance between these fields. We will discuss the case when the fields are not exactly admissible. We show that the errors introduced can be estimated with computable error constants and hence one obtains an asymptotically exact estimator.

Generalized Finite Element Method: Its conditioning and the effect on the associated iterative solvers

Uday Banerjee

(joint work with Ivo Babuška, Kenan Kergrene)

The Generalized Finite Element Method (GFEM) is used to approximate nonsmooth solutions of PDEs, e.g., interface problems, problems involving voids and inclusions, crack propagation problems etc. GFEM is an extension of the standard

Finite Element Method (FEM) where the trial space is obtained by *augmenting* the space of standard finite element piecewise linear functions, $\mathcal{S}_{FEM}$, by an *enrichment space*, $\mathcal{S}_{ENR}$. The space $\mathcal{S}_{FEM}$ is based on a simple mesh that may not conform to the "features" of the problem and the shape functions of $\mathcal{S}_{ENR}$ are often non-polynomials but with compact supports. The GFEM, with a simple mesh but with a smartly chosen $\mathcal{S}_{ENR}$ (problem dependent) yields an accurate approximation of the non-smooth solution of the underlying problem. Thus it avoids the difficult mesh generation, which could be prohibitive for time dependent problems, especially in 3D, with changing features that requires re-meshing at each time step. However, the linear system associated with the GFEM could be badly conditioned, in fact the conditioning of the GFEM could be much worse than that of the standard FEM. Furthermore, the conditioning of GFEM may not be *robust* with respect to the position of mesh. Thus the ill-conditioning of the GFEM may adversely affect the use of direct or iterative methods to solve the underlying linear system.

An improper choice of $\mathcal{S}_{ENR}$ is the main reason for the bad conditioning of GFEM. The goal is to choose an $\mathcal{S}_{ENR}$ such that the associated GFEM yields accurate approximation and its conditioning is not worse than that of the standard FEM. A GFEM satisfying these two conditions is called an Stable-GFEM (SGFEM).

In this talk we presented theoretical results showing that if the chosen $\mathcal{S}_{ENR}$ satisfies two axioms, then the conditioning of the GFEM is not worse than that of the standard FEM. Moreover, the conditioning is robust with respect to the position of the mesh. One of the crucial axioms states that the "angle" between the spaces $\mathcal{S}_{FEM}$ and $\mathcal{S}_{ENR}$ stays bounded away from zero, uniformly with respect to the mesh parameter h and the position of the mesh. We also presented an "element-wise" sufficient condition to check these axioms for a chosen $\mathcal{S}_{ENR}$.

We illuminated these theoretical results by numerical experiments on a simple interface problem. We considered 3 different $\mathcal{S}_{ENR}$s such that the associated GFEMs yielded optimal order of convergence, i.e., $O(h)$. We showed that the scaled condition number (SCN) of the stiffness matrix of the GFEM associated with one of these enrichment spaces (1^{st} $\mathcal{S}_{ENR}$) is $O(h^{-4})$, which is much worse than that of the standard FEM which is $O(h^{-2})$. The computed "angle" between $\mathcal{S}_{FEM}$ & the 1^{st} $\mathcal{S}_{ENR}$ approached zero as $h \to 0$. On the other hand, the SCN associated with the 2^{nd} $\mathcal{S}_{ENR}$ is $O(h^{-2})$ (similar to the FEM). However, for a particular mesh where the interface is close to the edges of the mesh, the SCN of the GFEM associated with the 2^{nd} $\mathcal{S}_{ENR}$ blows up; the "angle" between $\mathcal{S}_{FEM}$ & 2^{nd} $\mathcal{S}_{ENR}$ also becomes very small for this mesh. This show that the conditioning of GFEM associated with the 2^{nd} $\mathcal{S}_{ENR}$ is not robust with respect to the position of the mesh. The 3^{rd} $\mathcal{S}_{ENR}$ was obtained by subtracting the linear interpolant (w.r.t. the finite element mesh) of the functions in the 2^{nd} $\mathcal{S}_{ENR}$. The SCN of the GFEM associated with the 3^{rd} $\mathcal{S}_{ENR}$ is $O(h^{-2})$ and it is robust with respect to the position of the mesh, i.e., the GFEM associated with the 3^{rd} $\mathcal{S}_{ENR}$ is indeed an SGFEM. We have also shown theoretically that the 3^{rd} $\mathcal{S}_{ENR}$ satisfies the two axioms mentioned before.

Finally we presented an iterative scheme, based on block Gauss-Seidel method, to solve the linear system of the GFEM. The efficiency of the scheme also depended on the "angle" between $\mathcal{S}_{FEM}$ & $\mathcal{S}_{ENR}$. The "angle" between $\mathcal{S}_{FEM}$ & the 3^{rd} $\mathcal{S}_{ENR}$ was shown to be bigger than than the angle between $\mathcal{S}_{FEM}$ & 2^{nd} $\mathcal{S}_{ENR}$. The SGFEM (3^{rd} $\mathcal{S}_{ENR}$) required less number of iterations and 8 times less "wall clock" time than the GFEM based on the 2^{nd} $\mathcal{S}_{ENR}$, for a given tolerance.

It is important to note that "subtracting the interpolant" may not yield an SGFEM for all applications. However subtracting the interpolant could be a basis for further modifications of the enrichment space to obtain an SGFEM.

A posteriori error analysis for C^0 interior penalty methods for fourth order variational inequalities

Li-yeng Sung
(joint work with Susanne C. Brenner, Joscha Gedicke and Yi Zhang)

Let $\Omega \subset \mathbb{R}^2$ be a bounded polygonal domain, $f \in L_2(\Omega)$, $\psi \in C^2(\Omega) \cap C(\bar{\Omega})$, $\psi < 0$ on $\partial\Omega$ and $K = \{v \in H_0^2(\Omega) : v \geq \psi \text{ on } \Omega\}$. The obstacle problem for clamped Kirchhoff plates is to find

$$u = \underset{v \in K}{\operatorname{argmin}} \Big[\frac{1}{2}a(v,v) - (f,v)\Big],$$

where

$$a(v,w) = \int_\Omega \sum_{i,j=1}^{2} w_{x_i x_j} v_{x_i x_j}\,dx \quad \text{and} \quad (f,v) = \int_\Omega f v\,dx.$$

Its unique solution is characterized by the fourth order variational inequality

$$a(u, v-u) \geq (f, v-u) \qquad \forall\, v \in K.$$

C^0 interior penalty methods [9, 5] are discontinuous Galerkin methods for fourth order elliptic boundary value problems that are based on standard Lagrange finite element spaces for second order problems. They were extended to the obstacle problem of clamped Kirchhoff plates in [7, 6].

In this talk we present a recent discovery that a residual based error estimator originally designed for fourth order elliptic boundary value problems [4, 2] is also reliable and efficient for the obstacle problem. The reasons behind this surprising phenomenon are (i) the discrete Lagrange multipliers can be naturally expressed as a sum of Dirac point measures supported at the vertices, (ii) the reliability estimates for clamped Kirchhoff plates can be carried over to a related boundary value problem defined in terms of the discrete Lagrange multipliers (à la Braess [1]) because the discrete Lagrange multipliers only act on functions that vanish at the vertices, and (iii) the efficiency estimates can also be carried over since bubble functions vanish at the vertices.

Numerical results indicate that adaptive quadratic and cubic C^0 interior penalty methods based on this error estimator and the Dörfler bulk marking strategy perform optimally for the obstacle problem. Similar results also hold for C^0 interior penalty methods for elliptic distributed optimal control problems with pointwise state constraints formulated as fourth order variational inequalities [8].

Details can be found in [3].

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On (weak) Trefftz discontinuous Galerkin methods: fundamentals and application to medium-frequency engineering problems (transient dynamics and acoustics)

Pierre Ladevéze

Recently, numerical predictions have made a forceful entry into design and analysis offices. However, carrying out such simulations on small-wavelength problems, such as mid- and high-frequency acoustics, vibration or transient dynamics problems, remains a challenge. In these cases, finite element techniques, which are well-established tools for larger-wavelength problems, are hampered by pollution errors and their computation costs can be prohibitive.

Our first solution was a wave approach called the Variational Theory of Complex Rays for mid-frequency problems, which we have improved over the years [2, 3].

This presentation deals with a reformulation of this approach as a Trefftz Discontinuous Galerkin (TDG) method, initially introduced for quasi-static linear problems in [1]. Among the classical DG methods [6], this general TDG method can be viewed as the Trefftz version of Baumann-Oden's DG formulation [5].

In this presentation, we also show new extensions, called weak Trefftz DG methods [4], based on weakened Trefftz constraints, which overcome some limitations of the TGD method. These extensions may pave the way to new computational techniques for the resolution of engineering problems; in particular, they can be used to couple different types of numerical models, including classical FE models. The state of the art will be illustrated by several examples, including engineering problems.

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Adaptive finite element approximation of mixed eigenvalue problems

Daniele Boffi

We consider the mixed approximation of Laplace eigenvalue problem: find $\lambda \in \mathbb{R}$ and $u \in L^2(\Omega)$ with $\|u\| = 1$ such that for some $\boldsymbol{\sigma} \in H(\mathrm{div};\Omega)$ it holds

$$\begin{cases} \displaystyle\int_\Omega \boldsymbol{\sigma}\cdot\boldsymbol{\tau}\,d\mathbf{x} + \int_\Omega u\,\mathrm{div}\boldsymbol{\tau}\,d\mathbf{x} = 0 & \forall\boldsymbol{\tau}\in H(\mathrm{div};\Omega) \\ \displaystyle\int_\Omega v\,\mathrm{div}\boldsymbol{\sigma}\,d\mathbf{x} = -\lambda\int_\Omega uv\,d\mathbf{x} & \forall v\in L^2(\Omega). \end{cases}$$

Under standard assumptions we prove the convergence and the optimality of the adaptive finite element approximation in terms of an error quantity that takes into account the $L^2(\Omega)$ norm of the error in the u variable and the $L^2(\Omega)$ norm of the error in a suitably defined variable corresponding to $\boldsymbol{\sigma}$. For the eigenvalues, double order of convergence is proved. This is the first proof of convergence and optimality of AFEM for mixed problems. In this case, one of the crucial aspects is that mixed methods don't fulfill the classical orthogonality property of standard Galerkin formulations. In this context we can prove that the solutions generated by the AFEM enjoy a quasi-orthogonality estimate which is consequence of a superconvergence property.

The obtained result is cluster robust in the sense of [3]. More precisely, it has been recently observed (see [4, 1]) that in presence of multiple eigenvalues an adaptive strategy should consider an error indicator based on the whole invariant space and not only on a part of it. In case of cluster of eigenvalues, the results of [3] show that a robust adaptive strategy should involve simultaneously the invariant spaces of all eigenvalues of the cluster. In this spirit, our result shows the optimal convergence of all eigenvalues/eigenfunctions in the approximating cluster towards the continuous ones.

The result holds in two and three space dimensions when standard Raviart–Thomas or Brezzi–Douglas–Marini schemes on simplicial meshes are used.

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Hybrid finite element methods in solid mechanics

Christian Wieners

We consider a weakly conforming variant of the DPG method [2] in its hybrid version, using the reduction to the skeleton $\Gamma = \bar{\Omega} \setminus \bigcup K = \bigcup \partial K$ analyzed in [4]. Here, we discuss the application to nonlinear elasticity, i.e., we aim to minimize the energy $\mathcal{E}(\mathbf{u}) = \int_\Omega W(\mathbf{u})\,\mathrm{d}x - \langle \ell, \mathbf{u}\rangle$ in the weakly conforming space

$$V_h = \Big\{\mathbf{u} \in \mathrm{L}_2(\Omega)^D \colon \mathbf{u}_K \in V_K \text{ and } \sum \int_{\partial K \setminus \Gamma_\mathrm{D}} \mathbf{u}_K \cdot \boldsymbol{\eta}\mathbf{n}\,\mathrm{d}a = 0 \text{ for } \boldsymbol{\eta} \in W\Big\}$$

with $V_K \subset \mathcal{P}(K)^D$, where continuity is approximated testing with $W \subset \mathrm{H}(\mathrm{div}, \Omega)^D$. Introducing the trace space $\hat{V}_h = \prod V_h|_{\partial K}$ and operators B_K and R_K with $\langle B_K \mathbf{u}, \boldsymbol{\eta}_K\rangle = \int_{\partial K} \mathbf{u} \cdot \boldsymbol{\eta}\mathbf{n}\,\mathrm{d}a$ and $\langle R_K \hat{\mathbf{u}}, \boldsymbol{\eta}_K\rangle = \int_{\partial K} \hat{\mathbf{u}} \cdot \boldsymbol{\eta}\mathbf{n}\,\mathrm{d}a$, this results into the following hybrid algorithm for the skeleton variable $\hat{\mathbf{u}}$.

S0) Choose $\hat{\mathbf{u}}_h^0 \in \hat{V}_h$ with $\hat{\mathbf{u}}_h^0 = \mathbf{u}_\mathrm{D}$ on Γ_D. Set $k = 1$.

S1) For given $\hat{\mathbf{u}}_h^k$ and every K, find a minimizer of $\mathbf{u}_K^k \in V_K$ of

$$\mathcal{E}_K(\mathbf{u}_K) = \int_K W(\mathbf{u}_K)\,\mathrm{d}x - \langle \ell_K, \mathbf{u}_K\rangle$$

subject to the constraint $B'_K\mathbf{u}_K = R_K\hat{\mathbf{u}}_h^k$:

L0) Select $(\mathbf{u}_K^{k,0}, \boldsymbol{\eta}_K^{k,0})$ with $B'_K\mathbf{u}_K^{k,0} = R_K\hat{\mathbf{u}}_h^k$. Set $m = 0$.

L1) If $\ell_K^{k,m} = \ell_K - \partial W(\mathbf{u}^{k,m}) - B_K\boldsymbol{\eta}_K^{k,m}$ is small enough,
set $\mathbf{u}_K^k = \mathbf{u}_K^{k,m}$, $\boldsymbol{\eta}_K^k = \boldsymbol{\eta}_K^{k,m}$, and $A_K^k = A_K^{k,m}$; go to S2).

L2) Evaluate $A_K^{k,m} = \partial^2 W(\mathbf{u}^{k,m})$ and compute $(\delta\mathbf{u}_K^{k,m}, \delta\boldsymbol{\eta}_K^{k,m})$ solving

$$\begin{aligned} A_K^{k,m}\delta\mathbf{u}_K^{k,m} + B_K\delta\boldsymbol{\eta}_K^{k,m} &= \ell_K^{k,m}\,, \\ B'_K\delta\mathbf{u}_K^{k,m} &= \mathbf{0}\,. \end{aligned}$$

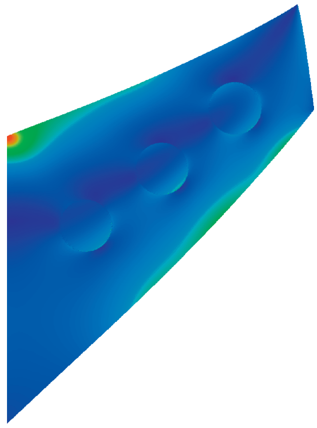
Update $(\mathbf{u}_K^{k,m+1}, \boldsymbol{\eta}_K^{k,m+1}) = (\mathbf{u}_K^{k,m}, \boldsymbol{\eta}_K^{k,m}) + (\delta\mathbf{u}_K^{k,m}, \delta\boldsymbol{\eta}_K^{k,m})$; go to L1).

S2) If $\hat{\ell}_h^k = \sum_K C'_K\boldsymbol{\beta}^k$ is small enough, STOP.

S3) Assemble $\hat{S}_h^k = \sum_K \begin{pmatrix} 0 \\ \hat{C}_K \end{pmatrix}' \begin{pmatrix} A_K^k & B'_K \\ B_K & 0 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ \hat{C}_K \end{pmatrix}$ and solve $\hat{S}_h^k\delta\hat{\mathbf{u}}_h^k = \hat{\ell}_h^k$.

Update $\hat{\mathbf{u}}_h^{k+1} = \hat{\mathbf{u}}_h^k + \delta\hat{\mathbf{u}}_h^k$ and go to S1).

This algorithm is tested for a composite material with Neo-Hooke type energy for poly-butylene terephthalate ($E = 2500$ and $\nu = 0.35$), and inclusions of linear elastic E-glass fibers ($E = 72000$ and $\nu = 0.2$). We use 4 degrees of freedom per face and cubic ansatz functions locally. In this configuration the weakly conforming generalization of Korn's inequality can be applied [1]. For the example we use 77 824 triangles and 468 352 degrees of freedom on the skeleton. The method is realized in the parallel finite element software system M++ [3].



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Low-memory discontinuous Galerkin methods for wave propagation on hybrid meshes

Jesse Chan

(joint work with Zheng Wang, Axel Modave, J.F. Remacle, and T. Warburton)

We introduce an adaptation of high order time-explicit discontinuous Galerkin (DG) methods to hybrid meshes with algorithmic aspects which yield efficient implementations on accelerators and Graphics Processing Units (GPUs) [2]. We extend earlier work for accelerating nodal DG on GPUs to meshes which contain predominantly hexahedral elements, combined with tetrahedra and transitional prism and pyramid elements for geometric flexibility. These meshes can potentially reduce costs by using exploiting the efficiency of hexahedra where possible. Recent developments in meshing have made it possible to create unstructured hex-dominant mixed element meshes for general geometries [6], which can leverage the fast tensor-product structure of hexahedral elements while maintaining the geometric flexibility of tetrahedral elements.

Efficient solvers for hexahedra and tetrahedra both rely on low-memory storage of mass matrix inverses. To extend such strategies to prismatic elements, we use a rational Low-Storage Curvilinear (LSC) approach [1], which defines a physical basis $\phi(x)$ by dividing the reference basis $\widehat{\phi}(x)$ by the geometric mapping factor J

$$\phi_i = \frac{\widehat{\phi}_i}{\sqrt{J}}, \qquad \int_K \phi_j \phi_i = \int_{\widehat{K}} \frac{\widehat{\phi}_j}{\sqrt{J}} \frac{\widehat{\phi}_i}{\sqrt{J}} J = \int_K \widehat{\phi}_j \widehat{\phi}_i,$$

which ensures that the mass matrix is identical over every element. Optimal convergence rates under LSC bases then depend on the growth of a high order Sobolev norm of J upon mesh refinement. While this quantity is controlled for prisms, these norms of J can be unbounded for non-affine pyramids, rendering LSC bases non-convergent. To address this, we construct a new high order basis which is orthogonal on vertex-mapped pyramids. On the bi-unit cube, this basis is given as follows:

$$\phi_{ijk}(a,b,c) = \ell_i^k(a)\ell_j^k(b)\left(\frac{1-c}{2}\right)^k P_k^{2k+3,0}(c), \qquad (a,b,c) \in [-1,1]^3,$$

where $\ell_i^k(a), \ell_j^k(b)$ are Lagrange basis functions at k-th degree Gaussian quadrature nodes, and $P_k^{2k+3,0}(c)$ is a weighted Jacobi polynomial. A collapsed-coordinate transform then maps the above to a reference pyramid.

By leveraging the above pyramidal and prismatic bases, GPU-accelerated DG methods can be efficiently extended to hybrid meshes [3]. Specific basis functions for each element achieve high order accuracy and low-storage simultaneously, while multi-rate timestepping circumvents restrictive global CFL conditions. The stability of the method is achieved through a variational formulation which is a-priori stable and a judicious choice of local timestep based on CFL constants. These local constants are derived from trace inequalities over each type of element, including new sharp face and surface trace inequalities for pyramidal and hexahedral elements [4, 3]. Different strategies for the optimization of computational kernels may then be applied for each element type.

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Hodge decomposition for two-dimensional time harmonic Maxwell's equations

Joscha Gedicke

(joint work with Susanne C. Brenner, Li-yeng Sung)

We extend the Hodge decomposition approach for the cavity problem of two-dimensional time harmonic Maxwell's equations [1, 4] to include the impedance boundary condition, with anisotropic electric permittivity ϵ and sign changing magnetic permeability μ.

Let $\Omega \subset \mathbb{R}^2$ be a bounded polygonal domain with boundary consisting of two disjoint closed subsets Γ_{pc} with perfectly conducting boundary and Γ_{imp} with the impedance boundary condition, $\mathbf{f} \in [L_2(\Omega)]^2$, $g \in L_2(\partial\Omega)$, μ and $1/\mu$ in $L_\infty(\Omega)$, ϵ smooth real symmetric positive-definite 2×2 tensor field defined on $\overline{\Omega}$, λ strictly positive on $\partial\Omega$, and $k > 0$.

We seek $\mathbf{u} \in H_{\mathrm{imp}}(\mathrm{curl};\Omega;\Gamma_{\mathrm{imp}}) \cap H_0(\mathrm{curl};\Omega;\Gamma_{\mathrm{pc}}) \cap H(\mathrm{div}^0;\Omega;\epsilon)$ such that for all $\mathbf{v} \in H_{\mathrm{imp}}(\mathrm{curl};\Omega;\Gamma_{\mathrm{imp}}) \cap H_0(\mathrm{curl};\Omega;\Gamma_{\mathrm{pc}}) \cap H(\mathrm{div}^0;\Omega;\epsilon)$,

$$(\mu^{-1}\nabla \times \mathbf{u}, \nabla \times \mathbf{v}) - k^2(\epsilon\mathbf{u}, \mathbf{v}) - ik\langle \lambda \mathbf{n} \times \mathbf{u}, \mathbf{n} \times \mathbf{v}\rangle_{\Gamma_{\mathrm{imp}}} = (\mathbf{f}, \mathbf{v}) + \langle g, \mathbf{n} \times \mathbf{v}\rangle_{\Gamma_{\mathrm{imp}}}$$

in Ω. In the case where Γ_{imp} is the outer boundary and Γ_{pc} is the inner boundary of Ω, this equation relates to a scattering problem where Γ_{pc} is the boundary of the scatterer and the impedance boundary condition acts as an absorbing boundary condition.

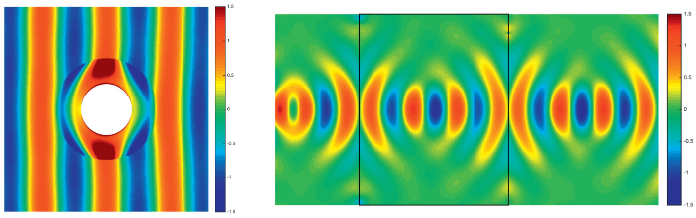

FIGURE 1. Cloaking (left) and flat lens (right) simulations.

Let $m \in \mathbb{N}$ denote the Betti number of the domain Ω with $m = 0$ for simply connected domains. The Hodge decomposition of $H(\mathrm{div}^0; \Omega; \epsilon)$ leads to

$$\mathbf{u} = \epsilon^{-1} \nabla \times \phi + \sum_{j=1}^{m} c_j \nabla \varphi_j,$$

where $\phi \in H^1(\Omega)$ satisfies $(\phi, 1) = 0$ and $c_1, \ldots, c_m$ are constants. The scalar functions $\varphi_1, \ldots, \varphi_m$ are harmonic functions and the function ϕ is determined by two scalar elliptic boundary value problems [1, 3].

We derive error estimates for a P_1 finite element method based on the Hodge decomposition approach [3] and develop a residual type *a posteriori* error estimator [2]. We show that adaptive mesh refinement leads empirically to smaller errors than uniform mesh refinement for numerical experiments that involve metamaterials and electromagnetic cloaking [2]. The well-posedness of the cavity problem when both electric permittivity and magnetic permeability can change sign is also discussed [3] and verified for the numerical approximation of a flat lens experiment, cf. Figure 1.

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A class of mixed finite element methods based on the Helmholtz decomposition

Mira Schedensack

Non-conforming finite element methods (FEMs) play an important role in computational mechanics. They allow the discretization of partial differential equations (PDEs) for incompressible fluid flows modelled in the Stokes equations, for almost incompressible materials in linear elasticity, and for low polynomial degrees in the ansatz spaces for the Kirchhoff plate problem. A generalization to higher polynomial degrees which also transfers the desirable properties of the scheme, however, has been an open question.

This presentation considers higher-order equations of the form $(-1)^m \Delta^m u = f$ and introduces novel formulations based on the new Helmholtz-type decomposition

$$L^2(\Omega;\mathbb{S}(m)) = D^m H^m_0(\Omega) \oplus \operatorname{symCurl} H^1(\Omega;\mathbb{S}(m-1)),$$

where $\mathbb{S}(m)$ denotes the set of symmetric m-tensors over $\mathbb{R}^2$, along with their discretizations of arbitrary (globally fixed) polynomial degree. The new formulation assumes that some function $\varphi \in H(\operatorname{div}^m,\Omega)$ is at hand, such that $(-1)^m \operatorname{div}^m \varphi = f$, and then decomposes

$$\varphi = \sigma + \operatorname{symCurl}\alpha \quad \text{and} \quad \sigma \perp_{L^2(\Omega)} \operatorname{symCurl} H^1(\Omega;\mathbb{S}(m-1)).$$

Then $\sigma = D^m u$. For the lowest-order polynomial degree, discrete Helmholtz decompositions of [1, 2] prove equivalence of the novel discretizations to the known famous non-conforming FEMs of Crouzeix and Raviart [3] for the Poisson equation for $m = 1$ and the Morley FEM [4] for the biharmonic problem for $m = 2$.

The direct approximation of $D^m u$ instead of u enables low order discretizations; only first derivatives appear in the symmetric part of the Curl and so the lowest order approach only requires piecewise affine functions. Mnemonic diagrams in Figure 1 illustrate lowest-order standard conforming FEMs and the lowest-order novel FEMs proposed in this presentation for $m = 1, 2, 3$. Since the proposed new FEMs differ only in the number of components in the ansatz spaces, an implementation of one single program, which runs for arbitrary order, is possible. Besides the a priori and a posteriori analysis, the presentation presents optimal convergence rates for adaptive algorithms for the new discretizations.

A generalization of non-conforming FEMs for the Stokes equations and linear elasticity can be found in [5].

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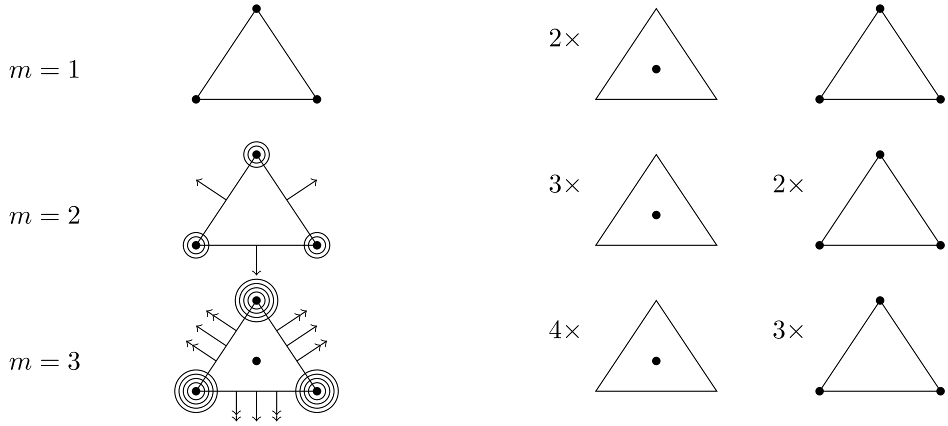

FIGURE 1. Lowest order standard conforming and novel FEMs for the problem $(-1)^m \Delta^m u = f$ for $m = 1, 2, 3$.

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Multiscale homogenization for the computational mechanics of cardiovascular structures: physiopathological behavior

MICHELE MARINO

(joint work with Peter Wriggers)

Cardiovascular structures are planar sheets of soft connective tissues which share a highly heterogeneous histology with a precise hierarchical organization from the nanoscale (molecules) through to the microscale (crimped periodic fibers) up to the macroscale (fiber-reinforced lamellae). Among the existing approaches, constitutive models based on a structural approach are usually employed in numerical simulations of macroscale biological structures [1]. In the structural approach, tissues are regarded as composite materials reinforced by fibers with an exponential mechanical behavior. Thereby, model parameters have indeed a phenomenological meaning with no straightforward correlation between histological/biochemical features and mechanical properties.

In this work, a novel approach for describing the constitutive response of cardiovascular tissues is proposed. The model is developed within a finite-strain anisotropic framework and it is based on the definition of tissue strain-energy (with particular attention to the collagenous constituents) by following a structural multiscale approach [2, 3, 4]. Accordingly, analytical and computational approaches are coupled in order to obtain the macroscale tissue response in function of both nanoscale mechanisms and microscale non-linearities.

Denoting with $\mathbf{C}$ the right Cauchy-Green deformation tensor, let $\lambda_4 = \sqrt{\mathrm{Tr}(\mathbf{CM})}$ be introduced where $\mathbf{M} = \mathbf{e}_C^o \otimes \mathbf{e}_C^o$ is the structural tensor associated with the main direction $\mathbf{e}_C^o$ of collagen fibers [5]. It is worth pointing out that λ_4 physically represents the stretch along the direction $\mathbf{e}_C^o$ of collagen fibers and that $\mathbf{M}$ results piecewise constant along tissue thickness due to tissue lamellar organization. The collagen-related contribution to tissue strain energy is defined as:

$$\Psi_C(\mathbf{C}) = \begin{cases} 0 & \text{for } \lambda_4 < 1 \\ \int_1^{\lambda_4} \int_1^{\xi} \frac{E_C(\eta)}{\eta} d\eta d\xi & \text{for } \lambda_4 \geq 1 \end{cases}, \tag{1}$$

where $E_C(\lambda_4)$ represents the tangent modulus of crimped collagen fibers correlating the perturbation of collagen-related stress with the perturbation of fibers configuration. Function $E_C(\lambda_4)$ is obtained as a results of a homogenization process involving:

- the application of the Principle of Virtual Power, in the framework of the classical beams' theory, for coupling the material and geometric non-linearities at the microscale associated with the straightening of crimped fibers;
- the definition of material non-linearities at the mesosocale between micro- and nanoscale, by coupling molecular and intermolecular effects in collagen fibrils;
- the refined modeling of collagen macromolecules at the nanoscale, accounting for the entropic effects associated with thermal fluctuations and for the energetic mechanisms related to the uncoiling of the triple helix and the stretching of molecular backbone.

In order to ensure the convergence properties of numerical schemes adopted in simulations, the polyconvexity of the proposed strain-energy term in Eq. (1) is discussed [5, 6]. For the sake of notation, let $\mathbb{R}^{++}$ the set of strictly positive numbers and $\mathbb{R}^{+} = \mathbb{R}^{++} \cup \{0\}$.

Remark 1. *For any given function $E_C : [1, +\infty) \mapsto \mathbb{R}^{++}$, the strain-energy term in Eq.* (1) *is polyconvex.*

For the proof of Remark 1, the following result is proved:

Remark 2. *Let $\mathbf{F} \in \mathbb{R}^{3\times3}$, $\mathbf{C} = \mathbf{F}^T\mathbf{F}$, and $\mathbf{M} = \mathbf{a} \otimes \mathbf{a}$ with $\mathbf{a} \in \mathbb{R}^3$. Function $f : \mathbb{R}^{3\times3} \mapsto \mathbb{R}^{+}$, $f(\mathbf{F}) = \mathrm{Tr}(\mathbf{CM})^k = |\mathbf{Fa}|^{2k}$ is convex if and only if $k \geq 1/2$.*

Remark 2 extends the results in [5] (holding for $k \geq 1$) and in [6] (for $k = 1/2$).

The effectiveness of the proposed approach is shown by comparison with available experimental data on the pressure/radius relationship of aortic segments from different age-groups [7]. Thanks to the employed multiscale framework, the model allows to correlate the variation of the macroscopic mechanical response with the one of tissue histological and biochemical properties. Finally, the approach is extended for the modeling of inelastic mechanisms in biological tissues, allowing to recover the peculiar features of collagen fibrils elasto-damage response [8].

In conclusion, the proposed approach opens to the development of numerical simulations where the constitutive behavior of biological tissues is developed within a patient-specific framework or following clinically-motivated considerations. For instance, the effects of collagen cross-linking enzymatic activity, metabolism and histological arrangement can be analyzed, providing an insight on physiological or pathological remodeling mechanisms.

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Finite element methods for the Von Kármán Equations

Neela Nataraj

(joint work with Gouranga Mallik)

Based on the thickness to length ratio, several plate models have been studied in literature; the most important ones being linear models like Kirchhoff and Reissner-Mindlin plates for *thin* and *moderately thick* plates respectively; and non-linear von Kármán plate model for *very thin* plates. In this report, a nonconforming Morley finite element method [2] is presented for the von Kármán equations. Optimal order error estimates in broken energy and H^1 norms are stated under minimal regularity assumptions on the solution. Over the last few decades, the finite element methodology has developed in various directions. For higher-order problems, nonconforming methods and discontinuous Galerkin methods are gaining popularity as they have a clear advantage over conforming finite elements with respect to simplicity in implementation. For the von Kármán plate model, theoretical and computational results can also be obtained using a conforming finite element method [1].

Let $\Omega \subset \mathbb{R}^2$ be a polygonal domain with boundary $\partial\Omega$. Consider the von Kármán equations for the deflection of very thin elastic plates defined by: for given $f \in L^2(\Omega)$, seek the vertical displacement u and the Airy stress function v such that

$$\Delta^2 u = [u, v] + f, \qquad \Delta^2 v = -\frac{1}{2}[u, u] \tag{1}$$

with clamped boundary conditions $u = \frac{\partial u}{\partial \nu} = v = \frac{\partial v}{\partial \nu} = 0$ on $\partial\Omega$, where the biharmonic operator Δ^2 is defined by $\Delta^2\varphi := \varphi_{xxxx} + 2\varphi_{xxyy} + \varphi_{yyyy}$, the von Kármán bracket $[\cdot,\cdot]$ is defined by $[\eta, \chi] := \mathrm{cof}(D^2\eta) : D^2\chi$, and ν denotes the unit outward normal to the boundary $\partial\Omega$ of Ω.

A vector form of the weak formulation is defined as: for $F = (f, 0)$ with $f \in L^2(\Omega)$, seek $\Psi = (u, v) \in \mathcal{V} := H_0^2(\Omega) \times H_0^2(\Omega)$, such that

$$A(\Psi, \Phi) + B(\Psi, \Psi, \Phi) = L(\Phi)\ \forall \Phi \in \mathcal{V}, \tag{2}$$

where $\forall\, \Xi = (\xi_1, \xi_2), \Theta = (\theta_1, \theta_2)$ and $\Phi = (\varphi_1, \varphi_2) \in \mathcal{V}$, $L(\Phi) = \int_\Omega f\varphi_1\, dx$,

$$A(\Theta, \Phi) := a(\theta_1, \varphi_1) + a(\theta_2, \varphi_2),$$
$$B(\Xi, \Theta, \Phi) := b(\xi_1, \theta_2, \varphi_1) + b(\xi_2, \theta_1, \varphi_1) - b(\xi_1, \theta_1, \varphi_2),$$

$\forall \eta, \chi, \varphi \in H_0^2(\Omega)$,

$$a(\eta, \chi) := \int_\Omega D^2\eta : D^2\chi\, dx,\ b(\eta, \chi, \varphi) := \frac{1}{2}\int_\Omega \mathrm{cof}(D^2\eta)D\chi \cdot D\varphi\, dx.$$

Assume that the solution Ψ is nonsingular. That is, the linearized problem defined by: for given $G = (g_1, g_2) \in \mathcal{V}'$, seek $\Theta = (\theta_1, \theta_2) \in \mathcal{V}$ such that
$A(\Theta, \Phi) + B(\Psi, \Theta, \Phi) + B(\Theta, \Psi, \Phi) = (G, \Phi)\ \ \forall \Phi \in \mathcal{V}$ is well posed.
The nonconforming formulation corresponding to (2) can be stated as: seek $\Psi_h = (u_h, v_h) \in \mathcal{V}_h$ such that

$$A_h(\Psi_h, \Phi) + B_h(\Psi_h, \Psi_h, \Phi) = L_h(\Phi)\ \ \forall \Phi \in \mathcal{V}_h, \tag{3}$$

where $\mathcal{V}_h := V_h \times V_h$, V_h is the Morley finite element space associated with a regular, quasi-uniform triangulation of $\bar{\Omega}$ defined by

$$\begin{aligned} V_h := \{&\varphi \in L^2(\Omega) : \varphi|_T \in P_2(T)\ \forall T \in \mathcal{T}_h,\ \varphi \text{ is continuous at the vertices of } \mathcal{T}_h,\\ &\text{the normal derivatives of } \varphi \text{ at the midpoint of the edges of } \mathcal{T}_h \text{ are continuous},\\ &\varphi = 0 \text{ at the vertices on } \partial\Omega,\ \partial\varphi/\partial\nu = 0 \text{ at the midpoint of the edges on } \partial\Omega\},\end{aligned}$$

and $A_h(\cdot,\cdot), B_h(\cdot,\cdot)$, $L_h(\cdot)$ are the piecewise versions of $A(\cdot,\cdot), B(\cdot,\cdot)$, $L(\cdot)$, respectively defined on $\mathcal{T}_h$. The main theorem is stated now.

Theorem. *Let Ψ be a nonsingular solution of* (2). *Then, for sufficiently small h, there exists a solution Ψ_h of the discrete problem* (3), *which is locally unique. The following error estimates hold true:*

$$|||\Psi - \Psi_h|||_{2,h} \le Ch^\alpha \text{ and } |||\Psi - \Psi_h|||_{1,h} \le Ch^{2\alpha},$$

# unknowns	$\|u-u_h\|_{2,h}$	Order	$\|u-u_h\|_{1,h}$	Order	$\|u-u_h\|_{L^2}$	Order
25	0.874685E-1	-	0.102155E-1	-	0.386068E-2	-
113	0.405787E-1	1.1080	0.257318E-2	1.9891	0.919743E-3	2.0695
481	0.209921E-1	0.9508	0.732470E-3	1.8127	0.248134E-3	1.8901
1985	0.106209E-1	0.9829	0.191118E-3	1.9383	0.636227E-4	1.9635
8065	0.532754E-2	0.9953	0.483404E-4	1.9831	0.160158E-4	1.9900
32513	0.266595E-2	0.9988	0.121213E-4	1.9956	0.401107E-5	1.9974

where $\alpha \in (1/2, 1]$ is the index of elliptic regularity and $|\!|\!|\cdot|\!|\!|_{2,h}$ and $|\!|\!|\cdot|\!|\!|_{1,h}$ denote the broken energy and H^1 norms in $\mathcal{V}_h$.

A working procedure to find an approximation for the discrete solution Ψ_h is defined now. Starting with an initial guess Ψ_h^0, the iterates of the Newton's method are defined by $\forall \Phi \in \mathcal{V}_h$,

$$A_h(\Psi_h^n, \Phi) + B_h(\Psi_h^{n-1}, \Psi_h^n, \Phi) + B_h(\Psi_h^n, \Psi_h^{n-1}, \Phi) = B_h(\Psi_h^{n-1}, \Psi_h^{n-1}, \Phi) + L_h(\Phi).$$

It can be established that the iterates of the Newton's method are well defined and converge quadratically to Ψ_h.

Next, the result of a numerical result that justifies the estimates is presented. Consider the problem with right hand side load function chosen such that the exact solution is given by $u(x,y) = x^2(1-x)^2y^2(1-y)^2;\quad v(x,y) = \sin^2(\pi x)\sin^2(\pi y)$ on the unit square. The Table above shows the errors and experimental convergence rates for the variable u_h. The computational order of convergences in broken H^2, H^1 norms are quasi-optimal and verify the theoretical results for $\alpha = 1$. The order of convergence with respect to L^2 norm is sub-optimal. Similar results can be obtained for v_h also.

An ongoing work is on reliable *a posteriori* error estimates for conforming and nonconfoming FEMs that drive the adaptive mesh refinements.

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Auxiliary Space Preconditioners for Discontinuous Galerkin Interior Penalty methods for $\boldsymbol{H}(\mathbf{curl};\boldsymbol{\Omega})$-elliptic problems

Blanca Ayuso de Dios

(joint work with Ralf Hiptmair, Cecilia Pagliantini)

Let $\Omega \subset \mathbb{R}^3$ be a simply connected bounded domain with Lipschitz boundary and let $\mathbf{f} \in L^2(\Omega)^3$. We consider the following $H_0(\mathbf{curl};\Omega)$-elliptic problem:

$$\nabla \times (\nu \nabla \times \mathbf{u}) + \beta \mathbf{u} = \mathbf{f} \quad \text{in } \Omega, \qquad \mathbf{u} \times \mathbf{n} = 0 \quad \text{on } \partial\Omega. \tag{1}$$

where $\nu = \nu(\mathbf{x}) > 0$ and $\beta = \beta(\mathbf{x}) > 0$ are assumed to be bounded functions in Ω but possibly discontinuous, and represent properties of the medium/material: ν is typically the inverse of the magnetic permeability and β is proportional to the ratio of electrical conductivity and the time step. Problems of this type arise in the modelling of magnetic diffusion phenomena (eddy current models) and also after implicit time discretisation of resistive magneto-hydrodynamics (MHD).

Let $\mathcal{T}_h$ be a shape-regular and local quasi-uniform partition of Ω, made of simplices or hexahedra, and let $\mathbf{V}_h = \{\mathbf{v} \in L^2(\Omega)^3 : \mathbf{v} \in \mathcal{M}(K), K \in \mathcal{T}_h\}$, with $\mathcal{M}(K)$ the local space of Nédélec elements of the second family, be the discontinuous finite element space. To approximate problem (1), we introduce a weighted symmetric Interior Penalty (IP) discontinuous Galerkin (DG) method, designed so that its stability is not jeopardized by the jumps in the coefficients and so it provides a robust approximation to (1) in all regimes. Upon discretization, it results in an ill-conditioned large sparse symmetric linear system of equations. Hence, suitable preconditioners to be accelerated within iterative solvers like CG are required, so that the overall convergence does not degrade with respect to mesh refinement and/or large jumps in the coefficients. For $H_0(\mathbf{curl};\Omega)$-conforming approximations of (1), a domain decomposition preconditioner has been studied in [8].

Here, we provide a simple family of preconditioners for the proposed IP-DG approximation of (1) and analyze their asymptotic convergence, addressing precisely the influence of possible discontinuities in the "diffusivity" ν and/or in the "reaction coefficient" β on their asymptotic performance. The construction and analysis of the proposed solvers hinges on the *Auxiliary Space Method* (ASM) [5, 7, 9, 6] and as starting point, we take for granted that good preconditioners for any $H_0(\mathbf{curl};\Omega)$-conforming finite element approximations of (1) are at hand. The proposed auxiliary space (AS) preconditioners, in their simpler additive version, consist of a relaxation operator in the DG space $\mathbf{V}_h$ and the solution of the finite element approximation to problem (1) using an auxiliary space of $H_0(\mathbf{curl};\Omega)$-conforming finite element functions. Two main preconditioners are considered:

- the former uses for the auxiliary space the corresponding $H_0(\mathbf{curl};\Omega)$-conforming finite element space $\mathbf{V}_h \cap H_0(\mathbf{curl};\Omega)$ combined with a simple pointwise smoother (pointwise Jacobi or non-overlapping block Jacobi),
- the latter AS-preconditioner, effective only if the underlying mesh partitioning consist of simplices, employs as auxiliary space the $H_0(\mathbf{curl};\Omega)$-conforming Nédélec first kind finite element space together with a patch smoother. We demonstrate that the use of an overlapping relaxation in this latter case is indeed essential to guarantee optimal convergence.

Both preconditioners are shown to be asymptotically optimal with respect to mesh refinement and robust with respect to large jumps in the coefficients ν and β except only when the problem changes from curl-dominated to reaction dominated and viceversa. We refer to [1] for all the details and further considerations.

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Geometric Multigrid Preconditioners for DPG Systems in Camellia

Nathan V. Roberts

The discontinuous Petrov-Galerkin finite element methodology of Demkowicz and Gopalakrishnan (DPG) [1, 2] offers a host of appealing features, including automatic stability and minimization of the residual in a user-controllable energy norm. DPG is, moreover, well-suited for high-performance computing, in that the extra work required by the method is embarrassingly parallel; the use of a discontinuous test space allows the computation of optimal test functions to be done element-wise. Additionally, the approach gives almost total freedom in the choice of basis functions, so that high-order discretizations can be employed to increase *computational intensity* (the number of floating point operations per unit of communication). Finally, since the method is stable even on a coarse mesh and comes with a built-in error measurement, it enables robust adaptivity which in turn means less human involvement in the solution process, a desirable feature when running large-scale computations.

Camellia [3] is a software framework for DPG with the aim of enabling rapid development of DPG solvers both for running on a laptop and at scale. Camellia supports spatial meshes in 1D through 3D; initial support for space-time elements is also available. Camellia supports h- and p-adaptivity, and offers distributed computation of essentially all the algorithmic components of a DPG solve. (One exception, which we plan to address, is the generation and storage of the mesh geometry; at present, this happens redundantly on each MPI rank.) Camellia supports static condensation for reduction of the global problem, and has a robust, flexible interface for using third-party direct and iterative solvers for the global solve.

Until recently, we have almost always solved the global DPG system matrix using parallel direct solvers such as SuperLU_Dist. This is not a scalable strategy, particularly for 3D and space-time meshes—for instance, SuperLU_Dist runs out of memory during a 3D Stokes solve involving approximately 7×10^5 degrees of freedom on 256 nodes of Argonne's Vesta machine—in total, those nodes have access to 4 terabytes of memory.

Both memory and time costs therefore motivate the present work, an exploration of iterative solvers in the context of Poisson and Stokes problems. Since Camellia's adaptive mesh hierarchy provides us with rich geometric information, we focus on *hp*-geometric multigrid preconditioners with additive Schwarz smoothers of minimal or small overlap. Preconditioning a conjugate gradient solve using such preconditioners, we are able to solve much larger problems within the same memory footprint.

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A novel mixed finite element for anisotropy - Basic Ideas

Jörg Schröder

(joint work with Nils Viebahn, Peter Wriggers, Daniel Balzani)

Unreliable results can occur in the approximation of boundary value problems due to distinct locking-phenomena, like the well-known *Poissonlocking*, see [1] and [2]. In order to overcome these locking effects for isotropic materials a volumetric-isochoric split of the deformation gradient has been successfully introduced [3]. This approach has been extended to a formulation based on different approximations of the minors of the deformation gradient, see [4]. Several authors, e.g. [5], have shown that the volumetric isochoric split for anisotropic materials could lead to unphysical results. Therefore, a novel approach is introduced here, preserving the structure of polyconvex energy functions. A separation of the approximation of the deformation measures, associated to the isotropic and anisotropic response, is introduced in order to relax the constraints resulting from anisotropy.

In the following we focus on free energy functions ψ formulated in terms of the right Cauchy-Green tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$, with the deformation gradient $\boldsymbol{F} = \nabla_X \boldsymbol{x}$. Here the actual placement $\boldsymbol{x}$ is interpolated with quadratic ansatz functions. Introducing of the structural tensor as $\boldsymbol{M} = \boldsymbol{a} \otimes \boldsymbol{a}$ following [6], where $\boldsymbol{a}$ denotes the preferred direction, free energy functions for transversely isotropic materials can be expressed as isotropic tensor functions $\psi = \psi(\boldsymbol{C}, \boldsymbol{M})$. Transversal isotropy may be formulated in the polynomial basis $\mathcal{P}_{ti} := \{I_1, I_2, I_3, J_4, J_5\}$ with $I_1,\ I_2,\ I_3$ as the principal invariants of $\boldsymbol{C}$ and the mixed invariants $J_4 = \text{tr}[\boldsymbol{C} \cdot \boldsymbol{M}]$ and $J_5 = \text{tr}[\boldsymbol{C}^2 \cdot \boldsymbol{M}]$. Considering a strain energy function, additively decoupled into an isotropic and an anisotropic part, a new deformation measure $\overline{\boldsymbol{\mathcal{C}}}$ is introduced

$$\psi = \psi^{iso}(\bullet) + \psi^{aniso}(\overline{\boldsymbol{\mathcal{C}}}). \tag{1}$$

For the isotropic part several formulations of the deformation measure are applicable. The Hu-Washizu functional follows as

$$\Pi(\boldsymbol{C}, \overline{\boldsymbol{\mathcal{C}}}, \overline{\boldsymbol{\mathcal{S}}}) = \int_{\mathcal{B}} \psi^{iso}(\boldsymbol{C}) dV + \int_{\mathcal{B}} \psi^{aniso}(\overline{\boldsymbol{\mathcal{C}}}) dV + \int_{\mathcal{B}} \frac{1}{2}\, \overline{\boldsymbol{\mathcal{S}}} : (\boldsymbol{C} - \overline{\boldsymbol{\mathcal{C}}}) dV + \Pi^{ext}(\boldsymbol{x}), \tag{2}$$

where $\overline{\boldsymbol{\mathcal{S}}}$ constitutes a second-order tensorial Lagrange-multiplier. Therefore, the Euler-Lagrangian equations can be identified by

$$\text{Div}(\boldsymbol{F}\ (2\ \partial_{\boldsymbol{C}} \psi^{iso} + \overline{\boldsymbol{\mathcal{S}}})) + \boldsymbol{f} = 0, \qquad \overline{\boldsymbol{\mathcal{S}}} = 2\ \partial_{\overline{\boldsymbol{\mathcal{C}}}} \psi^{aniso} \quad \text{and} \quad \overline{\boldsymbol{\mathcal{C}}} = \boldsymbol{C}. \tag{3}$$

The first variations $\delta_{\overline{\boldsymbol{\mathcal{C}}}} \Pi = 0$ and $\delta_{\overline{\boldsymbol{\mathcal{S}}}} \Pi = 0$ yield with a constant ansatz for $\overline{\boldsymbol{\mathcal{C}}}$, $\overline{\boldsymbol{\mathcal{S}}}$

$$\overline{\boldsymbol{\mathcal{C}}} = \frac{1}{V_0^e} \int_{\mathcal{B}^e} \boldsymbol{C}\ dV \qquad \text{and} \qquad \overline{\boldsymbol{\mathcal{S}}} = \frac{2}{V_0^e} \int_{\mathcal{B}^e} \partial_{\overline{\boldsymbol{\mathcal{C}}}} \psi^{aniso}\ dV, \tag{4}$$

where V_0^e denotes the volume of a typical element in the reference configuration. Inserting eq. (4) into the variation $\delta_{\boldsymbol{u}} \Pi = 0$ leads to a condensed formulation with the displacements as the only unknowns. Solving a boundary value within an iterative Newton-Raphson scheme requires a consistent linearization of $\delta_{\boldsymbol{u}} \Pi$.

The robustness of this formulation is compared with classical FE formulations by an academical simulation of arterial walls, here applying an unphysiological high pressure in order to analyze the performance of the variational scheme. The chosen polyconvex material model goes back to [7]. Fig. 1a depicts the discretized body and fig. 1b the norm of the displacements $|\boldsymbol{u}|$ of a specified point (dot in fig. 1a) versus the applied pressure p in fig. 1b. In case of the displacement based

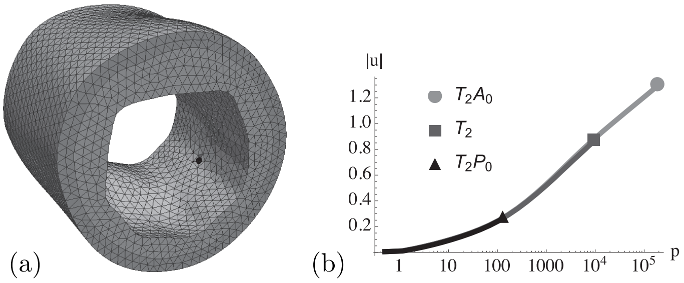

FIGURE 1. Arterial wall simulation.

element T_2 a maximal pressure of $p_{max} = 9592$ kPa can be applied, considering the $T_2 P_0$-element the maximal pressure corresponds to $p_{max} = 131$ kPa. In contrast to these results, a pressure even higher than $p = 200000$ kPa is applicable using the novel element formulation, denoted as $T_2 A_0$.

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A superconvergent HDG method for the Incompressible Navier-Stokes Equations on general polyhedral meshes

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(joint work with Ke Shi)

We present a superconvergent hybridizable discontinuous Galerkin (HDG) method for the steady-state incompressible Navier-Stokes equations on general polyhedral meshes. For arbitrary conforming polyhedral mesh, we use polynomials of degree $k+1$, k, k to approximate the velocity, velocity gradient and pressure, respectively. In contrast, we only use polynomials of degree k to approximate the numerical trace of the velocity on the interfaces. Since the numerical trace of the velocity field is the only globally coupled unknown, this scheme allows a very efficient implementation of the method. The design of the stabilization function corresponding to diffusion operator comes from Lehrenfeld in Remark 1.2.4 in [1]. In [3, 2], this kind of stabilization functions is used for HDG methods for linear elasticity and diffusion problem with complete error analysis. However, the analysis used in [3, 2] can not be generalized for nonlinear problems like the Navier-Stokes equations because of lack of the corresponding discrete energy stability. In [4], we provide the discrete energy stability for HDG method for convection diffusion problem, which uses the same stabilization function for the diffusion operator. In this paper, by generalizing the discrete energy stability in [4], for the stationary case, and under the usual smallness condition for the source term, we prove that the method is well defined and that the global L^2-norm of the error in each of the above-mentioned variables and the discrete H^1-norm of the error in the velocity converge with the order of $k+1$ for $k \geq 0$. We also show that for $k \geq 1$, the global L^2-norm of the error in velocity converges with the order of $k+2$. From the point of view of degrees of freedom of the globally coupled unknown: numerical trace, this method achieves optimal convergence for all the above-mentioned variables in L^2-norm for $k \geq 0$, superconvergence for the velocity in the discrete H^1-norm without postprocessing for $k \geq 0$, and superconvergence for the velocity in L^2-norm without postprocessing for $k \geq 1$.

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Time Dependent Scattering from a Diffraction Grating

Peter Monk

(joint work with Li Fan)

Computing the electromagnetic field in a periodic grating due to light from the sun is critical for assessing the performance of thin film solar voltaic devices. This calculation needs to be performed for many angles of incidence and many frequencies across the solar spectrum. To compute at multiple frequencies one approach is to use a broad band incoming wave and solve the time domain scattering problem for a grating. The frequency domain response for a band of frequencies can then be computed by a Fourier transform.

In this presentation we discuss a two dimensional model problem derived from Maxwell's equations by assuming that the fields and grating are translation invariant in one coordinate direction. This results in a wave equation with coefficients appearing as convolutions in the time domain. Assuming plane wave incidence, and the space-time transformation of [5] we then arrive at a time dependent second order hyperbolic problem posed on a infinite strip with periodic boundary conditions. Two complications occur: first, as already mentioned, materials used in practical devices have frequency dependent coefficients. In fact, at optical frequencies, commonly used metals have a frequency domain permittivity with negative real part but positive imaginary part which describes conductivity. Secondly the spatial domain for the problem is an infinite strip.

Using the Laplace transform and techniques from [1], we provide a proof of existence and uniqueness in the time domain for a general class of such frequency dependent materials [3]. In the Laplace domain we can also derive a simple expression for the Dirichlet-to-Neumann map (D-t-N), and hence reduce the Laplace domain problem to a bounded domain containing the grating. Then using Convolution Quadrature we can construct a discrete D-t-N map to truncate the spatial computational domain after time discretization, and we prove fully discrete error estimates using a class of multistep methods in time and finite elements in space. Because of the use of Convolution Quadrature [4], the discrete time domain D-t-N map t is perfectly matched to the time stepping scheme.

We end with some preliminary numerical results that demonstrate the convergence and stability of the scheme. We show that using the Backward Differentiation Formula-2 (BDF2) in time and finite elements in space we can compute the time dependent solution for a metal modeled by a Drude law, and for a dielectric modeled by the Sellmeier equation.

The main contributions of this paper are a general criterion on the frequency dependent coefficients in the wave equation under which the continuous problem is well-posed, and a demonstration that Convolution Quadrature schemes can be used to compute the fields arising in this problem for two classes of frequency dependent materials.

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Kinetic Methods for Computational Engineering

Manfred Krafczyk

(joint work with Martin Geier, Andrea Pasquali, Martin Schönherr, Konstantin Kutscher)

Although there has been quite some progress in terms of numerical methods, distributed hardware and turbulence models, the computation of complex flow problems in mechanical or environmental engineering is still a challenge when addressing time-dependent three-dimensional flows based on e.g. Large Eddy Simulation (LES) models. In our presentation we describe kinetic approaches to solve such problems based on the Lattice-Boltzmann (LBM) approach. We introduce the modeling hierarchy which allows to obtain approximate solutions of the Navier-Stokes equations from simplified Boltzmann models. These schemes have the favorable property that advection is exact and conservative while all non-linearities are local and thus compute bound instead of memory bound.

After the introduction of the basic concepts we describe in some more detail our recent development, the so-called cumulant LBM [1] which shows improved properties in terms of dispersion properties, Galilean invariance and numerical stability. Several benchmarks will be discussed which indicate the superiority of this approach over other LBM methods.

In addition to improvements of the new scheme the approach allows the efficient implementation on modern many-core hardware such as General Purpose Graphics Processing Units (GPGPUs). Using advanced implementation techniques we demonstrate how the cumulant LBM on a single GPGPU allows e.g. to compute the external aerodynamics of a car with an accuracy of about 1 % in about one day as compared to other proprietary codes which require the use of a midsize compute cluster to solve the same problem.

Our talk concludes by indicating the potential of our method for three-dimensional time-dependent coupled flow in urban systems with a spatial resolution of about one meter on a GPGPU-based desktop system.

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Mixed methods for degenerate elliptic problems

Ricardo G. Durán
(joint work with María E. Cejas and Mariana I. Prieto)

Given $\Omega \subset \mathbb{R}^n$ a bounded Lipschitz polytope and ω a non-negative measurable function, we consider mixed finite element approximations of $-\mathrm{div}\,(\omega\nabla u) = f$ with homogeneous Dirichlet boundary conditions (although other conditions can be treated analogously).

We are interested in non-uniformly elliptic problems, that is, the coefficient ω can vanish or become infinity in subsets of $\overline{\Omega}$ with vanishing n-dimensional measure. We will assume that ω belongs to the Muckenhoupt class A_2. Recall that a non-negative function ω defined in $\mathbb{R}^n$ belongs to A_2 if

$$[\omega]_{A_2} := \sup_Q \left(\frac{1}{|Q|}\int_Q \omega\,dx\right)\left(\frac{1}{|Q|}\int_Q \omega^{-1}\,dx\right) < \infty,$$

where the supremum is taken over all cube Q with faces parallel to the coordinate axes. Moreover, to prove anisotropic error estimates we will work with the stronger class $A_2^s \subset A_2$ defined in an analogous way but taking supremum over all parallelepipeds with faces parallel to the coordinate axes.

We will denote with L^2_ω the L^2 space with measure $\omega(x)dx$ and with H^1_ω the corresponding weighted Sobolev space.

Introducing the vector variable $\boldsymbol{\sigma} = -\omega\nabla u$, the mixed finite element approximation is given by $(\boldsymbol{\sigma}_h, u_h) \in \boldsymbol{S}_h \times V_h$ satisfying

$$\int_\Omega \omega^{-1}\,\boldsymbol{\sigma}_h\cdot\boldsymbol{\tau}\,dx - \int_\Omega u_h\,\mathrm{div}\,\boldsymbol{\tau}\,dx + \int_\Omega v\,\mathrm{div}\,\boldsymbol{\sigma}_h\,dx = \int_\Omega f v\,dx \quad \forall(\boldsymbol{\tau}, v) \in \boldsymbol{S}_h \times V_h$$

We consider the lowest order Raviart-Thomas approximation in rectangular elements. In this case, given a partition $\mathcal{T}_h$ the finite element spaces are,

$$\boldsymbol{S}_h = \{\boldsymbol{\tau} = (\tau_1, \ldots, \tau_n) \in H(\mathrm{div}\,, \Omega) : \, \tau_j|_R \in \mathbb{R} + x_j\mathbb{R}\,,\, \forall R \in \mathcal{T}_h\}$$

and

$$V_h = \{v \in L^2(\Omega) : \, v|_R \in \mathbb{R}\,,\, \forall R \in \mathcal{T}_h\}$$

It is well known that there exists Π_h (the so called Raviart-Thomas interpolation operator) satisfying the commutative diagram property $\mathrm{div}\,\Pi_h = P_h \mathrm{div}$, where P_h is the orthogonal L^2-projection onto V_h. To simplify notation we will write $\Pi_h\sigma_j$ instead of $(\Pi_h\boldsymbol{\sigma})_j$.

In many problems in which the coefficient ω degenerates near some part of the boundary, it is of interest to have error estimates involving the distance to the boundary or to a subset of it.

For a rectangular element $R = [a_1, b_1] \times \cdots \times [a_n, b_n]$ define, for $i = 1, \cdots, n$, $d_{i,R}(x) := \min\{(b_i - x_i), (x_i - a_i)\}$. Assuming that $\omega \in A_2^s$ we obtain the following error estimates for the Raviart-Thomas interpolation and for the L^2-projection:

$$\|\sigma_j - \Pi_h\sigma_j\|_{L^2_{\omega^{-1}}(R)} \le C \sum_{i=1}^{n} \left\| d_{i,R} \frac{\partial \sigma_j}{\partial x_i} \right\|_{L^2_{\omega^{-1}}(R)}$$

and

$$\|u - P_h u\|_{L^2_\omega(R)} \le C \sum_{i=1}^{n} \left\| d_{i,R} \frac{\partial u}{\partial x_i} \right\|_{L^2_\omega(R)}$$

where C is a constant that depends on ω and n. The main tool to prove these inequalities is a weighted improved Poincaré estimate proved in [1].

In view of these estimates, error estimates for the mixed finite element approximation are a consequence of

$$\|\boldsymbol{\sigma} - \boldsymbol{\sigma}_h\|_{L^2_{\omega^{-1}}(\Omega)} \le 2\|\boldsymbol{\sigma} - \Pi_h\boldsymbol{\sigma}\|_{L^2_{\omega^{-1}}(\Omega)}$$

and

$$\|u - u_h\|_{L^2_\omega(\Omega)} \le C \left\{ \|u - P_h u\|_{L^2_\omega(\Omega)} + \|\boldsymbol{\sigma} - \Pi_h\boldsymbol{\sigma}\|_{L^2_{\omega^{-1}}(\Omega)} \right\}$$

These estimates can be proved as in the non degenerate case. For the second one we make use of a weighted inf-sup, or equivalently, of the existence of right inverses of the operator $\mathrm{div} : H^1_{\omega^{-1}}(\Omega) \to L^2_{\omega^{-1}}(\Omega)$. This can be proved using the theory of singular integrals (see [2]).

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DPG method for a singularly perturbed reaction-diffusion problem

Norbert Heuer
(joint work with Michael Karkulik)

The discontinuous Petrov-Galerkin (DPG) method with optimal test functions aims at generating finite element approximations for singularly perturbed problems in a robust way. This has been successfully pursued in different variants for convection-dominated diffusion problems, see [1, 2, 3, 4].

We study the following singularly perturbed problem of reaction-dominated diffusion,

$$-\epsilon\Delta u + u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \Gamma. \tag{1}$$

Here, $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ is a bounded, simply connected Lipschitz polygonal/polyhedral domain with boundary $\Gamma := \partial\Omega$. We assume that $\epsilon > 0$ and $f \in L_2(\Omega)$. Such problems appear in applications, for instance, in implicit time-discretizations with small time steps of parabolic reaction-diffusion problems, and when solving nonlinear reaction-diffusion problems by the Newton method. We develop a DPG method that gives a robust (i.e., uniform in ϵ) approximation of the solution u to (1), and other field variables. The challenge is to find a setting that leads to this robust control in a norm that is stronger than the natural norm $(\|\cdot\|^2 + \epsilon\|\nabla\cdot\|^2)^{1/2}$ (induced by the Dirichlet bilinear form). Here, $\|\cdot\|$ denotes the $L_2(\Omega)$-norm. Indeed, in [6], Lin and Stynes argue that a balanced norm (in terms of ϵ) for this problem is $(\|\cdot\|^2 + \epsilon^{1/2}\|\nabla\cdot\|^2 + \epsilon^{3/2}\|\Delta\cdot\|^2)^{1/2}$. It turns out that a successful approach is to rewrite (1) as the first order system

$$\epsilon^{-\alpha}\sigma - \nabla u = 0, \quad \rho - \operatorname{div}\sigma = 0, \quad -\epsilon^{1-\alpha}\rho + u = f,$$

with parameter $\alpha \geq 0$, and to formulate this in an ultra-weak sense by testing the third equation also with the (piecewise) Laplacian of (piecewise) smooth functions. In this formulation we introduce another parameter $\beta \geq 0$ to equilibrate the influence of ϵ. We then develop a completely localizable test norm which induces the norm $(\|u\|^2 + \|\sigma\|^2 + \epsilon^{2\beta}\|\rho\|^2)^{1/2}$ on the ansatz side. Main result is that this norm is robustly controlled by the energy norm of the method when selecting $\alpha = 1/4, \beta = 1/2$. This yields the balanced norm proposed by Lin and Stynes, for the field variables u, $\sigma = \epsilon^{1/4}\nabla u$, and $\epsilon^{1/2}\rho = \epsilon^{3/4}\Delta u$. As a consequence, the DPG method with optimal test functions converges in this norm, robustly controlled by the energy norm. Note that, by design, the DPG method is optimal in the energy norm.

We present several numerical experiments that underline the robustness of the method, for smooth and non-smooth solutions, and very small ϵ. Generally, adaptivity driven by the energy norm (which is automatically local) delivers optimal convergence rates, once boundary and interior layers are sufficiently resolved.

A detailed analysis and description of the numerical results can be found in [5].

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Alternative energy space based approach for the finite element approximation of the Dirichlet boundary control problem

Thirupathi Gudi

(joint work with Sudipto Chowdhury, Thirupathi Gudi, A. K. Nandakumaran)

We consider the Dirichlet boundary control problem formulated as follows: Find $(u,q) \in H^1(\Omega) \times H^1(\Omega)$ such that

$$J(u,q) = \min_{(w,p)\in H^1(\Omega)\times H^1(\Omega)} J(w,p)$$

subject to

$$\begin{aligned} w &= w_0 + p \quad w_0 \in H_0^1(\Omega) \\ (\nabla w_0, \nabla v) &= (f,v) - (\nabla p, \nabla v) \quad \forall v \in H_0^1(\Omega), \end{aligned}$$

where $f \in L^2(\Omega)$ is given and $J : H^1(\Omega) \times H^1(\Omega) \to R$ is defined by

$$J(w,p) = \frac{1}{2}\|w - u_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|\nabla p\|^2_{L^2(\Omega)}, \quad w \in H^1(\Omega),\ p \in H^1(\Omega),$$

for given desired state $u_d \in L^2(\Omega)$ and regularizing parameter $\alpha > 0$. The optimal control problem has a unique solution and the following optimality system is obtained: There exists a unique state $u \in H^1(\Omega)$, adjoint state $\phi \in H_0^1(\Omega)$ and control $q \in H^1(\Omega)$ such that

$$\begin{aligned} u &= u_f + q, \quad u_f \in H_0^1(\Omega), \\ (\nabla u_f, \nabla v) &= (f,v) - (\nabla q, \nabla v) \quad \forall v \in H_0^1(\Omega), \\ (\nabla v, \nabla \phi) &= (u - u_d, v) \quad \forall v \in H_0^1(\Omega), \\ \alpha(\nabla q, \nabla p) &= (\nabla p, \nabla \phi) + (u_d - u, p) \quad \forall p \in H^1(\Omega). \end{aligned}$$

The approach with the aforementioned formulation provides the sufficient smooth control and the state on polygonal domains unlike in the case of Dirichlet control problem seeking the control variable form $L^2(\partial\Omega)$. We discretize the optimality system using piecewise linear conforming finite element method for approximating the state, adjoint state and the control. Optimal order a priori error estimates are derived in the energy and the L^2 norm for all the three variables. The L^2 norm error estimate requires an auxiliary optimal control problem and a post-processed control. Further, a reliable and efficient residual based *a posteriori* error estimator is derived. Numerical experiments show optimal order of convergence on uniform as well as on adaptively refined meshes. It is also observed that if the regularizing parameter is taken to be small, the state converges to the desired state u_d.

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Mixed Finite Element Method for Elasticity Problems

Jun Hu

We developed a new framework to design and analyze the mixed FEM for elasticity problems by establishing the following three main results:

A structure of the discrete stress space: on simplicial grids, the discrete stress space can be selected as the symmetric matrix-valued Lagrange element space, enriched by a symmetric matrix-valued polynomial $H(\mathrm{div})$ bubble function space on each simplex; a corresponding choice applies to product grids.

Two basic algebraic results: (1) on each simplex, the symmetric matrices of rank one produced by the tensor products of the unit tangent vectors of the $n(n+1)/2$ edges of the simplex, form a basis of the space of the symmetric matrices; (2) on each simplex, the divergence space of the above $H(\mathrm{div})$ bubble function space is equal to the orthogonal complement space of the rigid motion space with respect to the corresponding discrete displacement space. (A similar result holds on a macroelement for the product grids.)

These define a two-step stability analysis which is new and different from the classic one in literature. As a result, on both simplicial and product grids, we were able to define he first families of both symmetric and optimal mixed elements with polynomial shape functions in any space dimension. Furthermore, the discrete stress space has a simple basis which essentially consists of symmetric matrix-valued Lagrange element basis functions.

A line-search assisted monolithic scheme for phase-field computing of brittle fracture

Laura De Lorenzis
(joint work with Tymofiy Gerasimov)

Phase-field modeling of brittle fracture in elastic solids dates back to the late 1990s and, since then, has been the subject of extensive theoretical and computational investigations. In general, the phase-field approach to model systems with sharp interfaces consists in incorporating a continuous field variable, the field order parameter, which differentiates between multiple physical phases within a given system through a smooth transition. In the context of fracture, such order parameter describes the smooth transition between the fully broken and intact material phases, thus approximating the sharp crack discontinuity, and is, therefore, referred to as the crack field. The evolution of this field as a result of the external loading conditions models the fracture process. The mathematical description consists of a coupled non-linear system of (quasi-static or dynamic) stress equilibrium equations and a gradient-type evolution equation for the crack phase-field. What makes the approach particularly attractive is its ability to elegantly simulate complicated fracture processes, including crack initiation, propagation, merging, and branching, in general situations and for 3D geometries, without the need for additional ad-hoc criteria. Propagating cracks are tracked automatically by the evolution of the smooth crack field on a fixed mesh. This leads to a significant advantage over the discrete fracture description, whose numerical implementation requires explicit (in the classical finite element setting) or implicit (within extended finite element methods) handling of the discontinuities. The possibility to avoid the tedious task of tracking complicated crack surfaces in 3D significantly simplifies the implementation. Recent publications of our research group on this topic are [1, 2, 3]. However, within the finite element framework, already a two-dimensional quasi-static phase-field formulation is computationally quite demanding, mainly for the following reasons: (i) the need to resolve the small length scale inherent to the diffusive crack approximation calls for extremely fine meshes, at least locally in the crack phase-field transition zone, (ii) due to non-convexity of the related free-energy functional, a robust, but slowly converging staggered solution scheme based on algorithmic decoupling is typically used. In this contribution we tackle problem (ii) and propose a faster and equally accurate approach for quasi-static phase-field computing of (brittle) fracture using a monolithic solution scheme which is accompanied by a novel line search procedure to overcome the iterative convergence issues of non-convex minimization. We present a detailed critical evaluation of the approach and its comparison with the staggered scheme in terms of computational cost, accuracy and robustness [4].

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Optimal discretization in Banach spaces

Ignacio Muga

(joint work with Kristoffer G. van der Zee)

In the setting of Banach spaces, we consider the abstract problem

$$\begin{cases} \text{Find } u \in \mathbb{U} \text{ such that} \\ Bu = f \text{ in } \mathbb{V}^*, \end{cases}$$

where $\mathbb{U}$ and $\mathbb{V}$ are Banach spaces, $B : \mathbb{U} \to \mathbb{V}^*$ is a continuous, bounded-below, linear operator, and the data $f \in \mathbb{V}^*$ is a given element in the dual space of $\mathbb{V}$. For a given discrete subspace $\mathbb{U}_n \subset \mathbb{U}$ (of dimension n), the objective of this talk is to present a Galerkin-based discretization technique which is guaranteed to provide a near-best approximation $u_n \in \mathbb{U}_n$ to the solution u, i.e., u_n satisfies the a priori error estimate

$$\|u - u_n\|_{\mathbb{U}} \leq C \inf_{w_n \in \mathbb{U}_n} \|u - w_n\|_{\mathbb{U}},$$

for some constant $C \geq 1$, independent of n. In this spirit, we initially propose a discretization method to achieve

$$u_n = \arg \min_{w_n \in \mathbb{U}_n} \|f - Bw_n\|_{\mathbb{U}}.$$

The method relies upon the duality map $J_{\mathbb{V}} : \mathbb{V} \to \mathbb{V}^*$ (cf. [1, 2, 3]), which extend to Banach spaces the concept of the well-known Riesz map of Hilbert spaces. However, in a non-Hilbert setting, the duality map is nonlinear. To make the method feasible, a discretization of the test space is needed. Hence, by considering a finite-dimensional subspace $\mathbb{V}_m \subset \mathbb{V}$, we end up with a discretization method that achieves

$$u_n = \arg \min_{w_n \in \mathbb{U}_n} \|f - Bw_n\|_{\mathbb{V}_m^*}.$$

We show the well-posedness of these methods, together with error estimates, and some basic numerical experiments in 1D.

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Low-Order dPG-FEMs for Linear Elasticity

Friederike Hellwig
(joint work with Carsten Carstensen)

Since the design of pointwise symmetric stress approximations in $H(\mathrm{div},\Omega;\mathbb{S})$ is cumbersome, especially in $3D$, the discontinuous Petrov-Galerkin methodology promises a low-order symmetric stress approximation. In [1], we use the ultraweak formulation of linear elasticity to introduce three new methods. This formulation seeks $x \in X$ with $b(x,y) = F(y)$ for all $y \in Y$, where

$$x = (\sigma,u,t,s) \in X = L^2(\Omega;\mathbb{S}) \times L^2(\Omega;\mathbb{R}^n) \times H^{-1/2}(\mathcal{T};\mathbb{R}^n) \times H_0^{1/2}(\mathcal{T};\mathbb{R}^n),$$
$$y = (\tau,v) \in Y = H(\mathrm{div},\mathcal{T};\mathbb{S}) \times H^1(\mathcal{T};\mathbb{R}^n),$$
$$b((\sigma,u,t,s),(\tau,v)) = (\sigma,\mathbb{C}^{-1}\tau - \varepsilon_{NC}(v))_\Omega + (u,\mathrm{div}_{NC}\,\tau)_\Omega - \langle t,v\rangle_{\partial\mathcal{T}} - \langle \tau\nu,s\rangle_{\partial\mathcal{T}}.$$

The methods differ from each other in the choice of norms and the occurence of some constraint. The practical dPG method [2, 3] seeks $x_h \in \arg\min_{\xi_h \in X_h} \|F - b(\xi_h,\bullet)\|_{Y_h^*}$. The discrete trial space $X_h \subseteq X$ consists of piecewise constant ansatz functions for the displacement and the stress variable and piecewise affine and continuous interface displacements and piecewise constant interface tractions. The minimal discrete test space $Y_h \subseteq Y$ is of lower order than those presented in [4, 5] and comprises piecewise (and, in general, discontinuous) symmetric parts of lowest-order Raviart-Thomas functions and piecewise affine functions. This space allows for a direct proof of the discrete inf-sup condition

$$0 < \beta_h := \inf_{x_h \in X_h} \sup_{y_h \in Y_h} \frac{b(x_h,y_h)}{\|x_h\|_X \|y_h\|_Y}$$

with explicit constant $0 < c \le \beta_h$ independent of the mesh-size and the critical Lamé parameter λ. A splitting lemma and analysis of the trace functions as in [6] prove the continuous inf-sup condition

$$0 < \beta := \inf_{x \in X} \sup_{y \in Y} \frac{b(x,y)}{\|x\|_X \|y\|_Y} .$$

This implies the equivalence of the discrete inf-sup condition and the existence of a linear and bounded projection $\Pi : Y \to Y_h$ with $b(X_h,(1-\Pi)Y) = 0$ and yields a complete a priori

$$\|x - x_h\| \le \|b\|/\beta_h \,\mathrm{dist}_X(x,X_h)$$

and a posteriori error analysis [5, 7]

$$\beta\|x-\xi_h\| \leq \|\Pi\|\|F-b(\xi_h,\bullet)\|_{Y_h^\star} + \|F\circ(1-\Pi)\|_{Y^\star} \leq 2\|b\|\|\Pi\|\|x-\xi_h\|.$$

which is robust in the incompressible limit as $\lambda \to \infty$. Numerical experiments with uniform and adaptive mesh-refinings investigate λ-robustness and confirm that the third scheme is locking-free. Similar schemes can be applied to Stokes and Maxwell equations as well.

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DPG applied to various variational formulations of linear elasticity

Brendan Keith

(joint work with Federico Fuentes, Leszek Demkowicz)

The DPG method of Demkowicz and Gopalakrishnan [2] has recently presented itself, through numerical studies, as a reliably stable finite element method in a wide class of linear problems and some nonlinear problems (see [3] and references therein).

Until lately, this method has been studied exclusively for variational formulations in the ultra-weak setting. However, the DPG method is applicable to all well-posed variational problems on Hilbert spaces. In light of the improved theory presented in [1], we re-examine the DPG method in the context of linear elasticity. This problem was first studied with the method in the ultra-weak setting in [4]. Our contemporary study is purely a proof-of-concept, the purpose of which is to demonstrate, through the means of direct numerical experiment, the fitness of the method in multiple variational formulations.

For our experiments, we have considered four variational formulations for linear elasticity in 3D; the trivial formulation (equivalent to the first order least squares method), the ultra-weak variational formulation, the (first) mixed formulation, and the primal formulation. In each case, we demonstrate that the expected convergence rates are obtained.

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Reliable and Efficient A Posteriori Error Analysis for the Obstacle Problem

Karoline Köhler

(joint work with Carsten Carstensen)

The obstacle problem is the simplest mathematical model of a variational inequality, with countless applications and relatives in free boundary value problems. The point of departure for the reliable and efficient a posteriori error analysis is the methodology presented in [2]. Given the exact solution u and any approximation $v \in H_0^1(\Omega)$, as well as the exact Lagrange multiplier λ and some approximation $\mu \in L^2(\Omega; (-\infty, 0])$, the a posteriori error analysis concerns the notion of the total error

$$\begin{aligned}\mathrm{Err} := \left(\int_\Omega \mu(\chi - u)\mathrm{d}x\right)^{1/2} + \left(\int_\Omega (-\lambda)(v-\chi)_+\mathrm{d}x\right)^{1/2} \\ + |||e||| + |||e+w||| + |||\lambda - \mu|||_*.\end{aligned}$$

The general situation involves the residual

$$\mathrm{Res}(\varphi) := F(\varphi) - \int_\Omega \mu\varphi\mathrm{d}x - a(v,\varphi) \quad \text{for all } \varphi \in V$$

and the gap function $w := \min\{0, v-\chi\}$, which vanishes when v is replaced by $\max\{v,\chi\}$. With the guaranteed upper bound

$$\mathrm{GUB} := |||\mathrm{Res}|||_* + \left(\int_\Omega (-\mu)(v-\chi)_+\mathrm{d}x\right)^{1/2} + |||w|||$$

this leads to reliable and efficient error control for the obstacle problem, even with known constants, in the following sense.

Theorem. *Any Sobolev function v with exact boundary conditions and any nonpositive Lebesgue function μ satisfy*

$$1/2\ \mathrm{GUB} \le \mathrm{Err} \le \sqrt{30/7}\ \mathrm{GUB}.$$

The presented approach provides a refined generalization of the known error control [1, 2, 3, 4, 5, 6, 7, 8] and includes error control also for nonconforming and mixed finite element methods. The error control of the residual Res may involve the solve of a linear problem, but circumvents the need of exact solve in the nonlinear obstacle problem. The general setting provides a larger flexibility for the choice of $\mu \in L^2(\Omega; (-\infty, 0]) := \{\mu \in L^2(\Omega) |\ \mu \leq 0 \text{ a.e. in } \Omega\}$. For lowest-order conforming, nonconforming, and mixed finite element methods this allows for the design of an efficient discrete Lagrange multiplier in the following sense.

Theorem. *The discrete lowest-order conforming, nonconforming, and mixed finite element method allow for the computation of* $v \in H_0^1(\Omega)$ *and* $\mu \in L^2(\Omega; (-\infty, 0])$ *to the solution* $u \in H_0^1(\Omega)$ *and the Lagrange multiplier* $\lambda := f + \Delta u \in L^2(\Omega; (-\infty, 0])$ *such that*

$$|||\lambda - \mu|||_* \lesssim |||u - v||| + \text{HOT}$$

holds with higher-order terms HOT.

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Contact and mesh-tying using mortar methods

Linus Wunderlich

(joint work with E. Brivadis, A. Buffa, O. Steinbach, B. Wohlmuth)

Domain decomposition techniques and mortar methods are used in many situations, including multi-physics and contact problems, and they provide flexible and powerful tools for the numerical approximation of partial differential equations.

The first part of the talk considers the approximation of mechanical contact problems, modeled by variational inequalities. While optimal a priori error estimates for contact problems in the natural energy norm do exist, see [3], only very few results are known for alternative norms. In addition to the primal variable u, the dual variable λ is also of interest. We consider as prototype a simple

Signorini problem and provide new optimal order a priori error estimates for the trace and the flux on the Signorini boundary Γ_S. Signorini-type problems are non-linear boundary value problems that can be regarded as a simplified scalar model of elastic contact problems. For piecewise linear finite element discretizations using biorthogonal basis functions, we obtain the following a priori estimates in the natural trace norms, see [4]:

$$\|u - u_h\|_{H_{00}^{1/2}(\Gamma_S)} + \|\lambda - \lambda_h\|_{H^{-1/2}(\Gamma_S)} \leq ch^{3/2-\varepsilon}\|u\|_{H^{5/2-\varepsilon}(\Omega)}.$$

The a priori analysis is based on an equivalent reformulation as a variational inequality posed on the Signorini boundary and the use of the continuous and a discrete Steklov–Poincaré operator. A Strang lemma relates the discretization error to the difference of the Steklov–Poincaré operators, which is itself characterized as a trace error of a linear problem. Then the trace estimate for a linear setting can be shown using modern Aubin–Nitsche type duality arguments. A direct consequence is an a priori bound for the L^2 error in the domain, up to the order of $h^{3/2-\varepsilon}$. However, numerical results presented in [4] show a gap between the theoretical and numerical results concerning the L^2 error, where the order h^2 could be observed.

In the second part of the talk, the application of mortar methods in the framework of isogeometric analysis, see [2], is presented. A weak coupling of multi-patch geometries is needed due to the limiting tensor product grid structure. Based on the results in [1], we present theoretical as well as numerical aspects of isogeometric mortar methods. For the Lagrange multiplier, the choice of trace spaces of different spline degrees is considered. Two pairings were found to be suitable in a domain decomposition context. In one case, we consider an equal order pairing for which a cross point modification, e.g. based on a local degree reduction, is required. In the other case, the degree of the dual space is reduced by two compared to the primal degree. This pairing is proven to be inf-sup stable without any necessary cross point modification. By partial integration, the stability condition can carefully be traced back to a stable equal order pairing. A degree reduction by one yields an unstable pairing and spurious oscillations can be numerically observed. Stable pairings are given by a degree reduction by any even number, but for a degree difference larger than two, the approximation properties of the Lagrange multiplier space are then controlling the error decay also of the primal variable. The optimality of the two suitable pairings and the suboptimality of a degree reduction by four are shown in a numerical example, see Figure 1.

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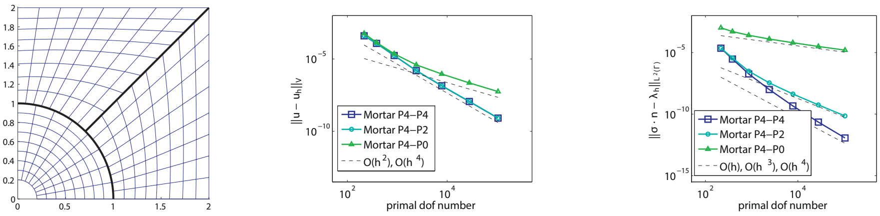

FIGURE 1. Error decay for different dual degrees, originally presented in [1]. Left: Mesh and domain partitioning. Middle: Error of the primal variable in the broken H^1 norm. Right: Error of the dual variable in the L^2 norm.

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Multiscale Petrov-Galerkin Finite Element Method for High-Frequency Acoustic Scattering

DIETMAR GALLISTL
(joint work with Daniel Peterseim)

The Helmholtz equation in an open bounded Lipschitz polygon $\Omega \subseteq \mathbb{R}^d$ ($d \in \{1, 2, 3\}$) with outer unit normal ν reads

$$\begin{aligned} -\Delta u - \kappa^2 u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \Gamma_D, \\ \nabla u \cdot \nu - i\kappa u &= g \quad \text{on } \Gamma_R. \end{aligned} \tag{1}$$

Here, the boundary $\partial\Omega$ is decomposed into disjoint parts $\partial\Omega = \Gamma_D \cup \Gamma_R$. Typically, the Dirichlet boundary Γ_D refers to a sound-soft obstacle whereas the Robin boundary Γ_R results from truncation of the full space problem to the bounded domain Ω. It is well known that standard finite element approximations to (1) exhibit the so-called *pollution effect* [1], which means that the ratio of the error of the finite element method and the best possible approximation in the finite element space becomes arbitrarily large as the real parameter $\kappa > 0$ (the wavenumber) increases. The mesh-size H for an accurate representation of the wave usually requires a fixed number of grid points per wavelength, written $\kappa H \approx 1$. The stability of the finite element method, however, requires a much finer mesh-size h with $h\kappa^\alpha \approx 1$ for some $\alpha > 1$. This makes high-frequency scattering simulations with standard methods problems computationally costly.

The talk presents a pollution-free Petrov-Galerkin multiscale finite element method for the Helmholtz problem with large wave number κ. The proposed method employs standard continuous Q_1 finite elements at a coarse discretization scale H as trial functions, whereas the test functions are computed as the solutions of local problems at a finer scale h. The diameter of the support of the test functions behaves like mH for some oversampling parameter m. Provided m is of the order of $\log(\kappa)$ and h is sufficiently small, the resulting method is stable and quasi-optimal in the regime where H is proportional to κ^{-1}. In homogeneous (or more general periodic) media, the fine scale test functions depend only on local mesh-configurations. Therefore, the seemingly high cost for the computation of the test functions can be drastically reduced on structured meshes. Numerical experiments in two and three space dimensions give empirical insight in the dependence of the parameters H, h, and m.

The talk is based on the recent works [2, 3].

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A Plane Wave Virtual Element Method for the Helmholtz Problem

Ilaria Perugia

(joint work with Paola Pietra, Alessandro Russo)

The virtual element method (VEM) is a generalisation of the finite element method recently introduced in [2, 3], which takes inspiration from mimetic finite difference schemes, and allows to use very general polygonal/polyhedral meshes.

My talk was concerned with a new method introduced in [15], based on inserting plane wave basis functions within the VEM framework in order to construct an H^1-conforming, high-order method for the discretisation of the Helmholtz problem, in the spirit of the partition of unity method (PUM, see e.g., [12, 13]).

Plane wave functions are a particular case of Trefftz functions for the Helmholtz problem, i.e., functions belonging to the kernel of the Helmholtz operator. Inserting Trefftz basis functions within the approximating spaces in finite element discretisations of the Helmholtz problem allows to obtain, compared to standard polynomial spaces, similar accuracy with less degrees of freedom, mitigating the the strong requirements in terms of number of degrees of freedom per wavelength due to the pollution effect [1]. There are in the literature several finite element methods for the Helmholtz problem which make use of Trefftz functions (for details, see the recent survey [8]). Besides the above mentioned PUM, which is H^1-conforming, other approaches use discontinuous Trefftz basis functions and impose interelement continuity with different strategies: by least square formulations [17, 14]); within a discontinuous Galerkin (DG) framework, like the ultra weak variational formulation [5, 4] or its Trefftz-DG generalisation [9]; by the use of Lagrange multipliers [10, 7]; through weighted residual formulations, like in the variational theory of complex rays [16, 11], or in the wave based method [6]).

The main ingredients of the plane wave VEM scheme(PW-VEM) are: *i)* a low order VEM space whose basis functions, which form a partition of unity and are associated to the mesh vertices, are not explicitly computed in the element interiors; *ii)* a proper local projection operator onto the plane wave space, which has to provides good approximation properties for Helmholtz solutions; *iii)* an approximate stabilization term. Convergence of the h-version of the PW-VEM was proved, and numerical results testing its performance on general polygonal meshes were presented.

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Mapped Tent Pitching Methods for Hyperbolic Conservation Laws

Joachim Schöberl
(joint work with Jay Gopalakrishnan, Christoph Wintersteiger)

We introduce a new class of methods called Mapped Tent Pitching (MTP) schemes for numerically solving hyperbolic problems. These schemes can be thought of as fully explicit or locally implicit schemes on unstructured space time meshes obtained by a process known in the literature as tent pitching. This process creates an advancing front in space time made by canopies of tent-shaped regions. Each such space time tent is erected (with time as the vertical direction in space time) so that causality constraints of the hyperbolic problem are never violated. Such meshing processes were named tent pitching.

Previous tent pitching methods were using Discontinuous Galerkin methods in space-time. We introduce a mapping from a cylinder in space-time to the diamond-shaped tent, and pull-pack the conservation law to the cylinder. This allows to separate space and time discretizations, such that existing Discontinuous Galerkin methods in combination with traditional Runge Kutta time-stepping methods can be applied. This reduces computing time as well as memory requirement. Numerical examples for the wave equation and Euler equations are presented.

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The finite cell method: A high-order immersed boundary method

Alexander Düster
(joint work with Stephan Heinze, Simeon Hubrich, Meysam Joulaian)

The finite cell method (FCM) [1, 2] is a combination of the fictitious domain approach with high-order finite elements. Thanks to the use of Cartesian meshes, the pre-processing, i.e. mesh generation is significantly simplified. However, due to the fact that the applied meshes do not conform to the geometry of the problem, special care has to be taken with respect to the numerical integration of the weak form, the local refinement of the approximation as well as the treatment of boundary conditions.

The FCM has been applied to several problems like linear elasticity [2] as well as to problems in biomechanics [3] or wave propagation [4]. Nonlinear problems such as geometrically nonlinearity [5] or elastoplasticity [6] have been addressed as well. The FCM has also been successfully applied to the numerical homogenization of materials with complicated microstructure [7] or to topology optimization [8] in structural mechanics. Instead of classical hierarchic shape functions, NURBS, which have become very popular thanks to the isogeometric analysis, can also be successfully used within the FCM. Local refinement strategies have been also developed for the FCM and it turned out that the *hp-d* method presents a general framework for local improvement of accuracy within the FCM, see [9].

The talk is intended to give an overview over the finite cell method, addressing also ongoing work and open questions. Several fields of applications will be presented, where the main advantages of the FCM can be exploited.

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Stress approximation and stress reconstruction for elasticity computations

Gerhard Starke
(joint work with Benjamin Müller)

Accurate stress approximations are of interest in many applications in solid mechanics due to the fact that large local stresses may cause inelastic material behavior or failure and also in order to get accurate approximations of surface traction forces. We investigate the suitability of different finite element methods regarding their ability to produce accurate stress approximations associated with elasticity problems. Starting from linear elasticity, the investigation of hyperelastic material models involving geometrical and material nonlinearities is also pursued. Of particular interest are approaches which remain uniformly accurate in the limit of incompressible materials.

From standard displacement-pressure finite element methods, accurate stress approximations can be reconstructed in a post-processing step. Particularly useful in this context are quadratic nonconforming finite elements [6, 5] since the associated stresses already obey certain local average momentum balance properties which give a good starting point for reconstruction algorithms (cf. [7]). In contrast to the lowest-order case, these elements satisfy a discrete Korn's inequality under reasonable assumptions on the prescribed boundary conditions (cf. [3]). An alternative approach consists in the use of variational formulations involving the stress as an independent variable which is approximated directly in suitable $H(div)$-conforming finite element spaces. Such approaches may either be of saddle-point type (cf. [2]) or of least-squares type (cf. [1, 4]) and relations between these two approaches will be investigated in detail. In particular, the error associated with momentum balance is proved to be of higher order than the overall error for the least-squares approach while it is well-known that the momentum balance is approximated in an optimal way for the saddle-point approach if appropriate finite element combinations are used. Stress-based variational principles for hyperelastic material models are studied based on the constructions in [8].

The approximations obtained from the stress-based finite element approaches are compared computationally with those obtained from a reconstruction procedure.

For all of the above approaches, stress approximations in Raviart-Thomas spaces of next-to-lowest order will be produced and compared. Computational results will be presented for some two- and three-dimensional model problems in the linearly elastic as well as in the hyperelastic setting focussing on incompressible materials.

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A general a posteriori estimation for variational inequalities of the second kind

Andreas Schröder
(joint work with Markus Bürg)

In this note, we briefly present a general residual-based a posteriori error estimation for variational inequalities of the second kind. The a posteriori error estimation is derived in [1]. The underlying idea is to express the residual in terms of discrete Lagrange multipliers which are associated with the constraints of the variational inequalities and which can be obtained, for instance, by some post-processing or by the discretization of a mixed formulation. The discretization error is estimated by the dual norm of the residual plus some computable remainder terms which capture typical error sources resulting, for instance, from the geometrical error, the violation of some complementarity conditions and the non-conformity of the discrete Lagrange multipliers. The dual norm of the residual can then be estimated by the error of an auxiliary problem which is given as a variational equation. Thus, well-known a posteriori error estimates for variational equations can be employed. In [1], this concept is applied to a variety of (frictional) contact problems, such as Signorini and obstacle problems, as well as to the Bingham fluid problem. Furthermore, the applicability of the estimates is confirmd by several numerical experiments in [1]. In particular, the general framework allows for the discretization with *hp*-adaptivity.

Variational inequalities of the second kind. We consider a Banach space V equipped with the norm $\|\cdot\|_V$ and a V-elliptic, continuous bilinear form $a : V \times V \to \mathbb{R}$. Let W_0 and W_1 be further Banach spaces, $\gamma_0 \in L(V, W_0)$ and $\gamma_1 \in L(V, W_1)$ with $\gamma_0(\ker \gamma_1) = W_0$ and $\gamma_1(\ker \gamma_0) = \gamma_1(V)$ where $\gamma_1(V)$ is assumed to be dense in W_1. Furthermore, let $g \in W_0$ and $K := \{v \in V \mid g - \gamma_0(v) \in G\}$ for a closed convex cone $G \subset W_0$ with $0 \in G$. We consider the variational inequality of the second kind: Find $u \in K$ such that

$$a(u, v - u) + j(v) - j(u) \geq \langle \ell, v - u \rangle$$

for all $v \in K$ where $j(v) := \sup_{\mu_1 \in \Lambda_1} \langle \mu_1, \gamma_1(v) \rangle$ with a closed, convex and bounded set $\Lambda_1 \subset W_1^*$.

A general a posteriori error estimation. Let $u_{hp} \in V$, $\tilde{\ell} \in V^*$, $\tilde{g} \in W_0$ and $(\lambda_{0,hp}, \lambda_{1,hp}) \in W_0^* \times W_1^*$ and let the residual $\mathrm{Res}(u_{hp}, \lambda_{0,hp}, \lambda_{1,hp}) : V \to V^*$ be defined as

$$\langle \mathrm{Res}(u_{hp}, \lambda_{0,hp}, \lambda_{1,hp}), v \rangle := \langle \tilde{\ell}, v \rangle - \langle \lambda_{0,hp}, \gamma_0(v) \rangle - \langle \lambda_{1,hp}, \gamma_1(v) \rangle - a(u_{hp}, v)$$

for $v \in V$. Note that u_{hp} is typically a discretization solution in some finite dimensional subspace, whereas $\lambda_{0,hp}$ and $\lambda_{1,hp}$ may serve as approximations of Lagrange multipliers. We define an error estimator by

$$\begin{aligned} \eta(\mu_0, \mu_1, z) := {}& \| \mathrm{Res}(u_{hp}, \lambda_{0,hp}, \lambda_{1,hp}) \|_{V^*}^2 + \|\lambda_{0,hp} - \mu_0\|_{W_0^*}^2 + \|\lambda_{1,hp} - \mu_1\|_{W_1^*}^2 \\ & + \|z\|_{W_0}^2 + \langle \lambda_{0,hp}, z \rangle + \langle \mu_0, \tilde{g} - \gamma_0(u_{hp}) \rangle + j(u_{hp}) - \langle \mu_1, \gamma_1(u_{hp}) \rangle \end{aligned}$$

for arbitrary $\mu_0 \in \Lambda_0 := G'$ (as the dual cone of G), $\mu_1 \in \Lambda_1$ and $z \in Z := \{z \in W_0 \mid \tilde{g} - \gamma_0(u_{hp}) + z \in G\}$. In [1, Thm.3.2] it is proven that there exists a constant $C > 0$ such that

$$\|u - u_{hp}\|_V^2 \leq C \left(\eta(\mu_0, \mu_1, z) + \|g - \tilde{g}\|_{W_0}^2 + \|\ell - \tilde{\ell}\|_{V^*}^2 \right).$$

Estimation of the residual. To estimate the dual norm of the residual, we find that $\kappa_a \|u^* - u_{hp}\|_V \leq \| \operatorname{Res}(u_{hp}, \lambda_{0,hp}, \lambda_{1,hp})\|_{V^*} \leq c_a \|u^* - u_{hp}\|_V$ where κ_a and c_a are the constants of ellipticity and continuity of a and $u^* \in V$ fulfills the variational equation $a(u^*, v) = \langle \tilde{\ell}, v \rangle - \langle \lambda_{0,hp}, v \rangle - \langle \lambda_{1,hp}, v \rangle$ for all $v \in V$. Hence, the estimation of $\| \operatorname{Res}(u_{hp}, \lambda_{0,hp}, \lambda_{1,hp})\|_{V^*}$ implies the estimation of $\|u^* - u_{hp}\|_V$ and vice versa. Assume $u_{hp} \in V_{hp}$ with V_{hp} as a subspace of V and let $\lambda_{0,hp}$ as well as $\lambda_{1,hp}$ be determined via the equation

$$\langle \lambda_{0,hp}, \gamma_0(v_{hp}) \rangle + \langle \lambda_{1,hp}, \gamma_1(v_{hp}) \rangle = \langle \tilde{\ell}, v_{hp} \rangle - a(u_{hp}, v_{hp})$$

for all $v_{hp} \in V_{hp}$. Then, u_{hp} may also be interpreted as a discrete approximation of u^* in the (finite-dimensional) discretization space V_{hp}. This means, $\| \operatorname{Res}(u_{hp}, \lambda_{0,hp}, \lambda_{1,hp})\|_{V^*}$ can be estimated by an a posteriori error estimation technique which is originally derived for variational equations.

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