

d-dimensional efficient P1-FEM implementation in Matlab and Julia

Stefanie Beuter¹ and Stefan A. Funken¹

¹*Institute of Numerical Mathematics, Ulm University, Germany*

We present an efficient implementation of the adaptive finite element method with continuous linear functions in arbitrary dimensions. Its strength lies in the applicability to any dimension without the necessity for any adjustments in the code. The routine includes all components of an adaptive FEM as the assembly of the stiffness matrix, calculation of the load vector, error estimation, and adaptive mesh refinement. The whole program is structured in six functions which have on average a length of no more than fifty lines. Due to singularities in a domain, adaptive methods are highly important to keep the computational cost low. This effect is even increased in higher dimensions. We refine a given mesh according to an error estimator by the Newest Vertex Bisection, i.e. any simplex that is marked for refinement is divided into two simplices by bisection of an edge. The achievement of a routine of almost linear complexity with respect to the number of elements is reinforced by numerical calculations. Our implementation is realized in Matlab and Julia and focuses on an efficient realization that can be easily adapted to other vectorized languages. Furthermore, the derived implementations allow for an analysis of the performance and data structures in high dimensions. For example, we investigate the sparsity of the stiffness matrix according to the dimensions.

Goal-oriented adaptive finite element method for semilinear elliptic PDEs

Roland Becker¹, Maximilian Brunner², Michael Innerberger², Jens Markus Melenk², and Dirk Praetorius²

¹*IPRA-LMAP, Université de Pau et des Pays de l'Adour, 64013 Pau Cedex, France*

²*Institute of Analysis and Scientific Computing, TU Wien, 1040 Vienna, Austria*

The talk presents our recent work [1]: For a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ and given $f, g \in L^2(\Omega)$, we aim to approximate the linear goal quantity

$$G(u) := \int_{\Omega} gu \, dx, \quad (1)$$

where $u \in H_0^1(\Omega)$ is the weak solution of the semilinear elliptic PDE

$$-\operatorname{div}(\mathbf{A}\nabla u) + b(u) = f \quad \text{in } \Omega \quad \text{subject to} \quad u = 0 \quad \text{on } \Gamma := \partial\Omega. \quad (2)$$

Here, the diffusion matrix $\mathbf{A} \in \mathbb{R}_{\text{sym}}^{d \times d}$ is uniformly positive definite, and the smooth nonlinearity $b(\cdot)$ is monotone and satisfies certain growth conditions. The weak formulation of the so-called *primal problem* [2] reads as follows: Find $u \in H_0^1(\Omega)$ such that

$$\langle \mathbf{A}\nabla u, \nabla v \rangle + \langle b(u), v \rangle = \langle f, v \rangle \quad \text{for all } v \in H_0^1(\Omega), \quad (3)$$

where $\langle v, w \rangle := \int_{\Omega} vw \, dx$ denotes the $L^2(\Omega)$ -scalar product. Existence and uniqueness of the solution $u \in H_0^1(\Omega)$ of [3] follow from the Browder–Minty theorem on monotone operators. Based on a conforming triangulation \mathcal{T}_H of Ω and a fixed polynomial degree $m \in \mathbb{N}$, let $\mathcal{X}_H := \{v_H \in H_0^1(\Omega) : \forall T \in \mathcal{T}_H: v_H|_T \text{ is a polynomial of degree } \leq m\}$. The FEM discretization of the primal problem [3] reads: Find $u_H \in \mathcal{X}_H$ such that

$$\langle \mathbf{A}\nabla u_H, \nabla v_H \rangle + \langle b(u_H), v_H \rangle = \langle f, v_H \rangle \quad \text{for all } v_H \in \mathcal{X}_H. \quad (4)$$

We approximate the sought goal quantity $G(u)$ by means of the computable quantity $G(u_H)$. The optimal error control of the goal error $G(u) - G(u_H)$ involves the so-called (*practical*) *dual problem*: Find $z[u_H] \in H_0^1(\Omega)$ such that

$$\langle \mathbf{A}\nabla z[u_H], \nabla v \rangle + \langle b'(u_H)z[u_H], v \rangle = G(v) \quad \text{for all } v \in H_0^1(\Omega). \quad (5)$$

Existence and uniqueness of $z[u_H]$ follow from the Lax–Milgram lemma. The FEM discretization of the dual problem [5] reads: Find $z_H[u_H] \in \mathcal{X}_H$ such that

$$\langle \mathbf{A}\nabla z_H[u_H], \nabla v_H \rangle + \langle b'(u_H)z_H[u_H], v_H \rangle = G(v_H) \quad \text{for all } v_H \in \mathcal{X}_H. \quad (6)$$

We prove the goal error estimate

$$C^{-1} |G(u) - G(u_H)| \leq \|u - u_H\|_{H^1(\Omega)} \|z[u_H] - z_H[u_H]\|_{H^1(\Omega)} + \|u - u_H\|_{H^1(\Omega)}^2. \quad (7)$$

Based on residual error estimators, we formulate a goal-oriented adaptive algorithm (GOAFEM), which guarantees convergence and, as the main contribution, optimal algebraic convergence rates.

References

- [1] R. Becker, M. Brunner, M. Innerberger, J. M. Melenk, and D. Praetorius, *Goal-oriented adaptive finite element method for semilinear elliptic PDEs*, [arXiv:2112.06687](https://arxiv.org/abs/2112.06687), 2021.

Numerical approximation of orthogonal maps with adaptive finite elements. Application to paper folding

Alexandre Caboussat

*Geneva School of Business Administration
University of Applied Sciences and Arts Western Switzerland (HES-SO)*

Orthogonal maps are the solutions of a first order fully nonlinear equation involving the gradient of the solution. It originated in the so-called origami problem [1], but has also several applications nowadays in material sciences. A Dirichlet problem is considered here, which consists of finding $\mathbf{u} : \Omega \subset \mathbb{R}^2 \rightarrow \mathbb{R}^2$ verifying

$$\nabla \mathbf{u} \in \mathcal{O}(2) \text{ in } \Omega, \quad \mathbf{u} = \mathbf{g} \text{ on } \partial\Omega.$$

where $\mathcal{O}(2)$ denotes the set of orthogonal matrix-valued functions, and \mathbf{g} is a given, sufficiently smooth, function. The solution to this problem is piecewise linear, with line singularities along the folding edges.

The numerical solution is obtained via a variational principle, which enforces a uniqueness of the solution. It relies on the minimization of a regularized objective function. We present a strategy based on a splitting algorithm for the flow problem derived from the first-order optimality conditions. It leads to solving a sequence of local nonlinear problems and a global variational problem at each time iteration. The local nonlinear problems are solved with mathematical programming techniques, while the variational problems are solved with a low order finite element method.

Within the splitting algorithm, anisotropic adaptive techniques are introduced for the solution of the variational problems. They rely on error estimate based techniques developed for the solution of linear Poisson problems [2], and show good convergence properties despite being sub-optimal. Anisotropic adaptive techniques allow to obtain refined triangulations near the folding edges while keeping the number of vertices as low as possible [4].

Numerical experiments validate the accuracy and efficiency of the adaptive method in various situations. Appropriate convergence properties are exhibited, and solutions with sharp edges are recovered. In particular, experiments with a fractal behaviour of the solution are exhibited.

This is a joint work with Prof. Marco Picasso (EPFL) and Dr Dimitrios Gourzoulidis (EPFL and HES-SO).

References

- [1] B. Dacorogna, P. Marcellini, and E. Paolini, *Origami and Partial Differential Equations*, Notices of the American Math. Soc., 57:598–606, 2010.
- [2] M. Picasso, *An anisotropic error indicator based on Zienkiewicz-Zhu error estimator: Application to elliptic and parabolic problems*, SIAM J. Sci. Comput., 24:1328–1355, 2003. DOI:[10.1137/S1064827501398578](https://doi.org/10.1137/S1064827501398578)
- [3] A. Caboussat, R. Glowinski, D. Gourzoulidis, and M. Picasso, *Numerical Approximation of Orthogonal Maps*, SIAM J. Sci. Comput., 41(6):B1341–B1367, 2019. DOI:[10.1137/19M1243683](https://doi.org/10.1137/19M1243683)
- [4] A. Caboussat, D. Gourzoulidis, M. Picasso, *An Anisotropic Adaptive Method for the Numerical Approximation of Orthogonal Maps*, J. Comput. Appl. Math., submitted, 2020.

Adaptive non-hierarchical Galerkin methods for parabolic problems with application to moving mesh and virtual element methods

Andrea Cangiani¹, Emmanuil H. Georgoulis^{2,3}, and Oliver J. Sutton²

¹*Mathematics Area, SISSA, Italy*

²*School of Mathematics and Actuarial Science at University of Leicester, UK*

³*School of Applied Mathematical and Physical Sciences, NTUA, Greece*

We extend classical *a posteriori* error estimates for Galerkin numerical solutions of parabolic problems by allowing the discrete spaces between time-steps to be completely unrelated from one another (*non-hierarchical discrete spaces*) [1]. As such, they can be used in conjunction with very general mesh modification for the first time. The *a posteriori* error estimates are derived for the error measured in the $L^2(H^1)$ and $L^\infty(L^2)$ norms using the elliptic reconstruction technique in an abstract framework requiring no particular compatibility between the computational meshes used on consecutive time-steps, thereby significantly relaxing this basic assumption underlying previous estimates.

The practical interest of this setting is demonstrated by applying our results to finite element methods on moving meshes and using the estimators to drive an adaptive algorithm based on a virtual element method (VEM) on very general polygonal meshes.

Our results are particularly relevant to the new velocity based moving mesh virtual element method, to be presented in [2], which combines moving meshes with the virtual element framework to solve porous medium equation free boundary problems. Here, polygonal meshes can be exploited to represent moving boundaries and interfaces with a minimal number of degrees of freedom and to produce efficient local mesh refinement when a change in mesh connectivity is required such as in contact problems.

References

- [1] A. Cangiani, E. H. Georgoulis, and O. J. Sutton. *Adaptive non-hierarchical Galerkin methods for parabolic problems with application to moving mesh and virtual element methods*. *Mathematical Models and Methods in Applied Sciences*. (2021) **31**(04): 711–751.
- [2] A. Cangiani, M. Hubbard, and H. Wells. *A velocity based moving mesh virtual element method*. In preparation.

An adaptive algorithm combining mesh and geometrical model refinement

Pablo Antolin¹, Annalisa Buffa^{1,2}, [Ondine Chanon](#)¹, and Rafael Vázquez^{1,2}

¹*MNS, Institute of Mathematics, EPFL, Lausanne, Switzerland*

²*IMATI ‘E. Magenes’ (CNR), Pavia, Italy*

Removing features from a complex geometry is a classical operation in computer aided design for manufacturing. It simplifies the meshing process, and it enables faster simulations with less memory requirements. However, given a partial differential equation defined on the geometrical model of interest, removing the wrong features may greatly impact the solution accuracy. For instance, in solid mechanics simulations, such features can be holes or fillets around stress concentration regions. This is why understanding well the effects of geometrical model simplification, also called defeaturing, is an important step to be able to adaptively integrate geometric design and analysis.

In this talk, we will present an adaptive strategy for analysis-aware defeaturing that is twofold. On the one hand, the algorithm performs standard mesh refinement steps in a (partially) defeatured geometry. On the other hand, the strategy also allows for geometrical refinement. That is, at each iteration, it is able to choose which missing geometrical feature should be added to the simplified geometrical model, in order to obtain a more accurate solution.

To drive this adaptive strategy, we will introduce an *a posteriori* estimator of the energy norm of the error between the exact solution defined in the exact fully-featured geometry, and the numerical approximation of the solution defined in the defeatured geometry. Using isogeometric analysis with hierarchical B-splines as numerical method to solve the problem at hand, this estimator is proven to be reliable for very general geometrical configurations. The dependence of the estimator upon the size of the features and upon the mesh size is explicit, and the effectivity index is independent from the number of considered features. The proposed estimator can be computed very efficiently, and it is also naturally parallelizable with respect to the number of features. During the talk, we will also show the results of some numerical experiments that illustrate the capabilities of the proposed adaptive strategy.

References

- [1] A. Buffa, O. Chanon and R. Vázquez, *Analysis-aware defeaturing: problem setting and a posteriori estimation*, Math. Models Methods Appl. Sci. 32(02):359–402, 2022. DOI:[10.1142/S0218202522500099](https://doi.org/10.1142/S0218202522500099)
- [2] A. Buffa, O. Chanon and R. Vázquez, *An a posteriori error estimator for isogeometric analysis on trimmed geometries* (submitted), 2022. [arXiv:2112.14661](https://arxiv.org/abs/2112.14661)
- [3] P. Antolin and O. Chanon, *Analysis-aware defeaturing in multifeature geometries for linear elasticity and Stokes equations*, in preparation.
- [4] A. Buffa, O. Chanon and R. Vázquez, *Adaptive analysis-aware defeaturing*, in preparation.

Analysis of gradient descent on wide two-layer neural networks

Lénaïc Chizat¹

¹*Institute of Mathematics, EPFL, Switzerland*

In this talk, we present an analysis of gradient descent on wide two-layer ReLU neural networks that leads to a better understanding of the function learnt by these models. The main idea is to study the training dynamics when the width of the hidden layer goes to infinity, which leads to a so-called Wasserstein gradient flow. We will discuss various aspects of those dynamics such as: (i) the crucial role of the scaling/parameterization when taking the limit, (ii) the convergence to global minimizers and (iii) algorithmic regularization.

Optimal adaptivity for inf-sup stable problems

Michael Feischl

Institute for Analysis and Scientific Computing, TU Wien, Austria

We prove new optimality results for adaptive mesh refinement algorithms for non-symmetric, indefinite, and time-dependent problems by proposing a generalization of quasi-orthogonality which follows directly from the inf-sup stability of the underlying problem. This completely removes a central technical difficulty in modern proofs of optimal convergence of adaptive mesh refinement algorithms and leads to simple optimality proofs for the Taylor-Hood discretization of the stationary Stokes problem, a finite-element/boundary-element discretization of an unbounded transmission problem, and an adaptive time-stepping scheme for parabolic equations. The main technical tool are new stability bounds for the LU -factorization of matrices together with a recently established connection between quasi-orthogonality and matrix factorization.

References

- [1] M. Feischl, *Inf-sup stability implies quasi-orthogonality*, accepted for publication at Math. Comp. Preprint at [arXiv:2008.12198](https://arxiv.org/abs/2008.12198), 2022.

Applications of a space-time first-order system least-squares formulation for parabolic PDEs

Gregor Gantner¹ and Rob Stevenson²

¹ *Institute of Analysis and Scientific Computing
TU Wien, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria*

² *Korteweg-de Vries Institute for Mathematics
University of Amsterdam, P.O. Box 94248, 1090 GE Amsterdam, The Netherlands*

Currently, there is a growing interest in simultaneous space-time methods for solving parabolic evolution equations. Main reasons are that, compared to classical time-marching methods, space-time methods are much better suited for a massively parallel implementation, are guaranteed to give quasi-optimal approximations from the employed trial space, have the potential to drive optimally converging simultaneously space-time adaptive refinement routines, and they provide enhanced possibilities for reduced order modelling of parameter-dependent problems. On the other hand, one important drawback of space-time methods is that they require more storage. This drawback however vanishes for problems of optimal control, for which the solution is needed simultaneously over the whole time interval anyway.

While the common space-time variational formulation of a parabolic equation results in a bilinear form that is non-coercive, [1] recently proved well-posedness of a space-time first-order system least-squares formulation of the heat equation. Least-squares formulations always correspond to a symmetric and coercive bilinear form. In particular, the Galerkin approximation from any conforming trial space exists and is a quasi-best approximation. Additionally, the least-squares functional automatically provides a reliable and efficient error estimator.

In [2], we have generalized the least-squares method of [1] to general second-order parabolic PDEs with possibly inhomogeneous Dirichlet or Neumann boundary conditions. For homogeneous Dirichlet conditions, we present in this talk convergence of a standard adaptive finite element method driven by the least-squares estimator, which has also been demonstrated in [2]. The convergence analysis is applicable to a wide range of least-squares formulations for other PDEs, answering a long-standing open question in the literature. Moreover, we employ the space-time least-squares method for parameter-dependent problems as well as optimal control problems. In both cases, coercivity of the corresponding bilinear form plays a crucial role.

References

- [1] T. Führer and M. Karkulik., *Space-time least-squares finite elements for parabolic equations*, *Comput. Math. Appl.* 92:27–36, 2021. DOI:[10.1016/j.camwa.2021.03.004](https://doi.org/10.1016/j.camwa.2021.03.004)
- [2] G. Gantner and R. Stevenson, *Further results on a space-time FOSLS formulation of parabolic PDEs*, *ESAIM Math. Model. Numer. Anal.* 55(1):283–299, 2021. DOI:[10.1051/m2an/2020084](https://doi.org/10.1051/m2an/2020084)

Nonlinear reduced models for parametric/random PDEs

Andrea Bonito¹, Albet Cohen², Ronald Devore¹, Diane Guignard³, Peter Jantsch⁴, and Guergana Petrova¹

¹*Department of Mathematics, Texas A&M University, United States*

²*Laboratoire Jacques-Louis Lions, Sorbonne Université, France*

³*Department of Mathematics and Statistics, University of Ottawa, Canada*

⁴*Weathon College, United States*

We consider model reduction methods for parametric/random partial differential equations. The usual approach to model reduction is to construct a linear space V_n of (hopefully low) dimension n which accurately approximates the *parameter-to-solution map*, and then use it to build an efficient forward solver. However, the construction of a suitable linear space is not always feasible. It is well-known that numerical methods based on nonlinear approximation may outperform linear methods in many contexts. In a so-called library approximation, the idea is to replace the linear space V_n by a collection of affine spaces V^1, \dots, V^N of dimension $m \leq n$.

In this talk, we briefly review standard linear methods for model reduction. Then, we present the strategy introduced in [1] which can be used to generate a nonlinear reduced model, namely a library based on piecewise (Taylor) polynomials. We provide an analysis of the method, illustrate its performance through numerical experiments, and, if time allows, discuss possible extensions.

References

- [1] A. Bonito, A. Cohen, R. DeVore, D. Guignard, P. Jantsch, and G. Petrova, *Nonlinear methods for model reduction*, ESAIM: Math. Model. Numer. Anal. 55(2):507–531, 2021. DOI:[10.1051/m2an/2020057](https://doi.org/10.1051/m2an/2020057)

A modified Kačanov iteration scheme for the numerical solution of quasilinear elliptic diffusion equations

Pascal Heid¹, Thomas P. Wihler²

¹*Mathematical Institute, University of Oxford, UK*

²*Mathematics Institute, University of Bern, Switzerland*

Kačanov's method is an efficient iterative solver for a class of quasilinear elliptic diffusion equations. However, in order to guarantee the convergence to a solution, the classical theorem requires the diffusion coefficient to be monotonically decreasing. In this talk, we introduce a modified Kačanov method, which allows for adaptive damping and, thereby, to derive a new convergence analysis, which no longer requires the standard monotonicity condition. We further present two different adaptive strategies for the practical selection of the damping parameter. Finally, the performance of the modified scheme is demonstrated with some numerical experiments in the context of piecewise affine finite element approximations.

References

- [1] L. M. Kačanov, *Variational methods of solution of plasticity problems*, J. Appl. Math. Mech. 23(3):616–617, 1959. DOI:[10.1016/0021-8928\(59\)90184-4](https://doi.org/10.1016/0021-8928(59)90184-4)
- [2] P. Heid and T. P. Wihler, *Adaptive iterative linearization Galerkin methods for nonlinear problems*, Math. Comp. 89:2707–2734, 2020. DOI:[10.1090/mcom/3545](https://doi.org/10.1090/mcom/3545)
- [3] P. Heid and T. P. Wihler, *A modified Kačanov iteration scheme with application to quasilinear diffusion models*, ESAIM: M2AN 56 (2022) 433–450, 2022. DOI:[10.1051/m2an/2022008](https://doi.org/10.1051/m2an/2022008)

AFC stabilization method for a cross-diffusion cancer invasion model

Shahin Heydari¹, Petr Knobloch¹, and Thomas Wick²

¹ *Charles University, Faculty of Mathematics and Physics, Czech Republic*

² *Leibniz University Hannover, Institute of Applied Mathematics, Germany*

In this work we investigate a model of the invasion of healthy tissue by cancer cells which is described by a system of nonlinear PDEs consisting of a cross-diffusion-reaction equation and two additional nonlinear ordinary differential equations. We then show that when the convective part of the system is dominant the straightforward numerical methods for the studied system may be unstable. We present an implicit finite element method using piecewise polynomial defined on rectangular meshes to discretize the model in space. The proposed method is based on algebraic flux-corrected (AFC) transport scheme which is positivity preserving. Moreover, the Crank-Nicolson method is used to discretize in time and the nonlinear terms in the system are treated with fixed-point iteration in the finite element scheme.

Adaptive FEM for parameter-errors in elliptic linear-quadratic parameter estimation problems

Roland Becker¹, Michael Innerberger², and Dirk Praetorius²

¹*IPRA-LMAP, Université de Pau et des Pays de l'Adour, France*

²*Institute of Analysis and Scientific Computing, TU Wien, Austria*

Many applications from science and engineering employ PDE models with a finite number of physical parameters. As particular model problem, we consider a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$ with polygonal boundary $\Gamma := \partial\Omega$ and consider the *state equation*

$$-\operatorname{div}(A\nabla u(\mathbf{p})) = b(\mathbf{p}, v) \quad \text{in } \Omega, \quad u(\mathbf{p}) = 0 \quad \text{on } \Gamma, \quad (1)$$

where $A(x) \in \mathbb{R}_{\text{sym}}^{n \times n}$ is a symmetric and uniformly positive definite matrix, and $b(\mathbf{p}, \cdot) \in H_0^1(\Omega)'$ depends linearly on some finite dimensional parameter $\mathbf{p} \in \mathcal{Q} \subseteq \mathbb{R}^{n_{\mathcal{Q}}}$ for some fixed $n_{\mathcal{Q}} \in \mathbb{N}$. We suppose that the parameter set \mathcal{Q} is convex and closed.

The parameter \mathbf{p} is typically unknown and usually determined by experimental measurements. We model these measurements by a linear vector-valued measurement operator $\mathbf{G}: H_0^1(\Omega) \rightarrow \mathbb{R}^{n_c}$ with $n_c \in \mathbb{N}$. A parameter $\mathbf{p}^* \in \mathcal{Q}$ is then chosen such that the simulated measurements $\mathbf{G}(u(\mathbf{p}^*))$ correspond to experimental measurements $\mathbf{G}^* \in \mathbb{R}^{n_c}$ in a least squares sense.

For a discretization \mathcal{T}_H of Ω into simplices, we solve (1) to obtain a \mathcal{T}_H -piecewise polynomial approximation $u_H(\mathbf{p})$ and find a corresponding discrete parameter estimate \mathbf{p}_H^* by fitting $\mathbf{G}(u_H(\mathbf{p}_H^*))$ to \mathbf{G}^* . In this talk, we present results from our recent work [1] and show that the error of the discrete parameter estimate can be bounded by

$$\begin{aligned} \|\mathbf{p}^* - \mathbf{p}_H^*\|_{\mathcal{Q}} &\lesssim \left[\sum_{i=0}^{n_{\mathcal{Q}}} \|u_i - u_{H,i}\|^2 \right]^{1/2} \left[\sum_{j=1}^{n_c} \|z_j - z_{H,j}\|^2 \right]^{1/2} \\ &\lesssim \left[\sum_{i=1}^{n_{\mathcal{Q}}} \eta_{H,i}^2 \right]^{1/2} \left[\sum_{j=1}^{n_c} \zeta_{H,j}^2 \right]^{1/2} =: \varrho_H, \end{aligned} \quad (2)$$

where u_i and z_j are quantities obtained by the state equation (1) and the *co-state equation*, which is the dual of (1) with the measurement functional \mathbf{G} as right-hand side; $\eta_{H,i}$ and $\zeta_{H,j}$ are corresponding energy norm residual error estimators.

We show that an adaptive algorithm driven by the upper bound ϱ_H from (2) is rate optimal. In particular, our upper bound (2) converges with a rate that is the sum of the rates of state and co-state and matches the rate of convergence of the parameter error, thus outperforming existing adaptive algorithms based on residual type estimators for energy norms; see, e.g., [2]. Numerical results underline our theoretical findings.

References

- [1] R. Becker, M. Innerberger and D. Praetorius, *Adaptive FEM for parameter-errors in elliptic linear-quadratic parameter estimation problems*, [arXiv:2111.03627](https://arxiv.org/abs/2111.03627), 2021.
- [2] R. Becker and S. Mao *Quasi-optimality of an adaptive finite element method for an optimal control problem* Comput. Methods Appl. Math. 11(2):107-128, 2011.

Discrete maximum principles and qualitative properties for nonlinear diffusion problems

Róbert Horváth¹, István Faragó², and János Karátson^{1,3}

¹*Dept. of Analysis, BUTE; Hungary*

²*Dept. of Diff. Eqns., BUTE; Hungary*

³*Dept. of Applied Analysis, ELTE; Hungary*

Qualitative properties of the discrete solutions of partial differential equations (PDEs) are of considerable interest. Namely, besides the convergence of a given method, it is also important that the numerical solution shall preserve the characteristic properties of the modeled phenomenon, thus guaranteeing the qualitative reliability of the method. For diffusion type PDEs, the most relevant properties are maximum/minimum principles and, in particular, nonnegativity/nonpositivity preservation, further, for time-dependent problems, also the maximum norm contractivity. For instance, for various models, violation of nonnegativity would mean that the obtained numerical solution contradicts basic physical laws. Consequently, a huge body of research has been carried out in this field.

In this talk we focus on our results on finite element discretizations of nonlinear parabolic problems. The elliptic case [1] serves as a motivation to show the importance of angle conditions of the space mesh, see also [5]. For parabolic problems, the preservation of the qualitative properties can be generally guaranteed with additional relations of the spatial discretization and the time-step. Discrete nonnegativity preservation and maximum principles will be summarized for a class of parabolic problems. Furthermore, it is also important to reveal the relations of the involved qualitative properties in an organized network. The results are based on [3, 4], which extend the properties of the linear case in [2]. Further research is intended to involve advection terms and boundary nonlinearities in this study.

References

- [1] J. Karátson, S. Korotov, *Discrete maximum principles for finite element solutions of nonlinear elliptic problems with mixed boundary conditions*, Numer. Math. 99(4):669–698, 2005.
- [2] I. Faragó, R. Horváth, *Discrete maximum principle and adequate discretizations of linear parabolic problems*, SIAM J. Sci. Comput. 28(6):2313–2336, 2006. DOI:[10.1137/050627241](https://doi.org/10.1137/050627241)
- [3] I. Faragó, J. Karátson, S. Korotov, *Discrete maximum principles for nonlinear parabolic PDE systems*, IMA J. Numer. Anal. 32(4):1541–1573, 2012. DOI:[10.1093/imanum/drr050](https://doi.org/10.1093/imanum/drr050)
- [4] R. Horváth, I. Faragó, J. Karátson, *Qualitative properties of discrete nonlinear parabolic operators*, Numer. Math. 143(3):529–554, 2019. DOI:[10.1007/s00211-019-01062-6](https://doi.org/10.1007/s00211-019-01062-6)
- [5] J. Brandts, S. Korotov, M. Krizek, *Simplicial partitions with applications to the finite element method*, Springer Monographs in Mathematics, Springer, Cham, 2020. DOI:[10.1007/978-3-030-55677-8](https://doi.org/10.1007/978-3-030-55677-8)

Numerical Analysis of a Time Filtered Scheme for a Linear Hyperbolic Equation Inspired by DNA Transcription Modeling

Lisa Davis¹, Faranak Pahlevani², Kadence Boatman², and Timmy Susai Rajan²

¹*Department of Mathematical Sciences, Montana State University, USA*

²*Division of Science and Engineering, Penn State University - Abington, USA*

The focus of this presentation is the development and analysis of a time filtering process for a linear hyperbolic equation motivated by the modeling of the transcription of ribosomal RNA in bacteria [1]. Recently the time filter has been combined with fully implicit schemes for nonlinear problems in order to increase accuracy with minimal modifications to existing code [2]. In this talk, we demonstrate that adding a time filter to explicit schemes for hyperbolic problems yields similar results. A new explicit implementation is presented, and increased accuracy of the filtered upwind scheme is observed for test problems. The typical treatments for explicit schemes for hyperbolic problems require calculations for CFL conditions in order for the filtered schemes to remain stable. A stability condition for the new algorithm is derived. Numerical computations illustrate stability and convergence as well as dissipation and dispersion of the filtered schemes.

References

- [1] L. Davis, F. Pahlevani, and T. Susai Rajan, *An Accurate and Stable Filtered Explicit Scheme for Biopolymerization Processes in the Presence of Perturbations*, *Applied and Computational Mathematics* 10(6):121–137, 2021. DOI:[10.11648/j.acm.20211006.1](https://doi.org/10.11648/j.acm.20211006.1)
- [2] A. Guzel, and W. Layton, *Time filters increase accuracy of the fully implicit method*, *BIT Numerical Mathematics* 58:301–315, 2018. DOI:[10.1007/S105543-018-0695-z](https://doi.org/10.1007/S105543-018-0695-z)

Anisotropic adaptive finite elements for linear and nonlinear elliptic problem with strongly varying diffusion coefficients

Samuel Dubuis¹, Paride Passelli¹, and Marco Picasso¹

¹*Institute of Mathematics, EPFL, Switzerland*

Anisotropic adaptive methods have shown to be very efficient, in particular for problems with boundary layers.

Two different problems will be considered, the linear elliptic equation $-\nabla \cdot (\mu \nabla u) = f$, where $\mu > 0$ is smooth but strongly varying and the nonlinear elliptic equation $-\nabla \cdot (\mu + |\nabla u|) \nabla u = f$ where μ is a non negative constant.

Using the anisotropic setting of [2, 3] an extension of [5] is proposed here for the linear elliptic equation, the error estimator being equivalent to the true error (up to some higher order terms). A posteriori error estimates for the nonlinear problem in the isotropic framework have been presented in [4, 1]. An upper bound will be presented in the anisotropic framework.

Finally a numerical study of the effectivity index will be presented for both the problems, on non-adapted and adapted anisotropic meshes.

References

- [1] C. Carstensen, W. Liu and N. Yan, *A posteriori FE error control for p-laplacian by gradient recovery in quasi-norm*, Math. of Comp., Vol. 75, No. 256, pp. 1599-1616 (2006). DOI:[10.1090/S0025-5718-06-01819-9](https://doi.org/10.1090/S0025-5718-06-01819-9)
- [2] L. Formaggia and S. Perotto, *New anisotropic a priori error estimates*, Numer. Math. 89, 641–667 (2001). DOI:[10.1007/s002110100273](https://doi.org/10.1007/s002110100273)
- [3] L. Formaggia and S. Perotto, *Anisotropic error estimates for elliptic problems*, Numer. Math. 94, 67–92 (2003). DOI:[10.1007/s00211-002-0415-z](https://doi.org/10.1007/s00211-002-0415-z)
- [4] W. Liu, N. Yan, *Quasi-norm local error estimators for p-laplacian*, SIAM J. NUMER. ANAL. Vol. 30, No. 1, pp. 100-127 (2001). DOI:[10.1137/S0036142999351613](https://doi.org/10.1137/S0036142999351613)
- [5] M. Picasso, *Adaptive finite elements with large aspect ratio based on an anisotropic error estimator involving first order derivatives*, Comput. Methods Appl. Mech. Eng. 196, 14–23 (2006). DOI:[10.1016/j.cma.2005.11.018](https://doi.org/10.1016/j.cma.2005.11.018)

A Posteriori Error Estimates for Boundary Value Problems in Measures Stronger than the Energy Norm

S. Repin

University of Jyväskylä, Finland

We discuss a posteriori estimates of the functional type which are derived by purely functional methods without using special properties of approximations and exact solutions to boundary value problems. Usually a posteriori estimates of this class are derived in terms of the natural energy norms. In this talk, an approach is proposed to obtain guaranteed and computable bounds for a wide spectrum of error measures, which are stronger than the energy norm. It is applicable provided that the exact solution and its approximation satisfy certain additional conditions (e.g., regularity). These measures include the standard energy norm as a simple special case. A general approach is proposed to construct various measures based on using an auxiliary variational problem. Two classes of measures whose properties are close to the L^q and L^∞ norms are studied in more detail. Their properties are established, and explicitly computable two-sided error bounds are derived.

Adaptive space-time goal-oriented methods for nonstationary Stokes flow

Julian Roth¹, Jan Philipp Thiele¹, Thomas Wick^{1,2}, Uwe Köcher³

¹*Leibniz University Hannover, Institute of Applied Mathematics, Germany*

²*Université Paris Saclay, ENS Paris Saclay, LMPS, France*

³*Faculty of Mechanical Engineering, Helmut Schmidt University, Germany*

In this presentation, the framework of the dual-weighted residual method is applied to a space-time formulation of nonstationary Stokes flow. Tensor-product space-time finite elements [1] are being used to discretize the variational formulation with discontinuous Galerkin finite elements in time and inf-sup stable Taylor-Hood finite element pairs in space. To estimate the error in a quantity of interest and drive adaptive refinement in time and space, we demonstrate how the dual-weighted residual method for incompressible flow [2] can be extended to a partition of unity based error localization [3, 4]. The presentation concludes with current developments and some preliminary findings of the extension of our methodology to the nonstationary Navier-Stokes equations.

References

- [1] M.P. Bruchhäuser, U. Köcher, and M. Bause, *On the implementation of an adaptive multi-rate framework for coupled transport and flow*, [arXiv:2202.03748](https://arxiv.org/abs/2202.03748), 2022.
- [2] M. Besier, and R. Rannacher, *Goal-oriented space-time adaptivity in the finite element Galerkin method for the computation of nonstationary incompressible flow*, *Int. J. Numer. Meth. Fluids* 70: 1139-1166, 2012. DOI:[10.1002/fld.2735](https://doi.org/10.1002/fld.2735)
- [3] T. Richter, and T. Wick, *Variational localizations of the dual weighted residual estimator*, *J. Comput. Appl. Math.* 279: 192–208, 2015. DOI:[10.1016/j.cam.2014.11.008](https://doi.org/10.1016/j.cam.2014.11.008)
- [4] J.P. Thiele, and T. Wick, *Space-time error control using a partition-of-unity dual-weighted residual method applied to low mach number combustion*, [arXiv:2112.12480](https://arxiv.org/abs/2112.12480), 2021, accepted for publication in ICOSAHOM 2020+1 proceedings, 2022.

Solvability of Discrete Helmholtz Equations

Stefan Sauter¹

¹*Institut für Mathematik, Universität Zürich, Switzerland*

In our talk, we discuss the unique solvability of the discretized Helmholtz problem with Robin boundary conditions using a conforming Galerkin hp-finite element method. Wellposedness of the discrete equations is typically investigated by applying a compact perturbation to the continuous Helmholtz problem so that a "sufficiently rich" discretization results in a "sufficiently small" perturbation of the continuous problem and well-posedness is inherited via Fredholm's alternative. The qualitative notion "sufficiently rich", however, involves unknown constants and is only of asymptotic nature. In our talk, we focus on a fully discrete approach by mimicking the tools for proving well-posedness of the continuous problem directly on the discrete level. In this way, a computable criterion is derived which certifies discrete well-posedness without relying on an asymptotic perturbation argument. By using this novel approach we obtain a) new stability results for the hp-FEM for the Helmholtz problem b) examples for meshes such that the discretization becomes unstable (stiffness matrix is singular), and c) a simple checking Algorithm MOTZ "marching-of-the-zeros" which guarantees in an a posteriori way that a given mesh is certified for a stable Helmholtz discretization.

This talk comprises joint work with Maximilian Bernkopf, Céline Torres, Alexander Veit

A posteriori error estimation for a projector-splitting scheme for dynamical low rank approximation of a random heat equation

Fabio Nobile, Eva Vidličková (EPFL, Switzerland)

Abstract: Dynamical Low Rank (DLR) approximation for time-dependent problems with random parameters can be seen as a reduced basis method, in which the solution is expanded as a linear combination of few well chosen deterministic functions with random coefficients. The distinctive feature of the DLR method is that the spatial basis is computed on the fly and is free to evolve in time, thus adjusting at each time to the current structure of the random solution. In this talk, we consider the DLR approximation for a random parabolic equation and propose a class of fully discrete numerical schemes. The problem is discretized by a stochastic collocation finite element method and advanced in time by a projector-splitting scheme. Similarly to the continuous DLR approximation, our schemes are shown to satisfy a discrete variational formulation. By exploiting this property, we derive a residual based a posteriori error estimation for a heat equation with a random forcing term and a random diffusion coefficient which is assumed to depend affinely on a finite number of independent random variables. The a posteriori error estimate consists of four parts controlling the finite element error, the time discretization error, the stochastic collocation error and the rank truncation error. These estimators can be used to drive an adaptive choice of finite element mesh, collocation points, time steps and rank.

SPDE-Net: Neural Network based prediction of stabilization parameter for SUPG technique

Sangeeta Yadav¹ and Sashikumaar Ganesan²

¹ sangeetay@iisc.ac.in, ² sashi@iisc.ac.in

^{1,2}Department of Computational and Data Sciences, Indian Institute of Science, Bangalore, India

Numerical techniques for solving Singularly Perturbed Differential Equations (SPDE) suffer low accuracy and high numerical instability in presence of interior and boundary layers. Stabilization techniques are often employed to reduce the spurious oscillations in the numerical solution. Such techniques are highly dependent on user chosen stabilization parameter. Streamline Upwind Petrov Galerkin (SUPG) technique is one such residual based stabilization technique. Here we propose *SPDE-Net* (as shown in Fig. 1), a novel neural network based technique to predict the value of optimal stabilization parameter for SUPG technique. The prediction task is modeled as a regression problem and is solved using Artificial Neural Network(ANN). Three training strategies for the ANN have been proposed i.e supervised, L^2 error minimization (global) and L^2 error minimization (local). It has been observed that the proposed method yields accurate results, and even outperforms some of the existing state-of-the-art ANN-based partial differential equation (PDE) solvers such as Physics Informed Neural Network (PINN). The training is based on error between the Finite Element Method(FEM) solution and the analytical solution of SPDE. Global and local variants of stabilization parameter τ are demonstrated. Experiments on a benchmark case of 1-dimensional convection diffusion equation show a reasonable performance of L^2 error minimization (global) as compared to the conventional supervised training. This makes the proposed technique eligible for extension to higher dimensions and other cases where the analytical formula for stabilization parameter is unknown, therefore making supervised learning impossible.

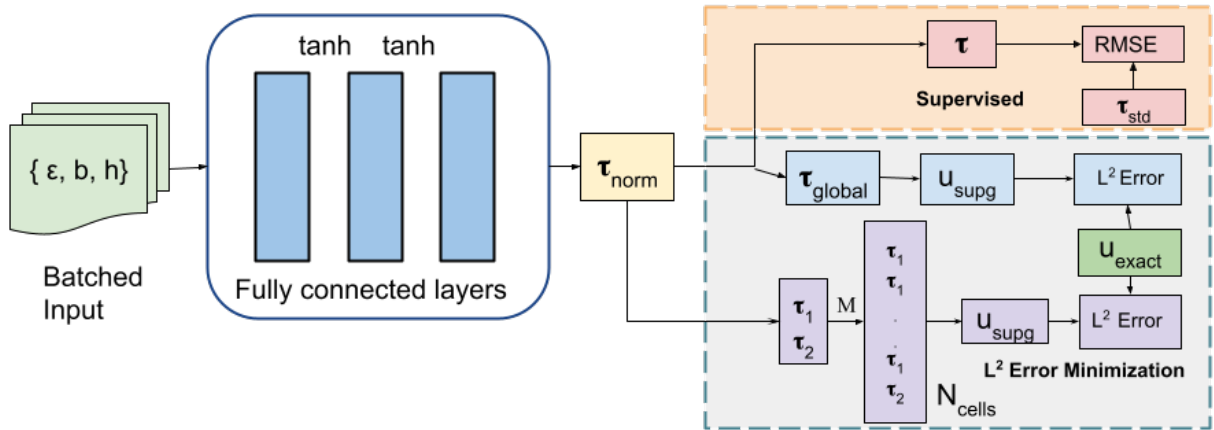


Figure 1: Schematic diagram of *SPDE-Net*: An end-to-end deep learning+FEM framework for solving SPDE

References

- [1] Sangeeta Yadav and Sashikumaar Ganesan, (2021). *SPDE-Net: Neural Network based prediction of stabilization parameter for SUPG technique*. Proceedings of The 13th Asian Conference on Machine Learning, Proceedings of Machine Learning Research 157:268-283 <https://proceedings.mlr.press/v157/yadav21a.html>.

The FVC scheme on non-uniform triangular meshes: Application to the multi-layers shallow water equation

M. Ziggaf^{1,2,3}, M. Boubekeur³, I. Kissami,² I. El Mahi^{1,2}, and F. Benkhaldoun³

¹ENSAO, LMCS, Complexe Universitaire, B.P. 669, 60000 Oujda, Morocco

²MSDA, Mohammed VI Polytechnic University Lot 660, 43150 Ben Guerir, Maroc

³Université Sorbonne Paris Nord, LAGA, CNRS, UMR 7539, F-93430, Villetaneuse, France

The multi-layer shallow water system with friction (1) are widely used to model tides, dam break, storms, tsunamis and in general, the various free surface geophysical flows in shallow water [1]. This system of PDEs was introduced in [2], it has been widely used in several works see e.g. [3, 4, 5] when supplemented with appropriate terms. The numerical solution of such models is a challenge due to their non-linear structure, additional source terms which are usually non-regular, the complicity of the exchange terms between layers without forgetting the complication of computational domain. In this study, we focus on the numerical solutions of the two-dimensional version of this system of equations with a topography source term using a new finite volume approach on unstructured meshes. We first present a simple and accurate homogeneous solver based on a finite volume predictor-corrector scheme with a characteristics method for the predictor. This scheme is called "Finite Volume Characteristics" (FVC) and was introduced in [6] to solve the one-dimensional version of this equation system. Then, we introduce a generalization of this scheme by preserving the properties of the homogeneous solver as a result, we end up with a well-balanced scheme satisfying the equilibrium of the lake at rest and taking in to into account the exchange terms between each layer of this system as well as the effect of the wind on the free surface and subsequently on all layers of the water mass. Finally, the proposed finite volume approach is verified on several benchmark tests and shows good agreement with solutions presented by other approaches as well as experimental observations.

$$\begin{cases} \partial_t h_\alpha + \nabla \cdot (h_\alpha \mathbf{u}) = 0 \\ \partial_t h_\alpha \mathbf{u}_\alpha + \nabla \cdot (h_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha) + g h_\alpha \nabla(h) = -g h_\alpha \nabla Z - \kappa_\alpha \delta_{1\alpha} \mathbf{u}_\alpha + F_\alpha, \end{cases} \quad (1)$$

such that α is the number of layer and the unknowns are the height of water in each layer $h_\alpha(t, x, y)$, such as $h = \sum_{\alpha=1}^N h_\alpha$ and the velocity vector $\mathbf{u}_\alpha(t, x, y) = (u_\alpha, v_\alpha)^T(t, x, y) \in \mathbb{R}^2$.

$$F_\alpha = \mathcal{F}_u + \mathcal{F}_b + \mathcal{F}_w + \mathcal{F}_\mu, \quad \alpha = 1, 2, \dots, N$$

where the first term \mathcal{F}_u is related to the momentum exchanges between the layers that are defined through the vertical discretization of the flow. The three last terms \mathcal{F}_b , \mathcal{F}_w and \mathcal{F}_μ are related to friction effects. Note that the bed friction forcing term \mathcal{F}_b is acting only on the lower layer, whereas the wind-driven forcing term \mathcal{F}_w is acting only on the upper layer. The internal friction term \mathcal{F}_μ models the friction between neighboring layers, see [2] for further details. Thus, \mathcal{F}_u represents the advection term. $\delta_{1\alpha}$ represents the Kronecker symbol.

References

- [1] Jean-Michel Hervouet. Hydrodynamique des écoulements à surface libre, modélisation numérique avec la méthode des éléments finis. Presses des Ponts et Chaussées 2003 (in French).
- [2] Emmanuel Audusse. A multilayer saint-venant model: derivation and numerical validation. *Discrete & Continuous Dynamical Systems-B*, 5(2):189, 2005.
- [3] Emmanuel Audusse, Marie-Odile Bristeau, Benoît Perthame, and Jacques Sainte-Marie. A multilayer saint-venant system with mass exchanges for shallow water flows. derivation and numerical validation. *ESAIM: Mathematical Modelling and Numerical Analysis*, 45(1):169–200, 2011.
- [4] Emmanuel Audusse, Fayssal Benkhaldoun, Jacques Sainte-Marie, and Mohammed Seaid. Multilayer saint-venant equations over movable beds. *Discrete & Continuous Dynamical Systems-B*, 15(4):917, 2011.
- [5] Saida Sari, Thomas Rowan, Mohammed Seaid, and Fayssal Benkhaldoun. Simulation of three-dimensional free-surface flows using two-dimensional multilayer shallow water equations. *Communications in Computational Physics*, 27(5):1413–1442, 2020.
- [6] Emmanuel Audusse, Fayssal Benkhaldoun, Saida Sari, Mohammed Seaid, and Pablo Tassi. A fast finite volume solver for multi-layered shallow water flows with mass exchange. *Journal of Computational Physics*, 272:23–45, 2014.