LONDON MATHEMATICAL SOCIETY
150 YEARS

UNIVERSITY OF BIRMINGHAM

Workshop

Adaptive algorithms for computational PDEs

School of Mathematics
University of Birmingham, UK
5 – 6 January, 2016

Organisers

Alex Bespalov, Daniel Loghin

Adaptive algorithms for computational PDEs

Adaptive algorithms and the associated software are ubiquitous in numerical solution of partial differential equations (PDEs). In many application areas, adaptive solution procedures offer the most efficient way to achieve the required accuracy in numerical simulations through effective use of available computational resources. The success of adaptive algorithms for computational PDEs relies on rigorous mathematical analysis of the underlying numerical methods.

The aim of this workshop is to discuss recent advances in mathematical foundations, design and implementation of adaptive algorithms for numerical solution of PDE problems.

Venue

The workshop will take place on the Edgbaston Campus at the University of Birmingham.

Key buildings (with their indices on the campus map, see next page):
Aston Webb Building (R5, R6), Bramall Music Building (R12), Staff House (R24).

Registration will take place in the Bramall Music Building from 8.45am until 9.20am on Tuesday, 5th January. The entrance to the building is from Chancellor's Court. Please go upstairs to the foyer on the first floor for registration and coffee.

Talks will take place in Lecture Room WG12 in the Aston Webb Building (west wing of the building – R5 on the map). The Bramall Music Building and the Aston Webb Building are connected by the gallery. The lecture room can also be accessed via the main entrance to the Aston Webb Building (building R6 on the map): enter the building from Chancellor's Court, walk past the reception area and then through double doors on the right, and continue walking through the corridor; the lecture room will be on the right-hand side.

Coffee breaks and lunches

Coffee/tea and refreshments will be provided at the times indicated in the programme in the foyer on the first floor of the Bramall Music Building.

We will go for lunch to the Staff House, the Noble Room (second floor). The details of the arrangements will be communicated during the meeting, and we will ask you to wear your badge when we go for lunch.

We suggest Cafe Aroma on the first floor of the Staff House for coffee/tea after lunch.

Dinner on Tuesday

We will go out for dinner on Tuesday evening. Further details will be communicated on the day.

Internet Access

Wireless access using EDUROAM is available in Aston Webb and Bramall Music Buildings, as well as in the Staff House.

Acknowledgement

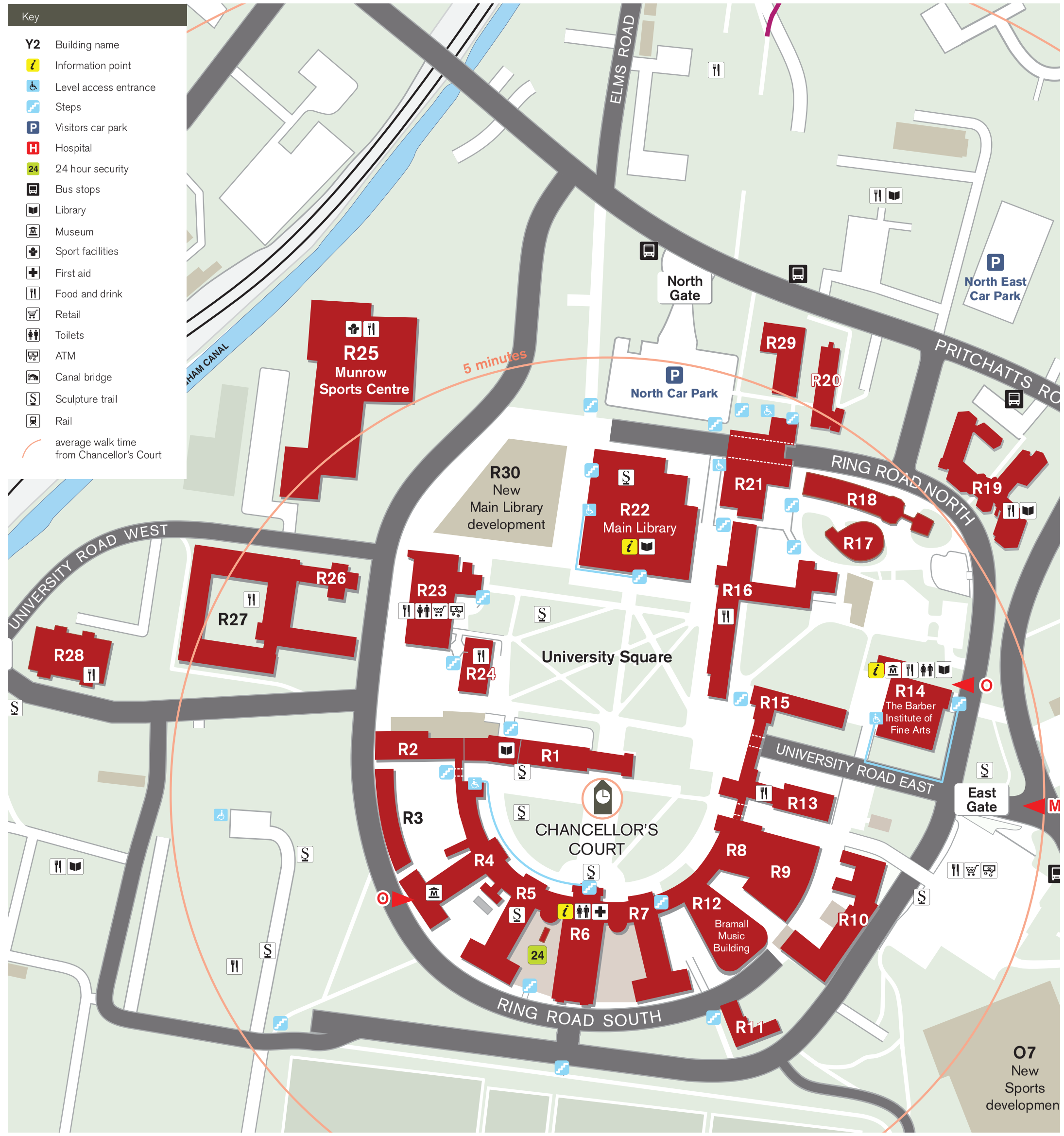
The organisers would like to thank the London Mathematical Society and the School of Mathematics at the University of Birmingham for financial support.

Edgbaston Campus Map

Index to buildings by zone

Red Zone

R1	Law Building
R2	Frankland Building
R3	Hills Building
R4	Aston Webb – Lapworth Museum (Reopening 2016)
R5	Aston Webb – B Block
R6	Aston Webb – Great Hall
R7	Aston Webb – Student Hub (Opening September 2015)
R8	Physics West
R9	Nuffield
R10	Physics East
R11	Medical Physics
R12	Bramall Music Building
R13	Poynting Building
R14	Barber Institute of Fine Arts
R15	Watson Building
R16	Arts Building
R17	Ashley Building
R18	Strathcona Building
R19	Education Building
R20	J G Smith Building
R21	Muirhead Tower
R22	Main Library
R23	University Centre
R24	Staff House
R25	Munrow Sports Centre
R26	Geography
R27	Biosciences Building
R28	Murray Learning Centre
R29	Postgraduate Centre (under construction)
R30	New Library (under construction)



Programme

Tuesday 5th January, 2016

8.45 – 9.20	Registration and coffee
9.25 – 9.30	Welcome and opening remarks
9.30 – 10.20	**Rob Stevenson** *Adaptive wavelet methods: quantitative improvements and extensions*
10.20 – 11.10	**Dirk Praetorius** *Axioms of adaptivity*
11.10 – 11.40	Coffee break
11.40 – 12.30	**Paul Houston** *Adaptive discontinuous Galerkin methods on polytopic meshes*
12.30 – 14.00	Lunch
14.00 – 14.50	**Natalia Kopteva** *Maximum-norm a posteriori estimates on anisotropic meshes*
14.50 – 15.40	**Gabriel Barrenechea** *Stabilised finite element methods in anisotropic quadrilateral meshes*
15.40 – 16.10	Coffee break
16.10 – 17.00	**Andreas Dedner** *A posteriori estimates for conservation laws*
17.00 – 17.25	**Uwe Köcher** *Software engineering aspects for a distributed-parallel and h-adaptive high-order space-time wave equation solver based on the deal.II library*
17.25 – 17.50	**Carlo Marcati** *h-p discontinuous Galerkin methods for electronic structure calculations*

Wednesday 6th January, 2016

9.00 – 9.50	**Martin Vohralík** *Localization of dual norms, local stopping criteria, and fully adaptive solvers*
9.50 – 10.40	**Mario Arioli** *The use of stopping criteria for iterative Krylov methods in designing adaptive methods for PDEs*
10.40 – 11.10	Coffee break
11.10 – 12.00	**David Silvester** *Adaptive algorithms driven by a posteriori estimates of error reduction for PDEs with random data*
12.00 – 12.25	**Philip Browne** *Adaptive mesh redistribution on the sphere for global atmospheric modelling*
12.25 – 14.00	Lunch
14.00 – 14.50	**Emmanuil Georgoulis** *Adaptivity and blow-up detection for nonlinear evolution PDEs*
14.50 – 15.40	**Omar Lakkis** *A posteriori error analysis of time-stepping schemes for the wave equation*
15.40 – 16.10	Coffee break and close

The use of stopping criteria for iterative Krylov methods in designing adaptive methods for PDEs

Mario Arioli

Wuppertal University, Germany

When using Krylov methods for solving linear systems that approximate PDEs the stopping criteria play a central role to identify at which iteration the approximate solution is satisfactory, i.e., the error between the exact solution of the PDE and the current approximation has the same order of the approximation error predicted by the finite-element method used.

We will give a few examples of how we can use the information computed by the stopping criteria in the design of adaptive methods. For the sake of simplicity, we will focus on elliptic problems approximated by both classical and mixed-hybrid finite-element methods.

Stabilised finite element methods in anisotropic quadrilateral meshes

Gabriel Barrenechea

University of Strathclyde, UK

In this talk I will review some recent results on the stabilisation of finite element methods in anisotropic quadrilateral meshes. Our first attempt is the family $Q_{k+1} \times P_{k-1}$. This pair is inf-sup stable, but their stability constant depends on the aspect ratio of the triangulation. Then, we identify the minimal amount of pressure modes which are responsible for this behaviour, and we propose a method that penalises them in such a way that the resulting scheme is stable independently of the aspect ratio. Next, we move to the, optimal and not inf-sup stable, $Q_1 \times P_0$ pair, and the Oseen equation.

This work has been done in collaboration with M. Ainsworth (Brown University) and A. Wachtel (University of Strathclyde).

Adaptive mesh redistribution on the sphere for global atmospheric modelling

Philip A. Browne

University of Reading, UK

Adaptive mesh redistribution, or *r*-adaptivity, has been demonstrated to be effective in cartesian coordinates for resolving fronts in PDEs such as Burger's equation and the Eady problem. The focus of a NERC project between Reading, Imperial and Bath is to develop adaptive mesh redistribution methods which can be applied to global atmospheric models.

To solve global atmospheric equations, the mesh adaptivity methods that have been developed on the interval $[0, 1]^n$ must be extended to a spherical shell. In this talk I will discuss the work we have done in order to prove the existance of optimally transported meshed on the sphere. I will discuss the numerical techniques we have developed in order to solve the associated equation of Monge-Ampère type on the sphere.

A posteriori estimates for conservation laws

Andreas Dedner

University of Warwick, UK

In this talk I will be discussing approaches for obtaining a-posteriori error estimates in the context of scalar and systems of non linear conservation laws. These estimates can be used like other similar estimates to drive grid adaptation but due to the typical structure of the solutions to these PDEs, the practical use of complex estimators in this context is debatable - heuristic indicators often do a good job without much computational overhead. Still one can learn a lot by studying the indicators and there are situations where heuristic indicators do not work so well. Another aspect is the use of these estimates as smoothness indicators for stabilizing higher order methods for the problems and I will discuss this aspect as well. I will discuss two different approaches for deriving such indicators derived for the time continuous version of the DG method. I will then briefly discuss how a fully discrete scheme could be analysed.

Adaptivity and blow-up detection for nonlinear evolution PDEs

Emmanuil Georgoulis

University of Leicester, UK

I will review some recent work on the problem of reliable automatic detection of blow-up behaviour for nonlinear parabolic PDEs. The adaptive algorithms developed are based on rigorous conditional a posteriori error bounds. The use of space-time adaptivity is crucial in making the problem computationally tractable. The results presented are applicable to quite general spatial operators, rendering the approach potentially useful in informing respective PDE theory.

The new adaptive algorithm is shown to accurately estimate the blow-up time of a number of problems, including ones exhibiting regional blow-up. Some brief comments on possible generalisation to interface problems will be also given.

Adaptive discontinuous Galerkin methods on polytopic meshes

Paul Houston

University of Nottingham, UK

In this talk we consider high-order/hp-version interior penalty discontinuous Galerkin methods for the discretization of second-order elliptic partial differential equations on general computational meshes consisting of polygonal/polyhedral elements. By admitting such general meshes, this class of methods allows for the approximation of problems posed on computational domains which may contain a huge number of local geometrical features, or micro-structures. While standard numerical methods can be devised for such problems, the computational effort may be extremely high, as the minimal number of elements needed to represent the underlying domain can be very large. In contrast, the minimal dimension of the underlying (composite) finite element space based on general polytopic meshes is independent of the number of geometric features. Here we consider both the a priori and a posteriori error analysis of this class of methods, as well as their application within Schwarz-type domain decomposition preconditioners.

Software engineering aspects for a distributed-parallel and *h*-adaptive high-order space-time wave equation solver based on the deal.II library

Uwe Köcher,[†] Markus Bause

[†]Helmut Schmidt University, University of the Federal Armed Forces, Germany

This contributed talk emphasises software engineering aspects for space-time finite element solutions of the time domain acoustic wave equation. The dimensionless first-order in time velocity-displacement form reads as

$$\begin{aligned} \partial_t v(\boldsymbol{x},t) - \nabla \cdot a(\boldsymbol{x}) \nabla u(\boldsymbol{x},t) &= f(\boldsymbol{x},t) \quad \text{in} \quad \Omega \times I\,, \\ \partial_t u(\boldsymbol{x},t) - v(\boldsymbol{x},t) &= 0 \quad \text{in} \quad \Omega \times I\,, \end{aligned}$$

equipped with appropriate initial and boundary values. We denote by v the velocity, by u the displacement and by $a \in L^\infty(\Omega)$ some positive bounded medium dependent coefficient function. The discretisation of the time-domain acoustic wave equation is done in a (high-order) space-time Galerkin framework to allow generally the application of space-time, and even duality-based, $hp\tau$-adaptive techniques; cf. for discretisation details [2, 1].

The implementation of such schemes must be done carefully for getting high-performance distributed-parallel, adaptive-ready and maintainable finite element codes. An overview of common and specific library toolchains will be outlined briefly. The implementations for space-time {cG(p), SIPG(p)}–{cG(1), dG(1), cG(2), cG-C1(3)} acoustic wave solvers are presented in a programming language independent way.

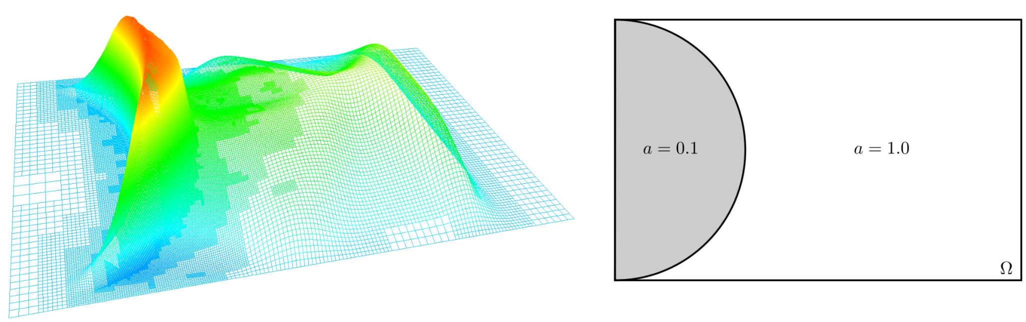


Figure 1: h-adaptive cG(3)–cG(1) acoustic wave simulation in a heterogeneous medium.

The Kelly error estimator is used for h-adaptivity, which computes space-cell local estimates

$$\eta_K^2 = \sum_{F \in \partial K} c_F \int_F \left[\!\!\left[a \frac{\partial u_h}{\partial \boldsymbol{n}} \right]\!\!\right]^2 \mathrm{d}o\,, \quad \text{using trace operator } [\![\cdot]\!] \text{ for the jump in the face } F\,.$$

This error estimator is implemented in deal.II; cf. [3].

Future prospects regarding recent developments of the research group on multi-physics solvers and duality based adaptivity for stabilised convection-dominated problems will be outlined.

References

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Maximum-norm a posteriori estimates on anisotropic meshes

Natalia Kopteva

University of Limerik, Ireland

Residual-type a posteriori error estimates in the maximum norm will be given for singularly perturbed semilinear reaction-diffusion equations posed in polygonal domains [1]. Linear finite elements are considered on anisotropic triangulations. The error constants are independent of the diameters and the aspect ratios of mesh elements as well as of the small perturbation parameter.

An inspection of standard proofs for shape-regular meshes reveals that one obstacle in extending them to anisotropic meshes lies in the application of a scaled traced theorem when estimating the jump residual terms (this causes the mesh aspect ratios to appear in the estimator). This, among a few other technical difficulties, will be addressed in the talk.

We shall also touch on that certain perceptions need to be adjusted for the case of anisotropic meshes. In particular, it is not always the case that the computed-solution error in the maximum norm is closely related to the corresponding interpolation error [2].

The talk will be concluded by a discussion of current and future work, including certain improvements of the results of [1] for the non-singularly perturbed case.

References

[1] KOPTEVA, N., *Maximum-norm a posteriori error estimates for singularly perturbed reaction-diffusion problems on anisotropic meshes*, SIAM J. Numer. Anal., 53 (2015), 2519-2544.

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A posteriori error analysis of time-stepping schemes for the wave equation

Omar Lakkis

University of Sussex, UK

A posteriori error estimates provide a rigorous foundation for the derivation of efficient adaptive algorithms for the approximation of solutions of partial differential equations. While the literature is rich as far as elliptic and parabolic equations are concerned, it is much less developed for the hyperbolic equations such as the wave equation. In this talk, I will review some of the "standard" a posteriori wave equation results, including those of [1] and [2], and present recent improvements and further developments to lower order Sobolev norms based on Baker's Trick [3] for backward Euler schemes. Subsequent focus will be given to practically relevant methods such as Verlet, or Cosine, methods, a popular example of which is the Leap-frog method [4].

This is based on joint work with E. H. Georgoulis, C. Makridakis and J. M. Virtanen.

References

[1] BANGERTH, W. AND RANNACHER, R., J. Comput. Acoust. 9(2):575–591, 2001.

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h-p discontinous Galerkin methods for electronic structure calculation

Carlo Marcati

UPMC, University of Paris VI, France

We analyze some models used in quantum chemistry for electronic structure computations and we provide some convergence results for the $h-P$ discontinuous Galerkin method on a model problem (Gross-Pitaevskii). We prove the exponential convergence of the approximation to the exact solution and analyze the asymptotics of the solution near its singularities to provide an *a priori* optimized approximation space.

In many real world problems in quantum chemistry, we are mainly concerned with the computation of the *ground state energy* of a system. We consider non linear eigenvalue problems of the form

$$\mathcal{F}u = \lambda u \tag{1}$$

where $\mathcal{F}$ is a self adjoint elliptic operator (depending on u) containing a potential V with singularities in a set of isolated points $\mathcal{C}$.

The solutions to (1) belong to the *countably normed Sobolev space*

$$\mathcal{K}^{\infty,\gamma} = \left\{u \in \mathcal{D}' : \ d(x,\mathcal{C})^{|\alpha|-\gamma}\partial^{\alpha}u \in L^2, \ |\alpha| = s, \ \forall s \in \mathbb{N}\right\}. \tag{2}$$

Since the solution is not regular in the “classical” (Sobolev) sense, the speed of convergence of widely used real space methods (such as the finite element (FE) or the spectral element (SE) methods) is bounded by the regularity of the solution. $h-P$ finite elements methods exploit the structure of the space (2) and provide approximations that are *exponentially convergent* to the solution. Moreover, by employing a Mellin transform of the problem considered, we obtain an asymptotic development of the solution near $\mathcal{C}$. We can therefore optimize the mesh grading parameters and the polynomial order slope using information that we derive on the eigenfunction.

Axioms of adaptivity

Dirk Praetorius

Vienna University of Technology, Austria

We present an axiomatic proof of optimal convergence rates for adaptive FEM [1, 2, 3, 7] as well as BEM [4, 5] in the spirit of [1]. For this purpose, an overall set of four axioms on the error estimator is sufficient and (partially even) necessary.

The four axioms are stability on non-refined element domains (A1), reduction on refined element domains (A2), general quasi-orthogonality (A3), and discrete reliability (A4). The presentation shall discuss those properties in very simple examples and motivate the different arguments which guarantee convergence with optimal rate in terms of certain nonlinear approximation classes which coincide from the literature, e.g., [2], if the error estimator is efficient.

Compared to the state of the art in the temporary literature [1, 2, 3, 4, 5, 7], the improvements of [6] can be summarized as follows: first, a general framework is presented which covers the existing literature on rate optimality of adaptive schemes for both, linear as well as nonlinear problems. This framework is fairly independent of the underlying (conforming, nonconforming, or mixed) FEM or BEM. Second, efficiency of the error estimator is not needed. Instead, efficiency exclusively characterizes the approximation classes involved in terms of the bestapproximation error plus data resolution. Third, some general quasi-Galerkin orthogonality is not only sufficient, but also necessary for the R-linear convergence of the error estimator, which is a fundamental ingredient in the current quasi-optimality analysis [1, 2, 3, 4, 5, 7]. Finally, the general analysis allows for various generalizations like equivalent error estimators and inexact solvers as well as different non-homogeneous and mixed boundary conditions.

The talk is based on joint work [6] with Carsten Carstensen (HU Berlin) and Michael Feischl (UNSW Sydney).

References

[1] STEVENSON, R., *Optimality of a standard adaptive finite element method*, Found. Comput. Math. 7 (2007), 245–269.

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Adaptive wavelet methods: quantitative improvements and extensions

Rob Stevenson

KdVI, University of Amsterdam, The Netherlands

Adaptive wavelet methods for solving operator equations were introduced by Cohen, Dahmen and DeVore in [1, 2] and further developed in e.g. [6, 3, 4, 5]. These methods were shown to converge to the solution with the best possible rate in linear computational complexity.

Compared to adaptive finite element methods, for which, for elliptic problems, similar theoretical results were proven, in a quantitative sense the results obtained with wavelet schemes are sometimes somewhat disappointing. The approximate matrix-vector multiplication routine, known as the **apply**-routine, is easily identified as the computational bottleneck. In this talk, it will be shown how the application of this routine can be avoided by writing the PDE as a first order system least squares problem.

The scope of adaptive wavelet methods is much larger than only elliptic problems. Promising applications include those to simultaneous space-time variational formulations of evolutionary PDEs as parabolic PDEs, or the instationary (Navier-) Stokes equations. Equipping the relevant function spaces with bases that consist of tensor products of temporal and spatial wavelets, the whole time evolution problem can be solved at a complexity of solving one instance of the corresponding stationary problem.

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Adaptive algorithms driven by a posteriori estimates of error reduction for PDEs with random data

David Silvester

University of Manchester, UK

An efficient adaptive algorithm for computing stochastic Galerkin finite element approximations of elliptic PDE problems with random data will be outlined in this talk. The underlying differential operator will be assumed to have affine dependence on a large, possibly infinite, number of random parameters. Stochastic Galerkin approximations are sought in a tensor-product space comprising a standard $h-$finite element space associated with the physical domain, together with a set of multivariate polynomials characterising a $p-$finite-dimensional manifold of the (stochastic) parameter space.

Our adaptive strategy is based on computing distinct error estimators associated with the two sources of discretisation error. These estimators, at the same time, will be shown to provide effective estimates of the error reduction for enhanced approximations. Our algorithm adaptively 'builds' a polynomial space over a low-dimensional manifold of the infinitely-dimensional parameter space by reducing the energy of the combined discretisation error in an optimal manner. Convergence of the adaptive algorithm will be demonstrated numerically.

This is joint work with Alex Bespalov (University of Birmingham) and Catherine Powell (University of Manchester).

Localization of dual norms, local stopping criteria, and fully adaptive solvers

Martin Vohralík

INRIA Paris-Rocquencourt, France

We show that dual norms of bounded linear functionals on the Sobolev space $W_0^{1,p}(\Omega)$ are localizable provided that the functional in question vanishes over locally supported test functions which form a partition of unity. This allows, a fortiori, to establish local efficiency and robustness for a posteriori analysis of nonlinear partial differential equations in divergence form. This result holds true even in presence of linearization and algebraic errors from fully adaptive inexact solvers, provided that local stopping criteria are used.