National University of Ireland, Galway

Numerical Methods for Problems with Layer Phenomena

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This workshop is dedicated to our friend and colleague Eugene O'Riordan on the occasion of his 60th birthday

Speakers

Uniform error estimates for general linear turning point problems on layer-adapted meshes

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We consider singularly perturbed linear boundary value problems of the type

$$\begin{aligned} -\varepsilon u''(x) + b(x)u'(x) + c(x)u(x) &= f(x), \qquad \text{for } x \in (\underline{a}, \overline{a}), \\ u(\underline{a}) = \nu_-, \quad u(\overline{a}) &= \nu_+, \end{aligned} \tag{1a}$$

where $0 < \varepsilon \ll 1$ and b, c, f are supposed to be sufficiently smooth. Furthermore, we assume

$$c(x) \geq \gamma > 0, \qquad \big(c - \tfrac{1}{2}b'\big)(x) \geq \tilde{\gamma} > 0, \quad \text{for all } x \in \overline{I} := [\underline{a}, \overline{a}]. \tag{1b}$$

A point $\bar{x} \in \overline{I}$ is called turning point of the problem if $b(\bar{x}) = 0$ and for every neighborhood U of $\bar{x}$ there is a point $x \in U \cap \overline{I}$ such that $b(x) \neq 0$. Note that the assumptions in (1b) on b and c allow an arbitrary number, location, and multiplicity of turning points.

As result of the general setting of problem (1), we have to be aware of many (possibly different) layers. It shows that exponential boundary layers, interior cusp-type layers, and certain power-type boundary layers could occur, see [1]. In order to treat these layers and to enable uniform estimates a convenient mesh construction strategy can be given. This one combines the well known Shishkin-type meshes with piecewise equidistant meshes proposed by Sun and Stynes in [2].

The mesh construction as well as some of the arising difficulties in proving uniform error estimates in the energy norm for higher order finite elements are discussed on the basis of several examples of problems with different layers. Note that the presented results and techniques can also be extended to a certain type of semilinear problems, see [3].

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Exponentially graded meshes and singularly perturbed problems

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By using a-priori defined layer-adapted meshes for singularly perturbed problems we are able to prove uniform convergence results for many variants of finite element methods. Some meshes allow for optimal convergence orders in the sense that the final estimate is $\mathcal{O}(N^{-p})$ for some number $p > 0$ where N is a mesh parameter. One such mesh is the exponentially graded mesh (eXp-mesh).

In this talk we look into some applications of this mesh to singularly perturbed problems and compare it to well known S-type meshes. Upon doing so, we generalise the class of S-type meshes and provide a new approach to analyse the eXp-mesh.

KEY WORDS: eXp-mesh, S-type meshes

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Numerical solution of convection-diffusion problems on annular and related domains

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We examine numerical methods for convection diffusion problems on annular domains, which combine polar coordinates, upwinding and a piecewise-uniform Shishkin mesh in the radial direction, and possibly some refinement in the axial direction. We examine computationally the effect of relaxing constraints on the data which are required to obtain parameter-uniform error bounds and also consider the application of the method to similar domains with non-circular boundaries. The numerical method is a variation of that considered in [1, 2], where the domain is circular and [3] in which numerical solutions are also obtained on annular domains.

KEY WORDS: annular domain, convection-diffusion, polar coordinates, mesh refinement

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Fully computable a posteriori error estimator using anisotropic flux equilibration on anisotropic meshes

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Fully computable a posteriori error estimates in the energy norm are given for singularly perturbed semilinear reaction-diffusion equations posed in polygonal domains. Linear finite elements are considered on anisotropic triangulations. To deal with the latter, we employ anisotropic quadrature and explicit anisotropic flux reconstruction. Prior to the flux equilibration, divergence-free corrections are introduced for pairs of anisotropic triangles sharing a short edge. We also give an upper bound for the resulting estimator, in which the error constants are independent of the diameters and the aspect ratios of mesh elements, and of the small perturbation parameter.

KEY WORDS: a posteriori error estimate, anisotropic triangulation, anisotropic flux equilibration, flux reconstruction, anisotropic quadrature, energy norm, singular perturbation, reaction-diffusion.

We consider linear finite element approximations to singularly perturbed semilinear reaction-diffusion equations of the form $-\varepsilon^2\triangle u + f(x, y; u) = 0$ posed in a, possibly non-Lipschitz, polygonal domain $\Omega \subset \mathbb{R}^2$. Here $0 < \varepsilon \leq 1$. We also assume that f is continuous on $\Omega \times \mathbb{R}$ and satisfies $f(\cdot; s) \in L_\infty(\Omega)$ for all $s \in \mathbb{R}$, and the one-sided Lipschitz condition $f(x, y; u) - f(x, y; v) \geq C_f[u - v]$ whenever $u \geq v$, with some constant $C_f \geq 0$.

Our goal is to give explicitly and fully computable a posteriori error estimates on reasonably general anisotropic meshes in the energy norm. This goal is achieved by a certain combination of explicit flux reconstruction and flux equilibration.

Flux equilibration for reaction-diffusion equations was considered in [1, 3, 4] on shape-regular meshes (see also [2, Chap. 6] for the case $\varepsilon = 1$), and in [5] on anisotropic meshes. The estimators in [3, 4] are based on flux reconstructions, while [1, 5] employ solutions of certain local problems.

Our approach in this paper differs from the previous work in a few ways.

- The fluxes are equilibrated within a local patch using anisotropic weights depending on the local, possibly anisotropic, mesh geometry.
- Prior to the flux equilibration, divergence-free corrections are introduced for pairs of anisotropic triangles sharing a short edge.
- A certain anisotropic quadrature is used on anisotropic elements. This is motivated by some observations made in [6], and also enables us to drop some mesh assumptions made in recent papers [7, 8].

- Our estimator is explicitly and fully computable in the sense that it involves no unknown error constants (unlike other estimators on anisotropic meshes, such as in [5, 7, 8]).
- In contrast to [5], an upper bound for our estimator involves no matching functions (which depend on the unknown error). In fact, the error constant C in our upper bound is independent not only of the diameters and the aspect ratios of mesh elements, but also of the small perturbation parameter ε.

For further details, we refer the audience to a recent paper [9].

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Collocation for singularly perturbed boundary-value problems

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A short summary of recent research into collocation methods for singularly perturbed boundary-value problems of reaction-diffusion type will be given. Both a priori and a posteriori error bounds will be presented.

KEY WORDS: collocation, a priori error analysis, a posteriori error bounds.

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Solving ill-posed problems for nonlinear singularly perturbed equations with internal and boundary layers

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We consider two approaches based on the asymptotic analysis [1] which are able to solve ill-posed problems for nonlinear singularly perturbed equations with internal and boundary layers.

The first approach is based on the idea that the asymptotic analysis allows to extract *a priory* information about interior layer (moving front), which appears in the direct problem, and boundary layers, which appear in the conjugate problem (in the case of using some gradient method for numerical solving of the considered problem). In this case we are able to construct so called *dynamically adapted mesh* based on this *a priory* information. The dynamically adapted mesh significantly reduces the complexity of the numerical calculations and improve the numerical stability in comparison with the usual approaches. The effectiveness of this approach are shown on the example of coefficient inverse problem for a nonlinear singularly perturbed reaction-diffusion-advection equation [2] with the final time observation data.

The second approach is based on the idea that in particular cases the asymptotic analysis allows to reformulate the initial ill-posed problem to the problem that is well-posed. The effectiveness of this approach are shown on the example of boundary inverse problem for a nonlinear singularly perturbed reaction-diffusion-advection equation [3] with the observation data based on the position of interior layer.

KEY WORDS: singularly perturbed problem, inverse problem, interior and boundary layers, dynamically adapted mesh, reaction-diffusion-advection equation.

AMS SUBJECT CLASSIFICATIONS: 65M32, 65L04, 65L12, 65L20, 65M20, 35G31.

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Tutorial on using Matlab to solve singularly perturbed systems of initial value problems

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In mathematical biology many systems of nonlinear differential equations arise, which are singularly perturbed. These may be found, for example, in the mathematical modelling of enzyme-substrate dynamics. It is necessary to solve these systems numerically. This is difficult because of the singular perturbations, but it is even more difficult when the system is large. In this tutorial, the use of standard packages in Matlab to solve such problems is demonstrated. This approach is then compared with the use of numerical methods based on specially constructed piecewise uniform meshes and appropriate standard finite difference operators.

KEY WORDS: initial value problems, large systems, singularly perturbed, Matlab packages, Shishkin meshes.

Initial boundary value problems for Burgers equation with nonlinear forcing: front motion and blow-up

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For the initial boundary value problems for reaction-diffusion-advection equations we prove the existence of fronts and give their asymptotic approximation including the new case of the blowing-up fronts. The last case we illustrate by the generalised Burgers equation.

KEY WORDS: boundary and interior layers, singular perturbations, comparison principle. moving fronts, blow-up.

We present recent results for some classes of IBVP (initial boundary value problem) where we investigate moving fronts by using the developed comparison technique. For these initial boundary value problems we proved the existence of fronts and give its asymptotic approximation. We proved that the principal term, describing the location of the moving front, is determined by the initial value problem

$$\frac{dx_0}{dt} = V(x_0), \quad x_0(0) = x_{00}, \tag{2}$$

where x_{00} is the initial location of the front, $V(x_0)$ is a known function, defined by the input data. We proved that the Lyapunov stability of steady points of equation (2) determine the Lyapunov stability of stationary solutions with interior layer of the IBVP. In the present paper we also have proved that under some conditions the blow-up of the solution problem (2) determine the blow-up of the interior layer solution of the IBVP.

We illusrate our results by the problem

$$\begin{gathered}\varepsilon\frac{\partial^2 u}{\partial x^2} - A(u,x)\frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} = f(u,x,\varepsilon), \quad x \in (0,1), t > 0, \\ u(0,t,\varepsilon) = u^0, \quad u(1,t,\varepsilon) = u^1, \quad t \in [0,T], \\ u(x,0,\varepsilon) = u_{init}(x,\varepsilon), \quad x \in [0,1].\end{gathered}$$

These results can be considered as an extension of the results of [1] - [5].

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Singularly perturbed convection-diffusion problems posed on an annulus

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A finite difference method is constructed for a singularly perturbed convection diffusion problem posed on an annulus. The method involves combining polar coordinates, upwinding and a piecewise-uniform Shishkin mesh in the radial direction. Constraints are imposed on the data in the vicinity of certain characteristic points to ensure that interior layers do not form within the annulus. Under these constraints, a theoretical parameter-uniform error bound is established. This approach is an extension of the method examined in [1, 2], where the problem was posed within a circle, as opposed to the problem examined here, where the problem domain is exterior to a circle.

KEY WORDS: annulus, convection-diffusion, characteristic points

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A two-scale sparse grid method for a singularly perturbed reaction-diffusion problem in three dimensions

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Standard finite element methods (FEMs), such as the Galerkin method, become impractical for large problems and in high dimensions. It is known that sparse grid methods have the ability to attain the accuracy of classical FEMs while requiring fewer degrees of freedom to do so. This is well-documented for both two-scale and multiscale sparse grid methods applied to singularly perturbed reaction-diffusion problems in two dimensions, (see, e.g., [1, 2]).

Sparse grid methods are important tools in the numerical solution of high-dimensional non-singularly perturbed problems because the computational cost associated with them is essentially independent of the dimension in which the problem is posed. However, little is known about the theoretical properties of sparse grid methods applied to singularly perturbed problems in more than two dimensions.

We investigate a two-scale sparse grid method applied to a three-dimensional singularly perturbed reaction-diffusion problem posed on the unit cube. To resolve the associated boundary layers a Shishkin solution decomposition and mesh are used to achieve a parameter-robust solution. By extending the ideas of [1] to the three-dimensional setting, we show that the two-scale sparse grid FEM we describe achieves essentially the same level of accuracy as the standard Galerkin FEM, while reducing the number of degrees of freedom required from $\mathcal{O}(N^3)$ to $\mathcal{O}(N^2)$. We conclude with the results of numerical experiments that support our theoretical findings.

KEY WORDS: sparse grids, finite elements, reaction-diffusion.

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Supercloseness of continuous interior penalty method for convection-diffusion problems with characteristic layers

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A singularly perturbed convection-diffusion problem posed on the unit square is solved using a continuous interior penalty (CIP) method with piecewise bilinears on a rectangular Shishkin mesh. A detailed analysis [1] proves a new stability bound for the CIP method, in a norm that is stronger than the usual CIP norm. This bound enables a new supercloseness result for the CIP method: the computed solution is shown to be second order (up to a logarithmic factor) convergent in the new strong norm to the piecewise bilinear interpolant of the true solution. As a corollary one obtains almost optimal order convergence in the L^2 norm of the CIP solution to the true solution. Numerical experiments illustrate these theoretical results.

KEY WORDS: Convection-diffusion, boundary layer, interior penalty finite element method, Shishkin mesh

AMS SUBJECT CLASSIFICATIONS: 65N30, 65N50.

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Singularly perturbed nonlinear time-dependent parabolic problem with singularly perturbed Neumann boundary conditions

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A singularly perturbed nonlinear reaction-diffusion equation with singularly perturbed Neumann boundary conditions is examined,

$$\varepsilon^2\left(\frac{\partial u}{\partial t}-\frac{\partial^2 u}{\partial x^2}\right)+f(x,t,u)=0,\quad (x,t)\in[0,1]\times[0,T],\, T\in\mathbb{R}^+,$$

$$\varepsilon\,\frac{\partial u}{\partial x}\bigg|_{x=0}=g_0(t),\quad \varepsilon\,\frac{\partial u}{\partial x}\bigg|_{x=1}=g_1(t)\quad \text{for } t\in[0,T],$$

and

$$u(x,0)=\varphi(x)\quad \text{for } x\in[0,1],$$

where $g_0(t)$, $g_1(t)$, $f(x,t,u)$ and $\varphi(x)$ are sufficiently smooth and $0<\varepsilon\ll 1$. Solutions to this equation involving boundary and initial layers will be discussed. This system is considered with a nonlinear function $f(x,t,u)$ and so the reduced problem, $f(x,t,u)=0$, has multiple solutions. The condition $f_u(x,t,u)>0$ is not assumed and instead weaker local assumptions are made. We consider [1] for assumptions that are necessary for existence of a boundary layer solution. In [1] an asymptotic expansion is constructed and existence of an exact solution is proven for a similar time dependent problem with periodic solutions. We enforce compatibility conditions at $x=0$, $t=0$ so that a sufficiently smooth solution can be obtained and by adding suitable conditions the existence of corner layer functions are removed. Discrete upper and lower solutions are constructed to prove existence and give accuracy of computed solutions.

Examples can be found which illustrate the difficulty of finding accurate solutions to this equation and give incorrect computed solutions. This problem is addressed by the introduction of artificial stabilisation previously considered by [2] for a time dependent problem with Dirichlet boundary conditions.

KEY WORDS: time dependent, boundary layers, singularly perturbed Neumann boundary conditions.

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Asymptotic-numerical method for the description of moving fronts in nonlinear two-dimensional reaction-diffusion models

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This work develops an analytic-numerical approach for the description of moving fronts in nonlinear singularly perturbed parabolic equations. We consider a singularly perturbed reaction-diffusion problem featuring the solutions with moving internal layers (moving fronts). It is important that the layer location and its speed are not known *a priori* and could be determined from the asymptotic procedure by smooth joining of asymptotic expansions. In quite general cases this procedure can be done explicitly and also explicit asymptotic formulas for the layers location or the front speed can be written. But for some classes of reaction-diffusion problems it can not be done explicitly and the asymptotic algorithm needs to be supplemented by the appropriate numerical calculations. The main purpose of this work is, on the one hand, to show the ideas of the asymptotic algorithm for the solutions with internal layers or moving fronts; on the other hand, to outline some problems which need to use numerical calculations on some steps of the asymptotic procedure.

Some combined asymptotic-numerical algorithm for the determination of moving fronts location in two-dimensional reaction-diffusion models is proposed. Asymptotic technique allows to reduce this two-dimensional nonlinear reaction-diffusion equation to a series of one-dimensional problems. This decomposition significantly decreases the complexity of numerical calculations for practical applications and allows the effective use of parallel computing. Some numerical experiments are presented to illustrate the proposed method.

We demonstrate our approach on the following problem:

$$\begin{aligned} &\varepsilon^2 \Delta u - \varepsilon \frac{\partial u}{\partial t} = f(u, x, y, \varepsilon), \\ &y \in (0, a), \qquad x \in (-\infty, +\infty), \qquad t > 0 \end{aligned} \tag{3}$$

with some boundary and initial conditions and the L–periodicity condition in the variable x.

In (3) the function $f(u, x, y, \varepsilon)$ is assumed to be sufficiently smooth and L–periodic in the variable x; $0 < \varepsilon \ll 1$ is small parameter, which is usually a consequence of the parameters

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of the physical problem. The appearance of small parameter before the spatial derivatives is determined by the characteristics of the physical system, while small parameter before the time derivative determines only the time scale, convenient for further consideration.

The problem of type (3) featuring the solution of moving front type which have been investigated, for example, in [1], [2] (see also the references therein). In these works some asymptotic procedure was developed and proof of the existence of such type solution was done. Also the equations for effective description of the front dynamics was obtained.

Asymptotic solution of the problem (3) could be constructed as a combination of the solutions of boundary value problems in two domains located at the opposite sides of some curve $\hat{C}(t)$. Front location (the curve $\hat{C}(t)$) and its speed are not known a priori and must be determined from the asymptotic procedure by the smooth joining of these two solutions ($C^{(1)}$–matching condition). As a result, the main problem for the front dynamics description can be written as

$$\begin{aligned} &\frac{\partial^2 \tilde{u}}{\partial \xi^2} + v_0 \frac{\partial \tilde{u}}{\partial \xi} = f(\tilde{u}, x, y, 0), \qquad && (x, y) \in \hat{C}(t) \\ &\tilde{u}(0) = \varphi^{(0)}(x, y), && \tilde{u}(\pm\infty) = \varphi^{(\pm)}(x, y), \end{aligned} \tag{4}$$

where the parameter v_0 provides a smooth joining of the solutions of (4) for $\xi > 0$ and $\xi < 0$ and determines the main term of the normal speed of the front's point with coordinates $(x; y)$. Note, that the problem (4) is a series of one-dimensional equations which depends on $(x; y)$ as a parameters considered on some curve (surface).

Explicit formulas for speed or location of the moving front can be written only for certain types of nonlinearities $f(u, y, x, \varepsilon)$. But in general case it can not be done explicitly. This work extends [2] and supplements the asymptotic procedure, based on the formulas from [2], by some numerical algorithm for the description of the moving front location and its dynamics in two-dimensional case.

It is important, that for two(or higher)–dimensional case the asymptotic procedure [1], [2] requires, that $C^{(1)}$–matching needs to be done only for the normal derivatives at each point $(x; y)$ on the curve $\hat{C}(t)$. So, the asymptotic approach allows to reduce numerical determination of the front location or speed to a series of one-dimensional problems. This fact enables to optimize computer calculations and effectively use parallel computing technologies.

KEY WORDS: singularly perturbed problem, interior and boundary layers, dynamically adapted mesh, reaction-diffusion-advection equation, coefficient inverse problem, final time observed data.

AMS SUBJECT CLASSIFICATIONS: 35G31, 65L04, 65L12, 65L20, 65M20.

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Adaptively Weighted Finite Element Methods for PDE with Boundary Layers

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The overall effectiveness of numerical methods may be limited by solutions that lack smoothness on a relatively small subset of the domain. This includes elliptic or parabolic systems with boundary or interior layers as a result of convection dominated diffusion, or problems with singularities induced by boundary conditions or nonsmooth coefficients. In particular, finite element methods may exhibit slow convergence, or in some cases, may fail to converge. There are a wide range of approaches to address these issues, from the use of exotic finite element spaces, to enhancing the finite element spaces with additional local basis functions, to mesh construction/refinement strategies, to a variety of strategies that weaken the variational problem. The approach we present here has similarities to each of these methodologies, where the underlying discrete variational problem is adaptively re-weighted by a sequence of approximate solutions. By changing the underlying metric of the numerical method, the choice of mesh and finite element space can better represent the solution. For problems with boundary layers, for example, an optimal metric has lower weight where sharp gradients develop. This effectively weakens the variational problem locally, reducing under/overshoot behavior in typical Galerkin formulations or excessive smoothing in typical least-squares formulations. For such problems where it is not known a priori where layers will form, an adaptive approach is necessary. In many cases the adaptively weighted approach can achieve optimal convergence rates (in both weighted and non-weighted norms) when the equivalent non-weighted solutions have significant defects. We present an overview of the approach and algorithmic framework as well as numerical examples that focus on problems with boundary layers.

KEY WORDS: adaptive, finite element, least-squares, boundary layers.

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On the finite element approximation of fourth order singularly perturbed eigenvalue problems

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We consider fourth order singularly perturbed eigenvalue problems in one-dimension and the approximation of their solution by the h version of the Finite Element Method (FEM). In particular, we use piecewise Hermite polynomials of degree $p \geq 3$ defined on an *exponentially graded* mesh. We show that the method converges uniformly, with respect to the singular perturbation parameter, at the optimal rate when the error in the eigenvalues is measured (in absolute value) and when the error in the eigenvectors is measured in the energy norm. We also illustrate our theoretical findings through numerical computations.

KEY WORDS: fourth order singulary perturbed eigenvalue problem, boundary layers, finite element method, exponentially graded mesh, uniform convergence.

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