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Special meshes and domain decomposition methods for evolutionary convection–diffusion–reaction problems

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SUMMARY

In this work we propose new parallel numerical methods to solve certain evolutionary singularly perturbed problems in a robust and efficient way. To get this, we firstly consider a semidiscretization in time using a simple fractional step Runge–Kutta method, where the splittings for the convection–diffusion–reaction operator and the source term are subordinated to a decomposition of the spatial domain in many smaller subdomains. Such semidiscretization procedure reduces the original problem to a set of elliptic problems (in smaller subdomains), which can be solved in parallel, and it avoids the use of Schwarz iterations. To discretize in space such problems we have considered classical linear finite elements on certain piecewise uniform meshes which have been constructed with a very simple *a priori* criterion, similar to the one introduced by Shishkin for one-dimensional stationary problems of this kind. We show that the use of these meshes permits to obtain uniformly convergent approximations even in the boundary layer regions. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: domain decomposition; Shishkin mesh; singularly perturbed problem; fractional step Runge–Kutta method

1. INTRODUCTION

Unsteady two-dimensional convection–diffusion–reaction phenomena can be modelled by initial boundary value problems which admit the following formulation:

$$\begin{array}{rccc} \text{Find } u: & [t_0, T] & \to & \mathscr{H} \quad \text{such that} \\ & t & \hookrightarrow & u(t) \equiv u(\bar{x}, t) \end{array}$$

$$\frac{\mathrm{d}u}{\mathrm{d}t} - \varepsilon \Delta u + \mathbf{a}(\bar{x}, t) \cdot \nabla u + b(\bar{x}, t)\, u = f(\bar{x}, t), \quad (\bar{x}, t) \in \Omega \times (t_0, T]$$

$$u(\bar{x}, t_0) = u_0(\bar{x}) \in \mathscr{H}, \quad \bar{x} \in \Omega$$

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$$u(\bar{x},t)=g(\bar{x},t)\in\mathscr{H}^b,\quad (\bar{x},t)\in\Gamma\times(t_0,T] \tag{1}$$

Here, we will assume that Ω is a bounded convex open subset of $\mathbb{R}^2$ ($\bar{x}\equiv(x,y)$) with a polygonal boundary Γ and that $\mathscr{H}$ and $\mathscr{H}^b$ are spaces of functions defined in Ω and Γ, respectively. We will suppose that the diffusion coefficient $\varepsilon>0$ can take small values and that the velocity field $\mathbf{a}\equiv\mathbf{a}(\bar{x},t)=(a_1(\bar{x},t),a_2(\bar{x},t))$ and the reaction term $b\equiv b(\bar{x},t)\geqslant 0$ are sufficiently smooth functions. We will also assume enough smoothness and compatibility among the source term $f(\bar{x},t)$ and the initial and boundary conditions u_0 and g, respectively, in order to guarantee that $u\in\mathscr{C}^{4,2}(\bar{\Omega}\times[t_0,T])$, i.e. that u is a function whose derivatives up to order 4 in space and up to order 2 in time are continuous functions on $\bar{\Omega}\times[t_0,T]$.

It is well known that, when ε is much smaller in size than $\|\mathbf{a}\|$, $|b|$ or both, the solution of (1) presents a multiscale character, i.e., certain narrow regions (called boundary or interior layers) appear and in such regions the solution varies (in space) much more rapidly than in the rest of the domain. The location and size of such layers depend on the behaviour of the velocity field $\mathbf{a}$. In this paper we will focus mainly on two cases: (1) $\mathbf{a}\equiv 0$, $b(\bar{x},t)\geqslant\beta>0$ (diffusion–reaction problem) and (2) $\|\mathbf{a}\|\geqslant\alpha>0$, where each component ($i=1,2$) verifies $\|a_i\|\geqslant\alpha_i>0$ or $a_i=0$ (convection–diffusion problem).

On the other hand, we consider a partition of Γ in three parts: $\Gamma=\Gamma_{\mathrm{i}}\cup\Gamma_{\mathrm{o}}\cup\Gamma_{\mathrm{c}}$, where $\Gamma_{\mathrm{i}}=\{\bar{x}\in\Gamma:\mathbf{a}(\bar{x},t)\cdot\mathbf{n}<0\}$, $\Gamma_{\mathrm{o}}=\{\bar{x}\in\Gamma:\mathbf{a}(\bar{x},t)\cdot\mathbf{n}>0\}$ and $\Gamma_{\mathrm{c}}=\{\bar{x}\in\Gamma:\mathbf{a}(\bar{x},t)\cdot\mathbf{n}=0\}$ are the input, output and characteristic boundaries, respectively ($\mathbf{n}$ denotes the unit outward normal to Γ). Assuming that the boundary condition imposed in (1) cannot have any discontinuity in Γ_{i} together with the previous hypotheses on the convection–reaction coefficients, it can be assured that interior layers are not present. With respect to boundary layers (see Reference [1]), in the convection–diffusion case we have a regular layer in Γ_{o}, which is $\mathscr{O}(\varepsilon)$ in width, and also a parabolic layer in Γ_{c} (if it is present), whose width is $\mathscr{O}(\sqrt{\varepsilon})$; in the diffusion–reaction case, a parabolic boundary layer, $\mathscr{O}(\sqrt{\varepsilon})$ in width, appears close to the whole boundary. Furthermore, in both cases, various corner layers use to be present in the corners of Γ.

Classical numerical methods on a uniform mesh provide solutions which approximate very badly to the exact solution in the layers. Moreover, in convection–diffusion problems, oscillations without any physical sense appear unless the chosen mesh is really fine. This unstable behaviour can be eradicated using more advanced techniques such as upwinding or streamline diffusion (see Reference [2]). In order to obtain schemes with the most desirable property, that is the ε-uniform convergence, two different techniques have been deeply studied providing fitted operator methods and fitted mesh methods (see Reference [1]). The first ones consist of difference operators on standard meshes which are exact for certain functions that characterize the singular behaviour of the solutions. The second ones use a classical method on a fitted mesh which is constructed using certain *a priori* or *a posteriori* criterions. In the field of *a priori* fitted meshes, where the Shishkin meshes are ones of the most used due to their simplicity and low cost of construction, the case of finite differences in simple domains has been deeply studied. Here, we will extend these ideas to more general domains by using simple finite elements, which is the classical choice for complicated geometries.

Concerning the ε-uniform convergence, Andreyev (see Reference [3]) proves for the one-dimensional convection–diffusion problem, that the use of suitable meshes implies that it is

not necessary to use upwind techniques. Moreover, if a classical centred difference scheme is used, although oscillations which are physically unrealistic continue appearing, they are negligible in size and a uniformly convergent behaviour of the numerical solutions is proven for a single linear problem like (1). We will apply these ideas to the two-dimensional case. Obviously, it is very interesting to avoid these oscillations not only because the numerical solution obtained possesses a better physical interpretation, but also because, as it is indicated in Reference [4] for stationary problems, the iterative methods used to solve the resulting linear systems converge much faster in the case of developing a monotone scheme. So, this is a task which we think of developing in the future.

2. SEMIDISCRETIZATION IN TIME

For the time integration of problem (1) we propose the use of a fractional step Runge–Kutta method (FSRK) which provides an algorithm of type domain decomposition whose cost in terms of computational complexity is lower than the one obtained using classical domain decomposition techniques (see References [5, 6]). In order to carry out such semidiscretization in time we need to consider an additive splitting for the elliptic operator $A(\bar{x},t)=\varepsilon\Delta-\mathbf{a}\cdot\nabla-b\mathscr{I}$ and for the source term f. To specify such splitting we start considering the spatial domain decomposed as follows: $\Omega=\bigcup_{i=1}^{m}\Omega_i$, where each subdomain Ω_i consists of a set of m_i disjoint components Ω_{ij} satisfying $\Omega_i=\bigcup_{j=1}^{m_i}\Omega_{ij}$. Associated with this decomposition, we construct a smooth partition of unity, $1=\sum_{i=1}^{m}\{\psi_i\}_{i=1}^{m}$, in such a way that

$$\psi_i(\bar{x})=\begin{cases}\left.\begin{array}{ll}0 & \text{if } \bar{x}\in\Omega\setminus\Omega_i,\\ 1 & \text{if } \bar{x}\in\Omega_i\setminus\bigcup_{\substack{j=1\\ j\neq i}}^{m}(\Omega_i\cap\Omega_j),\end{array}\right\} & \text{non-overlapped zones}\\ h_i(\bar{x}) \text{ if } \bar{x}\in\bigcup_{\substack{j=1\\ j\neq i}}^{m}(\Omega_i\cap\Omega_j), & \text{overlappings}\end{cases} \tag{2}$$

$$\text{with } 0\leqslant h_i(\bar{x})\leqslant 1 \text{ and } \sum_{i=1}^{m}h_i(\bar{x})=1 \ \forall\ \bar{x}\in\bigcup_{\substack{j=1\\ j\neq i}}^{m}(\Omega_i\cap\Omega_j)$$

The chosen splittings are $A(\bar{x},t)=\sum_{i=1}^{m}A_i(\bar{x},t)$, where $A_i(\bar{x},t)=\varepsilon\,\mathrm{div}(\psi_i(\bar{x})\cdot\nabla)-\psi_i(\bar{x})\mathbf{a}\cdot\nabla-\psi_i(\bar{x})b\mathscr{I}$ and $f(\bar{x},t)=\sum_{i=1}^{m}f_i(\bar{x},t)$, where $f_i(\bar{x},t)=\psi_i(\bar{x})f(\bar{x},t)$.

Using these partitions, an FSRK method provides semidiscrete approximations of the exact solution $u_n\equiv u_n(\bar{x})(\approx u(\bar{x},t_n))$ which are obtained as follows:

$$\begin{cases}U^{n,j}=u_n+\tau\sum_{k=1}^{j}a_{jk}^{i_k}\left(A_{i_k}(\bar{x},t_{n,k})U^{n,k}+f_{i_k}(\bar{x},t_{n,k})\right) & \text{in } \Omega\\ U^{n,j}=g(\bar{x},t_{n,j}) \quad \text{in } \Gamma, \ \text{for } j=1,\ldots,s\end{cases} \tag{3}$$

$$u_{n+1}=u_n+\tau\sum_{j=1}^{s}b_j^{i_j}\left(A_{i_j}(\bar{x},t_{n,j})U^{n,j}+f_{i_j}(\bar{x},t_{n,j})\right), \quad n=1,2,\ldots,N$$

where $i_\bullet\in\{1,\ldots,m\}$, $t_n=t_0+n\tau$, $t_{n,j}=t_n+c_j\tau$ and $N=[T/\tau]$.

It is interesting to notice that in the calculus of $U^{n,j}$ (internal jth stage), $A_{i_j}(\bar{x},t_{n,j})$ is the only part of the operator $A(\bar{x},t_{n,j})$ which acts implicitly; due to its construction, this operator is null in practically the whole domain. Consequently, when we combine one of these methods with

a suitable spatial discretization, we obtain algorithms which in the jth fractionary step must solve a linear system just in the subdomain Ω_{i_j}. Moreover, if this subdomain consists of the union of several disjoint connected components, we can parallelize the necessary calculations. Note also that this technique does not require the use of iterative Schwarz processes as it happens in the classical domain decomposition techniques (see Reference [6]).

3. SEMIDISCRETIZATION IN SPACE

In order to obtain a totally discrete scheme, which approximates the exact solution of the original problem (1), we must combine the previous time integration with a suitable discretization of the spatial variables. It is shown in Reference [7] that if we combine an FSRK method which satisfies suitable absolute stability properties with a classical spatial discretization scheme, the resulting numerical algorithm is unconditionally convergent, i.e. there is no restriction between the sizes of the time step τ and the mesh parameter h to obtain convergence.

In this case, we have chosen to use linear finite elements on certain special meshes based on Shishkin proposals (see Reference [1]) that we describe below; the use of finite elements instead of finite differences permits us to deal with problems whose spatial domain geometry can be much more complicated. Note that the construction of a special mesh using an *a priori* criterion requires to possess quite deep knowledge of the continuous solution behaviour. In the well studied one-dimensional singularly perturbed problems, Shishkin proposes the following special meshes (see Reference [1]). For a diffusion–reaction problem, we define $\sigma_1 = \min\{\frac{1}{4}, \frac{1}{\beta}\sqrt{\varepsilon}\log(N)\}$, and the following piecewise uniform meshes (see Figure 1) are considered for a segment l in length (N is the number of segment partitions, $N = \dot{4}$). On the other hand, for a one-dimensional convection–diffusion problem which has positive or negative convective term ($|a(x)| \geqslant \alpha > 0$), the following special meshes (see Figure 2) are considered, where $\sigma_2 = \min\{\frac{1}{4}, \frac{1}{\alpha}\varepsilon\log(N)\}$.

We have extended these ideas to two-dimensional polygonal domains, starting from a coarse triangulation, which defines the geometry, and performing a piecewise uniform or quasi uniform triangulation, where the transition segments are at a distance of the boundary segments determined by the same parameters (σ_1 for the parabolic layers and σ_2 for the regular ones). In Figures 3 and 4 we plot these meshes for a regular hexagon considering $\varepsilon = 0.02$ and $N = 16$.

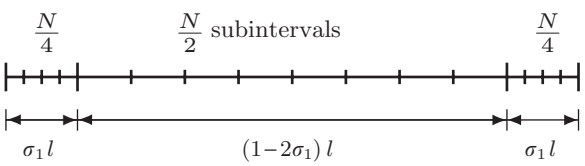

Figure 1. Diffusion–reaction case.

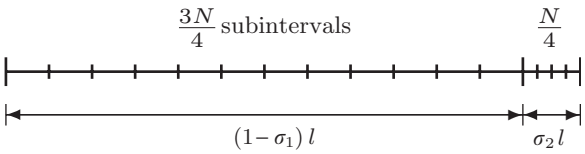

Figure 2. Convection–diffusion case.

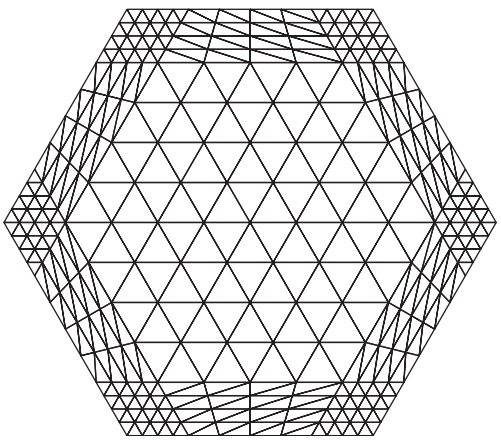

Figure 3. Diffusion–reaction with $\beta = 1$.

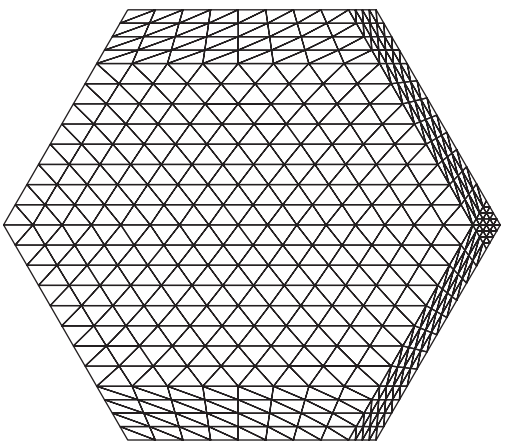

Figure 4. Convection–diffusion with $\mathbf{a} = (1, 0)$.

4. NUMERICAL EXPERIMENTS

In the examples included in this section we have chosen as spatial domain Ω the regular hexagon with vertices $(-\frac{1}{2}, \frac{\sqrt{3}}{2})$, $(\frac{1}{2}, \frac{\sqrt{3}}{2})$, $(1, 0)$, $(\frac{1}{2}, -\frac{\sqrt{3}}{2})$, $(-\frac{1}{2}, -\frac{\sqrt{3}}{2})$, $(-1, 0)$. We will present numerical results concerning the ε-uniform convergence and not the computing speedup ad-

vantages provided by the possible parallelization of the necessary calculations. That is the reason why we consider a very simple domain decomposition in six subdomains: $\Omega = \bigcup_{i=1}^{6} \Omega_i$, each one of them consisting of just one connected component. Concretely, in both examples, $\{\Omega_i\}_{i=1}^{6}$ are six equilateral triangles (whose three vertexes are the two vertices of one side of the hexagon and its centre) extended with a band, which is d in width,[‡] added along the two sides of these triangles, which are inside of Ω, to form the overlappings.

Using the auxiliary function

$$g(w) = \begin{cases} 0 & \text{if } -\dfrac{\sqrt{3}}{2} \leqslant w \leqslant -\dfrac{\sqrt{3}d}{2} \\ \dfrac{1}{2} + \dfrac{\sqrt{3}}{2d} w - \dfrac{2\sqrt{3}}{9d^3} w^3 & \text{if } -\dfrac{\sqrt{3}d}{2} \leqslant w \leqslant \dfrac{\sqrt{3}d}{2} \\ 1 & \text{if } \dfrac{\sqrt{3}d}{2} \leqslant w \leqslant \dfrac{\sqrt{3}}{2} \end{cases}$$

we can define the following smooth partition of unity related to such domain decomposition:

$$\begin{aligned} \psi_1(x,y) &= g(w_1)\, g(w_2)(1 - g(w_3)), & \psi_4(x,y) &= (1 - g(w_1))(1 - g(w_2))\, g(w_3) \\ \psi_2(x,y) &= g(w_1)\, g(w_2)\, g(w_3), & \psi_5(x,y) &= (1 - g(w_1))(1 - g(w_2))(1 - g(w_3)) \\ \psi_3(x,y) &= (1 - g(w_1))\, g(w_2), & \psi_6(x,y) &= g(w_1)(1 - g(w_2)) \end{aligned}$$

where $w_1 = y$, $w_2 = \frac{1}{2}(y + \sqrt{3}x)$, and $w_3 = -\frac{1}{2}(y - \sqrt{3}x)$.

Once the splitting for the operator and the source term is defined, as it was indicated in Section 2, we will use as time integrator the first-order Fractionary Implicit Euler scheme defined as

$$\begin{aligned} U^{n,0} &= u_n \\ U^{n,j} &= U^{n,j-1} + \tau(A_j(t_{n+1})U^{n,j} + f_j(t_{n+1})), \quad j = 1, \ldots, 6 \\ u_{n+1} &= U^{n,6} \end{aligned}$$

combined with linear finite elements on the special meshes introduced in Section 3.

4.1. Diffusion–reaction example

We have considered a problem of type (1) where $T = 2$, $\mathbf{a} \equiv 0$, $b = 1$, and f, u_0 and g are data chosen such that

$$\begin{aligned} u(x,y,t) = {} & \mathrm{e}^{-t}(c_1 + c_2\mathrm{e}^{-(\sqrt{3}-2y)/2\sqrt{\varepsilon}} + c_3\mathrm{e}^{-(\sqrt{3}+2y)/2\sqrt{\varepsilon}})(c_1 + c_2\mathrm{e}^{-(\sqrt{3}(1-x)-y)/2\sqrt{\varepsilon}} \\ & + c_3\mathrm{e}^{-(\sqrt{3}(1+x)+y)/2\sqrt{\varepsilon}})(c_1 + c_2\mathrm{e}^{-(\sqrt{3}(1+x)-y)/2\sqrt{\varepsilon}} \\ & + c_3\mathrm{e}^{-(\sqrt{3}(1-x)+y)/2\sqrt{\varepsilon}}), \quad (c_1, c_2, c_3 \text{ real constants}) \end{aligned}$$

[‡]For these numerical experiences we have chosen $d = \frac{1}{8}$.

Table I. Global errors for the diffusion–reaction case.

	$N=4$	$N=8$	$N=16$	$N=32$	$N=64$	$N=128$	$N=256$
$\varepsilon=1$	9.975E-2	2.889E-2	9.931E-3	5.910E-3	3.936E-3	2.348E-3	1.261E-3
$\varepsilon=10^{-2}$	1.942E-2	1.336E-2	7.886E-3	4.262E-3	1.104E-3	4.141E-4	2.090E-4
$\varepsilon=10^{-4}$	5.489E-2	1.876E-2	7.931E-3	6.807E-3	2.994E-3	1.030E-3	3.372E-4
$\varepsilon=10^{-6}$	5.904E-2	2.087E-2	8.000E-3	6.808E-3	2.994E-3	1.030E-3	3.371E-4
$\varepsilon=10^{-8}$	5.947E-2	2.108E-2	8.008E-3	6.808E-3	2.994E-3	1.030E-3	3.371E-4

Table II. Global error estimates for the convection–diffusion case.

	$N=4$	$N=8$	$N=16$	$N=32$	$N=64$
$\varepsilon=1$	1.285E-2	3.288E-3	1.105E-3	5.740E-4	3.098E-4
$\varepsilon=10^{-2}$	1.855E-1	6.129E-2	2.368E-2	6.443E-3	1.537E-3
$\varepsilon=10^{-4}$	2.128E-1	1.183E-1	8.397E-2	4.983E-2	2.938E-2
$\varepsilon=10^{-6}$	2.120E-1	1.184E-1	8.495E-2	5.108E-2	3.109E-2
$\varepsilon=10^{-8}$	2.118E-1	1.182E-1	8.495E-2	5.108E-2	3.110E-2

is the exact solution. In Table I, we show the maximum global errors obtained for several values of N (τ is chosen in such a way that $\tau N = 0.2$).

4.2. *Convection–diffusion example*

We consider now a problem of type (1) without known exact solution where $T=2$, $\mathbf{a}=(1,0)$, $b=1$, $u_0(\bar{x}) \equiv 0$, $g(t) \equiv 0$ and $f(x,y,t) = 3\,t\,\mathrm{e}^{-3t+1}\cos(\pi x)\cos(\pi\frac{x+\sqrt{3}y}{2})\cos(\pi\frac{x-\sqrt{3}y}{2})$.

In Table II, we show the maximum global errors estimated for several values of N ($\tau N = 0.4$), such estimations have been computed using the double mesh principle in time and space (see Reference [8]).

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