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Adaptive multiresolution schemes for reaction-diffusion systems

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This note outlines a fully adaptive multiresolution scheme with local time stepping for the efficient numerical solution of (possibly degenerate) reaction-diffusion systems. A new numerical example showing Turing-type pattern formation is presented.

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1 Introduction

In [1] we present a fully adaptive multiresolution (MR) scheme for spatially 2D, possibly degenerate reaction-diffusion systems, focusing on models of combustion, pattern formation, and chemotaxis. Solutions of these equations in these applications exhibit steep gradients, and in the degenerate case, sharp fronts and discontinuities. This calls for a concentration of computational effort in zones of strong variation. The MR scheme is based on finite volume discretizations with explicit time stepping. The MR representation of the solution is stored in a graded tree ("quadtree"), whose leaves are the non-uniform finite volumes on the borders of which the numerical divergence is evaluated. By a thresholding procedure, namely the elimination of leaves that are smaller than a threshold value, substantial data compression and CPU time reduction is attained. Our version of the MR method includes a locally varying adaptive time stepping strategy similar to that by Müller and Stiriba [5]. Numerical experiments presented in [1] illustrate the effectiveness of the adaptive MR method. It turns out that local time stepping accelerates the adaptive MR method by a factor of two, while the error remains controlled.

2 Reaction-diffusion system, multiresolution scheme and numerical example

We consider the domain $Q_T := \Omega \times (0,T)$, $\Omega := (0,1)^2$, its boundary $\Sigma_T := \partial\Omega \times (0,T)$, and the reaction-diffusion system

$$u_t = \gamma f(u,v) + \Delta u, \quad v_t = \gamma g(u,v) + d\Delta v \quad \text{on } Q_T\,, \tag{1}$$

$$u(\boldsymbol{x},0) = u_0(\boldsymbol{x}), \qquad v(\boldsymbol{x},0) = v_0(\boldsymbol{x}) \quad \text{on } \Omega, \quad \nabla u \cdot \boldsymbol{n} = \nabla v \cdot \boldsymbol{n} = 0 \quad \text{on } \Sigma_T. \tag{2}$$

In [1], this system is studied with more general degenerate diffusion terms. This system models several phenomena including combustion [1, 7], but is considered here as a well-known model of pattern formation in mathematical biology. Under a number of structural conditions relating the functions $f(u,v)$ and $g(u,v)$ and their derivatives to the parameters γ and d, the system produces stationary solutions with Turing-type spatial patterns (see [6] for details). To produce this effect, we select the kinetics $f(u,v) = a - u + u^2 v$ and $g(u,v) = b - u^2 v$, with the parameters $a = -0.5$, $b = 1.9$, $d = 4.8$, and $\gamma = 800$ [6].

We employ a standard finite volume scheme to discretize, which is described here for a uniform grid. The domain Ω is partitioned into control volumes $(\Omega_{ij})_{(i,j)\in\Lambda}$, where Λ is an index set, defining $\Omega_{ij} := [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}]$, $\Delta x := x_{i+1/2} - x_{i-1/2}$, $\Delta y := y_{j+1/2} - y_{j-1/2}$, for all $(i,j) \in \Lambda$, and $\widetilde{\Delta x} := \min\{\Delta x, \Delta y\}$. Let $\bar{q}_{ij}(t)$ denote the cell average over Ω_{ij} of a quantity q at time t. The FV scheme is described here for the first equation of (1); for the second equation, we replace u by v and $f(u,v)$ by $g(u,v)$. Integrating the respective equation and averaging over Ω_{ij} yields the folowing expression, where $\mathcal{D}$ denotes the RHS of the PDE except for the reaction term:

$$\frac{1}{|\Omega_{ij}|}\iint_{\Omega_{ij}} u_t(\boldsymbol{x},t)\,d\boldsymbol{x} = \frac{1}{|\Omega_{ij}|}\iint_{\Omega_{ij}} \mathcal{D}\big(u(\boldsymbol{x},t), \nabla u(\boldsymbol{x},t)\big)\,d\boldsymbol{x} + \frac{1}{|\Omega_{ij}|}\iint_{\Omega_{ij}} f\big(u(\boldsymbol{x},t), v(\boldsymbol{x},t)\big)\,d\boldsymbol{x}.$$

We discretize $\mathcal{D}$ via $\bar{\mathcal{D}}_{ij} := -\frac{1}{\Delta x}(\bar{F}_{i+1/2,j} - \bar{F}_{i-1/2,j}) - \frac{1}{\Delta y}(\bar{F}_{i,j+1/2} - \bar{F}_{i,j-1/2})$ defining $\bar{F}_{i+1/2,j} := -\frac{1}{\Delta x}(\bar{u}_{i+1,j} - \bar{u}_{ij})$ and $\bar{F}_{i,j+1/2} := -\frac{1}{\Delta y}(\bar{u}_{i,j+1} - \bar{u}_{ij})$. The reaction term is approximated by $\bar{f}_{ij} \approx f(\bar{u}_{ij}, \bar{v}_{ij})$. A first-order Euler time discretization yields the formula $\bar{u}_{ij}^{n+1} = \bar{u}_{ij}^n + \Delta t\gamma\bar{f}_{ij} + \Delta t\bar{\mathcal{D}}_{ij}(\mathcal{S}(\bar{u}_{ij}^n), \widetilde{\Delta x})$, $\bar{v}_{ij}^{n+1} = \bar{v}_{ij}^n + \Delta t\gamma\bar{g}_{ij} + d\Delta t\bar{\mathcal{D}}_{ij}(\mathcal{S}(\bar{v}_{ij}^n), \widetilde{\Delta x})$, where $\mathcal{S}(\cdot)$ denotes the stencil used for computing $\bar{\mathcal{D}}_{ij}$. This scheme is stable under the CFL condition

$$\lambda\gamma(\|f_u\|_\infty + \|f_v\|_\infty + \|g_u\|_\infty + \|g_v\|_\infty) + 8\mu d \le 1, \quad \lambda := \Delta t/\widetilde{\Delta x}, \quad \mu := \Delta t/\widetilde{\Delta x}^{\,2}. \tag{3}$$

The adaptive MR method is an efficient space-time adaptive implementation of the FV scheme, which relies on storing the numerical solution on a sequence of nested dyadic grids defined on Ω. Basically, we define a finest grid on Ω with the

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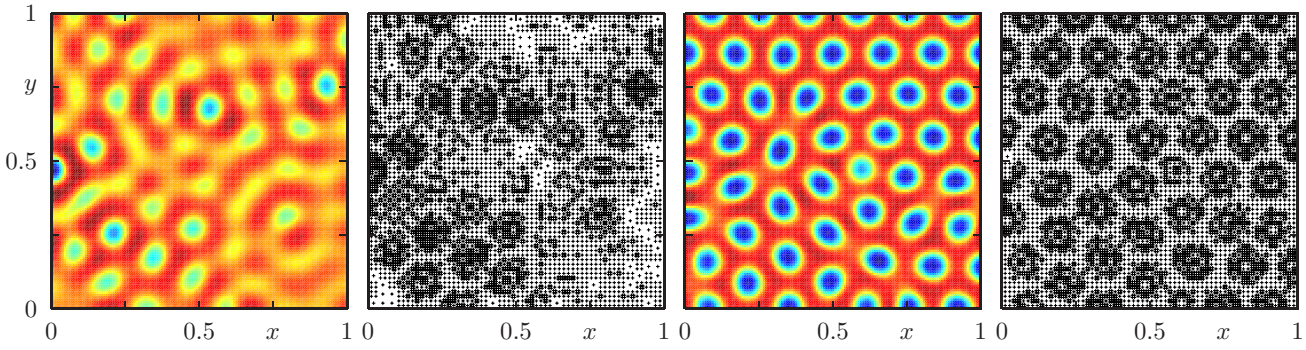

Fig. 1 Numerical simulation of Turing-type pattern formation. From left to right: component u at $t = 0.05$, adaptive mesh at $t = 0.05$, component u at $t = 1.5$ and adaptive mesh at $t = 1.5$. The solution assumes values $0.8 < u < 1.7$ and $0.1 < u < 2.1$ for $t = 0.05$ and $t = 1.5$, respectively. The adaptive mesh is represented by the centers of the finite volumes.

t	$\mathcal{V}$	η	L^1-error in (u,v)	L^2-error in (u,v)	$L^\infty-$error in (u,v)
0.05	7.94	12.2072	$(5.83 \times 10^{-4}, 4.02 \times 10^{-4})$	$(3.89 \times 10^{-4}, 2.46 \times 10^{-4})$	$(1.95 \times 10^{-3}, 9.08 \times 10^{-4})$
0.5	10.63	11.7857	$(5.91 \times 10^{-4}, 4.77 \times 10^{-4})$	$(4.97 \times 10^{-4}, 4.31 \times 10^{-4})$	$(9.59 \times 10^{-4}, 8.44 \times 10^{-4})$
1.5	12.23	11.9140	$(7.62 \times 10^{-4}, 5.75 \times 10^{-4})$	$(8.08 \times 10^{-5}, 3.32 \times 10^{-4})$	$(1.22 \times 10^{-3}, 1.16 \times 10^{-3})$

Table 1 Turing model: Corresponding simulated time, speedup $\mathcal{V}$, data compression rate η, and normalized errors.

meshwidth $\Delta x = \Delta y = \widetilde{\Delta x} = 2^{-L}$, $L \in \mathbb{N}$. We may represent the cell averages of a function defined on the finest grid by storing the average of four neighbouring cells that form a cell of the next coarsest grid, plus three independent differences, called *details*. Repeating this process successively for all coarser levels eventually leads to the *multiresolution representation* of the solution, which consists of one average value for each cell of the coarsest grid plus a sequence of details corresponding to finer levels. For a sufficiently smooth function, the details diminish when we proceed from coarser to finer levels of resolution. The decisive benefit of the MR representation accrues from an operation called thresholding, that is, we set to zero all details that are smaller in absolute value than a tolerance $\varepsilon_l = 2^{2(l-L)}\varepsilon_{\mathrm{R}}$, where ε_{R} is a reference tolerance and $l = 0, 1, \ldots, L$ are the levels of multiresolution ($l = L$ is the finest). Roughly speaking, the numerical solution in the graded tree is re-organized after each time iteration, and the additional error introduced by thresholding will not deteriorate the rate of convergence of the FV scheme if ε_{R} is chosen in a particular way that is compatible with the CFL condition (3), see [4] for a rigorous analysis for the case of conservation laws and [1, 2, 3] for further details on our implementation. Clearly, this procedure naturally suggests that we employ a graded tree data structure for the representation of the solution. In this so-called quadtree (i.e., a node will have up to four sons), the leaves correspond to the finest level of resolution and form the finite volumes on which the numerical discretization is eventually applied.

The performance of the MR device is measured by the speedup $\mathcal{V}$ and the data compression rate η, which are defined by

$$\mathcal{V} = \frac{\text{CPU time of FV scheme on finest grid}}{\text{CPU time of MR version of FV scheme}}, \quad \eta = \frac{\#\{\text{cells of finest grid}\}}{\#\{\text{cells of finest grid}\} \cdot 2^{-2L} + \#\{\text{leaves}\}}.$$

An additional speedup of a factor of roughly two is attained by *local time stepping* (first proposed by Müller and Stiriba [5]). The basic idea is to advance parts of the solution corresponding to leaves lying on coarser levels of resolution by larger time steps than those corresponding to fine levels, and to ensure stability by strictly enforcing the CFL condition. This requires a careful synchronization after each coarse-level time iteration; this task is, however, greatly facilitated by the graded nature of the tree. See [1] for further technical details that have been omitted in this note, and which also include the precise evaluation of numerical fluxes and the creation of a safety zone in the graded tree.

Our example (Figure 1) starts from a random perturbation of the steady state ($u^0 = a + b = 1.4, v^0 = b/(a + b)^2 = 0.96939$). We use $L = 8$ and $\varepsilon_{\mathrm{R}} = 7.82 \times 10^{-4}$. The effectiveness of the MR method is illustrated in Table 1.

References

[1] M. Bendahmane, R. Bürger, R. Ruiz, K. Schneider, Preprint 2007-35, DIM, U. de Concepción; submitted.
[2] R. Bürger, R. Ruiz, K. Schneider, M. Sepúlveda, J. Engrg. Math. **60** (2008) 365–385.
[3] R. Bürger, R. Ruiz, K. Schneider, M. Sepúlveda, M2AN Math. Model. Numer. Anal., to appear.
[4] A. Cohen, S. Kaber, S. Müller, M. Postel, Math. Comp. **72** (2002) 183–225.
[5] S. Müller, Y. Stiriba, J. Sci. Comput. **30** (2007) 493–531.
[6] J.D. Murray, Mathematical Biology II: Spatial Models and Biomedical Applications, Third Edition, Springer-Verlag, New York, 2003.
[7] O. Roussel, K. Schneider, Combust. Theory Modelling **10** (2006) 273–288.

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