Numerical techniques for differential equations with multiple scales in space or time

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In this report we discuss recently developed numerical methods for multiscale problems in time (a numerical integrator for stiff advection-diffusion-reaction equations with or without noise) and multiscale problems in space (a numerical homogenization algorithm that combines different physics at different scales).

Numerical methods for stiff advection-diffusion-reaction equations with or without noise. Consider a system of (stochastic) ordinary differential equations originating from space discretized partial differential equations (PDEs)

$$\dot{y} = F(y) = F_D(y) + F_A(y) + F_R(y) + \sum_{j=1}^{m} F_G^j(y)\dot{\xi}_j, \qquad y(0) = y_0, \tag{1}$$

where $F_D(y), F_A(y), F_R(y), F_G^j \in \mathbb{R}^n$ and $\xi_j, j = 1, \ldots, m$ are independent one-dimensional Wiener processes. Here $F_D(y)$ represent a diffusion term with eigenvalues close to the negative real axis, $F_A(y)$ advection terms with eigenvalues close to the imaginary axis, $F_R(y)$ stiff (reaction) terms and F_G^j (stiff) noise terms, respectively. Classical numerical methods usually face the following issues

- a step size restriction for *explicit methods* due to the F_D term ("CFL-type" restriction), F_R term (multiple reaction rates that can vary over order of magnitudes) and F_G^j term ("stiff" mean-square stable problems) [2],[8];
- large nonlinear systems at each time steps when using *implicit methods* that can become quite involved, particularly for systems involving complicated nonlinear structure [9].

In [6] we present a new partitioned implicit-explicit orthogonal Runge-Kutta (RK) method (PIROCK) for the time integration of (1). Due to the use of a *stabilized* explicit second order orthogonal RK Chebyshev method (ROCK2) [1] for the F_D term, the severe restriction of the CFL condition for explicit schemes can be relaxed. A second order singly diagonally implicit RK that is unconditionally stable is used for the F_R term and a third order explicit method (stable on a portion of the imaginary axis) is taken for the F_A term. Finally an explicit stabilized method is also used for the F_G^j terms following the methods developed in [2],[5].

Other implicit-explicit or partitioned method have been proposed for (1)[1], and we mention the implicit-explicit Runge-Kutta-Chebyshev method (IRKC) derived in [10] and the fully explicit partitioned Runge-Kutta-Chebyshev method (PRKC) proposed in [11] (see [10],[11],[6]) for a more comprehensive literature review. For problems with stiff reactions, the PIROCK method is more efficient than the IRKC method as the number of function evaluations of the reaction terms F_R (solved implicitly) is independent of the (possibly high) stage number used in the stabilized explicit method for the diffusion terms F_D (it has also a better behavior for advection dominated problems than IRKC). Compared to the PRKC method

[1]However, none of them have been developed for equations including (stiff) noise terms.

(that can only handle non stiff reaction terms) the PIROCK method has larger stability domains on both the real and the imaginary parts. PIROCK implemented in a single black-box FOTRAN code available at `http://anmc.epfl.ch`, is fully adaptive, provides a posteriori error estimators, and requires from the user solely the right-hand side of the differential equation.

An adaptive numerical homogenization method for a Stokes problem. Consider the Stokes problem in heterogeneous media with pore sizes ε that can be several orders of magnitude smaller than the macroscopic size of the computational domain of interest Ω. Then, a full Stokes solver over Ω is often too expensive. For such problems we propose in [7] an adaptive multiscale micro-macro homogenization method, using the framework of the finite element heterogeneous multiscale method (FE-HMM) [4] with an adaptive strategy [3]. The new method relies on adaptive mesh refinement on macro and micro problems and on rigorous residual-based a posteriori error estimates derived in [7]. We propose a strategy to adequately couple macro and micro error indicators (a challenging issue) in order to achieve a desired accuracy with minimal computational cost on both the macro and the micro scales.

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