LSMS Conference 2017 - Lebanon

"Adaptive time-space algorithms for the simulations of multi-scale reaction waves"

Marc Massot

Centre de Mathématiques Appliquées, Ecole Polytechnique, UMR CNRS 7641
and formerly at
CentraleSupélec - Laboratory EM2C – UPR CNRS 288
Fédération de Mathématiques de l'Ecole CEntrale Paris – FR CNRS 3487

Abstract:

Numerical simulations of multi-scale phenomena are commonly used for modeling purposes in many applications such as combustion or plasmas physics. These models raise several difficulties created by the high number of unknowns, the wide range of temporal scales due to detailed chemical kinetic mechanisms, as well as steep spatial gradients associated with very localized fronts of high chemical activity. Furthermore, a natural stumbling block to perform 3D simulations with all scales resolution is either the unreasonably small time step due to stability requirements or the unreasonable memory requirements for implicit methods. In this work, we introduce a new resolution strategy for multi-scale reaction waves based mainly on time operator splitting and space adaptive multiresolution. It considers high order time integration methods for reaction, diffusion and convection problems, in order to build a time operator splitting scheme that exploits efficiently the special features of each problem. Based on theoretical studies of numerical analysis, such a strategy leads to a splitting time step which is not restricted neither by fast scales in the source term nor by restrictive stability limits of diffusive or convective steps, but only by the physics of the phenomenon. Moreover, this splitting time step is dynamically adapted taking into account a posteriori error estimates, carefully computed by a second embedded and economic splitting method. The main goal is then to perform computationally efficient as well as accurate in time and space simulations of the complete dynamics of multi-scale phenomena, considering large simulation domains with conventional computing resources and splitting time steps dictated by the physics of the phenomenon and not by stability constraints associated with mesh size or source time scales. Applications will be presented in the fields of combustion waves and plasma discharges dynamics and the question of high-performance computing using such numerical methods will be discussed and illustrated.

Biosketch:

Marc Massot obtained his PhD in Applied Mathematics from Ecole Polytechnique, France, in 1996. After a year at Yale University, Department of Mechanical Engineering, he obtained a CNRS position in the Applied Mathematics Laboratory of the University of Lyon, France, where he stayed until 2005. He was offered an Associate Professor position at Ecole Centrale Paris when he installed a mathematics team in the EM2C mechanical engineering laboratory. He was Visiting Professor at the Center for Turbulence Research, Stanford University, in 2011-2012 and created and chaired the Fédération de Mathématiques de l'Ecole Centrale Paris between 2013 and 2016. He initiated the Computing Center (Mésocentre) of Ecole Centrale Paris in 2010, of which he was the deputy director until 2016 and he is scientific adviser at ONERA DEFA and scientific collaborator at Maison de la Simulation since 2013. Full Professor since 2011, he has been recruited on a full Professor position at Ecole Polytechnique, Centre de Mathématiques Appliquées in 2017. His main fields of research are mathematical modeling and numerical analysis, analysis of PDEs and dynamical systems for multi-scale systems, scientific computing and high performance computing with applications in combustion, two-phase flows, plasma physics and biomedical engineering.

References on the subject of the talk:

[1] **S. Descombes, M. Duarte, M. Massot**, *Operator splitting methods with error estimator and adaptive time-stepping. Application to the simulation of combustion phenomena*. Roland Glowinski; Stanley Osher; Wotao Yin. Operator splitting and alternating direction methods, Springer (2017) 1-13 https://hal.archives-ouvertes.fr/hal-01183745

[2] **S. Descombes, M. Duarte, T. Dumont, T. Guillet, V. Louvet, M. Massot**, *Task-based adaptive multiresolution for time-space multi-scale reaction-diffusion systems on multi-core architectures*, submitted to SMAI - JCM (2016) 1-24 https://hal.archives-ouvertes.fr/hal-01148617

[3] **M. Duarte, Z. Bonaventura, M. Massot, and A. Bourdon**, *A Numerical strategy to discretize and solve Poisson equation on dynamically adapted multiresolution grids for time-dependent streamer discharge simulation*, Journal of Computational Physics, 289 (2015) 129-148

[4] **S. Descombes, M. Duarte, T. Dumont, F. Laurent, V. Louvet, M. Massot**, *Analysis of operator splitting in the non-asymptotic regime for nonlinear reaction diffusion equations. Application to the dynamics of premixed flames*, SIAM Journal of Numerical Analysis, Vol. 52, No. 3 (2014) 1311-1334

[5] **M. Duarte, S. Descombes, C. Tenaud, S. Candel, M. Massot**, *Time-space adaptive numerical methods for the simulation of combustion fronts*. Combustion and Flame, Vol. 160, No. 6 (2013) 1083-1101

[6] **T. Dumont, M. Duarte, S. Descombes, M.-A. Dronne, M. Massot, V. Louvet**, *Simulation of human ischemic stroke in realistic 3D geometry : a numerical strategy*, Communications in Nonlinear Science and Numerical Simulation, Vol. 18, Issue 6 (2013) 1539-1557

[7] **M. Duarte, A. Bourdon and M. Massot, Z. Bonaventura**, *Derivation of a merging condition for two interacting streamers in air*, Plasma Sources Science and Technology, Vol. 21, No. 5 (2012) 052001 1-5

[8] **M. Duarte, Z. Bonaventura, M. Massot, A. Bourdon, S. Descombes, T. Dumont**, *A new numerical strategy with space-time adaptivity and error control for multi-scale streamer discharge simulations*, Journal of Computational Physics, 231, 3 (2012) 1002-1019

[9] **M. Duarte, M. Massot, S. Descombes**, *Parareal operator splitting techniques for multi-scale reaction waves: numerical analysis and strategies*, M2AN, Vol. 45, No. 5 (2011) 825-852

[10] **M. Duarte, M. Massot, S. Descombes, C. Tenaud, T. Dumont, V. Louvet, and F. Laurent**. *New resolution strategy for multi-scale reaction waves using time operator splitting, space adaptive multi-tiresolution and dedicated high order implicit/explicit time integrators*. SIAM J. Sci. Comput., 34, 1 (2012) 76-104

[11] **S. Descombes, M. Duarte, T. Dumont, V. Louvet, and M. Massot**. *Adaptive time splitting method for multi-scale evolutionary PDEs*. Confluentes Mathematici, Numéro Spécial en hommage à Michelle Schatzman, Vol. 3, No. 3 (2011) 1-31

[12] **S. Descombes, T. Dumont, V. Louvet, M. Massot**, *On the local and global errors of splitting approximations of reaction-diffusion equations with high spatial gradients*, International Journal of Computer Mathematics, Special Issue on Splitting Methods for Differential Equations, Ed. Q. Sheng Vol. 84, No. 6(2006) 749-765

[13] **S. Descombes, M. Massot**, *Operator splitting for nonlinear reaction-diffusion systems with an entropic structure: singular perturbation and order reduction*, Numerische Mathematik, Vol. 97, No. 4 (2004) 667-698