

**PARAREAL SIMULATION OF MULTI-SCALE EVOLUTION EQUATIONS : FROM
POLARISABILITY OF NANOPARTICLES TO REACTING WAVES WITH COMPLEX
CHEMISTRY**

Advisorship:

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1 Context of the study

1.1 Location and collaboration network for an interdisciplinary project

The two laboratories J. A. Dieudonné and EM2C, two reknown laboratories of the CNRS are involved in the PITAC project the aim of which is the study and demonstration of the possibilities of parareal computations for various applications. They are involved in both departments of CNRS in France : ST2I (Engineering) and MPPU (Mathematics and Physics), and the post-doctoral position involves an interdisciplinary scientific project : introducing new algorithms and their numerical analysis into key applications in physics and engineering. It will be located at Laboratory EM2C with a high level of exchanges with the laboratory J. A. Dieudonné, Nice.

The EM2C laboratory provides an ideal framework for such a project since it involves a group of applied mathematicians within a laboratory mainly devoted to engineering and physics studies and guaranties the quality of the applications fields : evaluation of the polarisability of nanoparticles by simulation of molecular dynamics and the numerical simulation of reacting flows involving complex chemistry mechanisms (typically 50 species and 250 reactions). These two applications require too intensive numerical simulations in most cases and constitute two stumbling blocks of the actual scientific investigations. The introduction of new algorithms and dedicated solvers should allow a major breakthrough in these two fields. The strong collaboration with both the Institut Camille Jordan (V. Louvet and T. Dumont) at the University of Lyon and with the Laboratoire J. A. Dieudonné at the University of Nice with S. Descombes [1, 2] in the field of numerical simulation and numerical analysis of multi-scale evolution equations provides a sound theoretical and computing background.

1.2 Principle of parareal simulations

The applications we focus on are modeled by evolution equations with multiple time scales and can be described most of the time by system of ordinary differential equations (ODE).

For a short presentation of parareal numerical methods we focus on ODE. Let us consider an ODE or a system of ODE that we want to solve on $[0, T]$, with $T > 0$; the parareal algorithm consists in, as an example, discretizing

the interval by using a fine time step, which governs the required final accuracy of the method, and a coarse time step, introduced to maximize speedup (maximal gain in time) or to optimally use a given number of processors (system efficiency). The algorithm then consists in many steps :

- The first time step consists in solving the ODE on the coarse discretization sequentially.
- The second step consists in solving the ODE on each coarse interval. It is worth insisting that this step is fully parallelizable.
- The last step consists of propagating the error between the coarse and fine discretizations through the whole time interval by using one more time the non-parallel coarse discretization.

The latter two steps may be repeated sequentially $k - 1$ times and is proved in a number of cases to converge to the solution in time. The main advantage of the algorithm is that it can provide a precise solution within less time than solving with the fine time step over the entire time range by using the system efficiency during the step which can be parallelized [3]. Such an algorithm can also be viewed as the replacement a scheme of order m on the coarse grid by a scheme of order km on that same grid and this replacement is made by using corrections obtained by steps fully parallelizable [4]. Another interpretation can be found in term of space-time multi-grid and multiple shooting methods [5].

One issue which is still not understood is the compatibility of the proposed method with the presence of multiple scales in the system.

2 Parareal simulations of multiscale phenomena

2.1 Objectives of the study

The objective of the post-doctoral position are threefold. First the candidate should become familiar with the parareal literature and implement the method in some basic configurations. Then, he would study the extension of parareal algorithms to multi-scale generic problems in connection with operator splitting techniques such as in [6], conduct the related numerical analysis and implement the algorithms on parallel architectures (the EM2C laboratory has a cluster of 20 nodes, with 2 AMD Opteron 64 bits dual core per node, that is 4 slots per node with 8 Go of shared memory, or overall 80 processors). Finally, he should get familiar with the modelling of both complex chemistry for combustion applications and nanothermal modelling and apply the identified techniques to both situations.

2.2 Two applications : Complex Chemistry and Nanothermal Modeling

The study of the structure of chemically reacting flows [7, 8, 9, 1] with complex chemistry naturally involves many temporal scales in the system and leads to very heavy numerical simulations even in the case of simplified configurations such as the one of pulsated counter premixed flames proposed in [10]. The numerical simulation of such models in the context of multi-dimensional configuration is still an open problem even if it has received some interesting contribution recently. Besides, simulating propagating flames also involve steep spatial gradients which can lead to another source of stiffness in the system [2]. It is thus interesting to study if the parareal capabilities can provide a new framework as well as a new generation of method in this field. Before getting to the full system of partial differential equations modelling such flows, many models intermediate in complexity have to be tackled in order to assess the numerical analysis and method developed such as in [6].

The polarisability of nanoparticles have been extensively studied in the frame of electric or semi-conducting materials. Dielectric materials were not targeted so far, whereas thermal absorption is at stake. The molecular dynamics technique [11, 12] allows for the determination of the polarisability in nanoclusters [13]. This technique consists in solving the classical motion equation of each atom in the system. The characteristic time of the material resonance is about a tenth of a picosecond whereas the time step is a tenth of a femtosecond. The simulations are costly in computation time because long range interactions are taken into account. We intend to apply the parareal numerical scheme to shorten this computation time. The effect of the nanoparticle size on the polarisability as well as the impact of a neighbouring nanocluster will be analysed.

3 Necessary Background

Numerical analysis (resolution of large/stiff ODE systems). Scientific programming and computing (parallel computing abilities). Interest for applications in the field of physics or mechanical engineering.

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