Campagne 2020 Contrats Doctoraux Instituts/Initiatives

Proposition de Projet de Recherche Doctoral (PRD)

Appel à projet ISCD-Institut des Sciences du calcul des Données 2020

Intitulé du Projet de Recherche Doctoral : Fast multiphase flows solvers

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Unité de Recherche :

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Code *(ex. UMR xxxx)* : UMR7598

Ecole Doctorale de rattachement de l'équipe & d'inscription du doctorant : ED386-Sciences Mathématiques Paris C

Doctorants actuellement encadrés par le directeur de thèse (préciser le nombre de doctorants, leur année de 1ere inscription et la quotité d'encadrement) : 0

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Code *(ex. UMR xxxx)* : UMR7190

Ecole Doctorale de rattachement : ED 391 - Sciences mécaniques, acoustique, électronique et robotique de Paris (SMAER)

Doctorants actuellement encadrés par le co-directeur de thèse (préciser le nombre de doctorants, leur année de 1ere inscription et la quotité d'encadrement) : 2

Serena Costanzo (2018, 50%, coencadrement Pascal Frey), Tomas Fullana (2019, 50%, coencadrement Bruno Després).

Cotutelle internationale : Non

Description du projet de recherche doctoral *(en français ou en anglais)*

3 pages maximum – interligne simple – Ce texte sera diffusé en ligne

Fast multiphase flows solvers:

The system of balance laws known as the Navier-Stokes equations (NSE) describes the physics of many fluid phenomena of scientific and engineering interest. Practical use of this model relies on the numerical resolution of large systems of equations. In the context of two-phase incompressible flows, **two aspects render the resolution/accuracy of such simulations challenging:**

(I) Differential algebraic structure: in the incompressible limit, the semi-discrete NSE consist of a set of equations that equate the rate of change of the differential variables (the velocity components) to the net force exerted on fluid particles. This net force includes the gradient of an additional field, the pressure, an algebraic variable which in turn enforces the conservation of fluid particles' volume. As a result, the semi-discrete incompressible NSE form an index 2 Differential Algebraic Equation, the resolution of which is significantly more challenging than the Ordinary Differential Equations that govern compressible flows. Block preconditioners have been proposed (Cahouet-Chabard and approximate commutators), but these methods either lack generality (e.g. not applicable to two-phase flows) and/or do not perform well at large scales. As a consequence, the vast majority of the incompressible fluid mechanics community approximates the DAE by a set of decoupled hyperbolic/parabolic equations for the velocity components, and an elliptic equation for the pressure field, all of which can be solved by standard resolution techniques. Unfortunately, this approximation gives rise to a number of numerical artifacts in the vicinity of interfaces and boundaries, that are detrimental to both the stability and the accuracy of the method.

(II) Piecewise constant physical properties in two-phase flows: in the context of two-phase flows the physical properties (density and viscosity) are piecewise constant (i.e. constant in each phase) with large jumps across the interface (itself part of the solution, featuring complex topologies such as sheets, ligaments, droplets and bubbles…). The two interacting fluids can either be treated as such (with immersed boundary methods) although dedicated techniques have yet to be developed, or as a single-phase flow with discontinuous properties. Regardless of the approach, in the interface vicinity where vorticity is generated, the discontinuity strongly couples the velocity components which can not be solved separately anymore. This coupling is not accounted for in the current generation of solvers, which results in slow convergence and/or numerical instabilities that ultimately impede the computation of realistic flow regimes.

Tackling these two bottlenecks can vastly improve the efficiency of two-phase flow simulations, as the resulting linear algebra typically accounts for 80% of the computational cost. An additional speed up is furthermore expected since fully implicit simulations also reduce time-step size restrictions, hence lowering the number of time-steps to simulate a given time horizon. These aspects combined could theoretically yield ten-fold speed up as well as provide stable algorithms to venture beyond current parameter limitations.

One way of reducing the cost of the resulting linear algebra, in the system of interest to this project, is using preconditioners. Over the years, the applied math community has devised efficient and scalable state-of-the-art preconditioning techniques, prime among them Multigrid and Domain Decomposition (DD) methods which, from an abstract point of view, are very similar. Algebraic Multigrid preconditioning can be the most efficient choice in some cases (two- and three-dimensional diffusion-dominated regimes), but it can also exhibit slow convergence and even diverge in convection-dominated regimes. We will therefore focus on DD methods, since it exposes better parallelism

and its mathematical foundations are well established.DD methods started as an effort to increase the parallelism of numerical solvers designed to simulate physical phenomena governed by partial differential equations. Contrary to direct methods, the appealing feature of domain decomposition methods is that they are naturally parallel. Using domain decomposition methodology the full simulation domain is decomposed into smaller subdomains, where each subdomain can be treated independently and concurrently. The resulting domain decomposed system is typically solved by iterating over a collocation of smaller problems, fueling research in areas, which insure that the number of these required iterations remain small. The method of interest to this project is based on two-level preconditioners of the GenEO type [Do15]. This method has proved to be robust with respect to the heterogeneity of the problem under consideration and the PhD director is one of the authors of the original method. This domain decomposition method guarantees a constant number of iterations regardless of the problem size, the domain decomposition methodology and of the heterogeneities of the parameters. It was first developed for symmetric positive definite problems and has recently been extended to saddle point problems [Nat, 2019], and is the first Schwarz type DD method with a mathematically guaranteed a priori chosen convergence rate, which works as well for substructured type methods ([Spi, 2013b] and [Man, 2007]). Large scale computations of heterogeneous three dimensional Darcy and elasticity problems on thousands of cores [Jol, 2013], show the GenEO method to perform on par with state of the art classical (*hypre*) and smoothed aggregation (GAMG) MG methods and to even outperform them in some problems [Jol, 2014 (section 5.2)]. In spite of these promising results, there remain open issues such as the treatment of the skew-symmetric contributions originating from convective transport. In practice, the size of the coarse space may grow to be very large in which case, the construction has to be recursive in order to add extra levels which will lead to efficient methods, [AlD, 2019]. **To the best of our knowledge however, documented applications of DD outside of the Finite Element community are scarce. However, the Finite Volume and Finite Difference communities, that represent the vast majority of the CFD applications, would benefit tremendously from the use of DD methods**. This is a strong incentive for collaborative research between the two communities, to adapt and showcase the applicability of DD methods to CFD applications.

Furthermore, for this endeavor to achieve its full potential, it should also embrace the shift of HPC from homogeneous to heterogeneous architectures by leveraging the benefits of GPU deployment. The use of GPU architecture is an extremely promising path for reducing our computing time, due to their ability to reduce the cost of some linear algebra operations. GPUs are energy efficient, allow multiple precision computations and are pervasive in modern heterogeneous computing platforms. The two most powerful supercomputers in the world (according to the last TOP500 list - November 2019) rely on GPUs, as well as about one fifth of those in the TOP500 list, highlighting the current extent of GPU usage in scientific computing. Independent of the method, the main result is usually a hybrid parallel CPU-GPUs algorithm. This makes the solver adaptable for applications running on both large scale supercomputers and on local workstations.

Therefore, the objective of this collaborative work is to speed up the computation of two-phase incompressible flows, by leveraging the aforementioned DD methods (suited for saddle-point systems with high contrast coefficients), with low-level linear algebra operations (inner products, matrix-vector multiplications…) operated on GPUs. The project will initially focus on the viscous limit of the incompressible two-phase NSE, namely the two-phase Stokes equations. This symmetric system retains the saddle-point structure as well as the high contrast coefficients. The GenEO method will be deployed to a single GPU for problems of moderate size. Different computation grain sizes will be considered to best fit the GPU architecture. As shown in [Pa11], very small subdomains will likely be required in

order to take full advantage of the GPU architecture. The second stage of the project will therefore consist of developing a three-level DD method best suited for GPUs. To the best of our knowledge, while the last decade has seen efforts to port other DD algorithms to GPUs [Pa11, St17, Ya14], no three-level DD has ever been investigated for GPU acceleration. A hybrid CPU-GPU deployment, with multi-core parallelism on CPU, could then be investigated for the rest of the flow solver, where computational geometry operations are best executed on CPU (pervasive use of branching). Finally, the algorithms will be deployed to multiple nodes, possibly with multiple GPUs on each node, where the three-level DD solver is expected to overcome the performance issue related to the numerous small subdomains. Using multiple GPUs to solve larger problems will indeed greatly increase the number of subdomains, which will thus exacerbate the second-level solving bottleneck.

The completion of such interdisciplinary work will be best supported under an infrastructure such as ISCD, where the team of one applied mathematician (F. Nataf, LJLL, SU), two thermofluid engineers (T. Sayadi, IJLRDA, SU & V. Le Chenadec, MSME, UGE) and one computer scientist (P. Fortin, LIP6, SU; see e.g. [FGG16], http://lip6.fr/Pierre.Fortin) will best be able to coordinate their efforts and supervise the Ph.D. candidate, expected to have a background in applied mathematics with strong programming skills.

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