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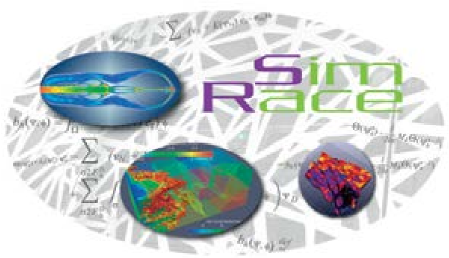

Numerical Methods and High Performance Computing for Industrial Fluid Flows - SimRace

IFPEN, Rueil-Malmaison, 8 - 10 December 2015

SimRace Conference Highlights

The aim of SimRace was to cover multi-disciplinary topics relating to scientific computing applied to the simulation of industrial fluid flows. Our objective was to bring together people from the sphere of computer science, applied mathematics and applications. Over these three days we tackled issues ranging from the upcoming OpenMp 5.0 norm to various industrial applications in chemical engineering, geosciences and automotive engines, as well as covering topics such as a multiscale DG method, virtual element or volume formulations, directive-based automatic code generation and many others.

The conference was organized around five sessions which will be briefly summarized here.

Session 1: High-performance computational and programming models for emerging architecture

We are currently facing on-going architectural changes to HPC systems. The number of nodes continues to grow, intra-node concurrency is greatly increasing and we are moving towards heterogeneous systems. Within this context, it is important to ensure performance portability of HPC applications, though it is difficult to predict performance in a dynamic execution environment.

One of the answers provided in this session is the need for a layered programming approach, from applications to hardware. In these layers, we find today's portable parallel programming APIs: MPI, OpenMP, PGAS, Charm++. These APIs are being adapted to follow the hardware evolution. For instance, version 4.5 of OpenMP has just been released and version 5.0 is already under discussion (Keynote by B. Chapman).

Another level coming over these parallel APIs is the Domain Specific Language level. Two different kinds of DSLs were illustrated during the session. A directive based language able to generate simulation codes with automatic adaptation and parallelization was presented. A framework based on advanced C++11 features dedicated to finite element formulations applied to incompressible Navier-Stokes simulations (Feel++) was also described.

Finally, at the top level we find the applications that are also trying to adapt to the various architectures. In this context, a performance model (for data and CPU) can be used to predict the efficiency of a numerical scheme algorithm. This model uses given information on the target machine: bandwidth and peak.

Session 2: Challenging exaflopic applications

Different challenging applications have been presented during the session in the field of chemical engineering and automotive engine simulations. Both industrial and academic fellows presented their simulation results. The applications described used distributed memory computations with MPI communications on up to several tens of thousands of cores on French and European HPC facilities (GENCI, PRACE). The use of HPC enables the simulation of cases at industrial scale with refined modeling, such as Large Eddy Simulations, and the study of transitional phenomena such as cyclic variation or knocks development in automotive engine simulations. It also enables us to simulate and gain insight into two-phase flow dynamics in a complex industrial reactor with moving parts.

Session 3: Multi-scale methods and model coupling

The first part of this session was devoted to turbulence and two-phase flow modeling and simulation. These flows occur, for instance, in liquid injection of aeronautical and automotive engines or in particulate flows in fluidized beds. Simulating these complex flows is highly challenging as the problem is truly multi-scale. Space scales go from micrometers to meters or even tens of meters for fluidized beds. The time scale goes from microseconds to days, months or even years! Furthermore, coupling problems often occur in such flows, as in the carrier gaseous phase in liquid injection problems, for example. An interesting approach to tackle these flows on an industrial scale is to use reduce-order models. A State of the art of Eulerian model for liquid injection flows has been proposed in the session (Keynote by M. Massot). Based on a statistical description these models use moment methods. High order moment methods are derived to handle modeling difficulties. The use of these moment methods requires specific numerical scheme development to ensure stability. To obtain closure for the reduced models, work has to be done on smaller scales. Micro-scale computations were presented for the study of heat and mass transfer and for the proposal of drag force closures in gas-solid flows. Fully resolved computations are still being developed and Direct Numerical Simulations of water jet destabilization were presented. Finally, the problem of obtaining boundary conditions at the wall for turbulent incompressible flows was tackled, in the framework of finite element methods.

In the second part of the session, multi-scale problems were also illustrated in the context of geoscience simulations. Tough nonlinear systems were resolved for reactive multi-space multi-species flows in porous media using active set methods or splitting algorithms. The study of a specific multi-scale DG method for transport modeling in porous media flows was presented, detailing the construction of the basis functions on agglomerated elements.

Session 4: Numerical schemes on general meshes for complex flows

New trends in numerical scheme derivations were presented in this session, dealing with new finite element or finite volume methods, applied to advection-diffusion, radiation and gas dynamics problems.

In the field of finite element methods, an introduction to the Virtual Element Method was presented (Keynote of L. Beirao da Veiga). The idea is to derive a new finite element method which is well suited for general meshes, based on the building of a new local approximation space. The basis functions are defined as solutions of well-chosen local problems inside each element, thus the scheme can be computed solely from the degrees of freedom. An extension of Virtual Element methods to a finite-volume-like formulation was brought to light in the session, allowing a conservative flux-based formulation using cell and vertex unknowns. An evaluation of this scheme against classical finite-volume multi-point schemes was displayed on advection-diffusion problem. Remaining in the field of diffusion problems, new developments of finite volume methods were also presented. A new non-linear positive scheme increasing the robustness of deformed mesh computations was presented on a parabolic radiation equation.

The remainder of the session was devoted to a Lagrangian remap method for gas dynamics. Two different aspects were raised. First a new conservative scheme dealing with all Mach regimes and any equations of state was presented. This scheme uses relaxation and separation between acoustic and transport operators. It enables a large time step and is compatible with asymptotic preserving techniques. The second contribution on Lagrange remap steps tries to build a "HPC-compatible" algorithm. Thanks to the performance analysis tool presented in session 1, the algorithm has been rewritten to minimize memory transfers and maximize vectorization compatibility. The new algorithm shows a good scalability using AVX extensions.

Session 5: Scalable linear solvers

The interdependence of linear and nonlinear solvers when studying the performance of a nonlinear problem was detailed in this session. The tradeoffs between linear and nonlinear solvers were first presented (Keynote by C. Woodward), when applied to groundwater flows and climate simulations. Several points have to be studied to increase the performance of the overall simulation: how to build the Jacobian (analytic, finite differences…), how to exploit symmetry, how to avoid oversolve in the linear solver. The different cost at the different levels: function evaluation, Jacobian evaluation and preconditioner evaluation, have to be compared to avoid useless optimization. It is then necessary to perform a global choice, keeping in mind that a slower outer method can be globally faster if the inner system is easier to solve. Finally moving to exascale will require a reconsideration what we need from a solver and how we can standardize information transfer from the user physics to the linear solver, passing through the nonlinear solver, in numerical libraries and software.

Some new numerical techniques derived to increase performance in a parallel context were then presented. In order to increase the scalability of linear solver, an s-step algorithm has been developed for BiCGStab solver, aiming at reducing significantly the need to communicate in parallel. To improve the convergence of domain decomposition methods, a two level method, based on eigenvalues problem resolution, has been developed and implemented in the parallel library HPDDM.

Finally the importance of optimizing the solvers has been illustrated in two geoscience applications of gas storage and reservoir simulation. In these applications, up to 80% of the simulation can be spent in the solver. Different techniques have been used to reduce this problem. Mesh refinement and coarsening techniques along with original a posteriori error estimates have been used in a first application to diminish the load of data to solve and prevent oversolving. A second application based on Induced Dimension Reduction methods (IDR(s) solver), shows, after a benchmark on several parallel strategies, some encouraging results with a GPU accelerator, obtaining a simulator response time reduced by a factor of 2.5 to 3.

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…SimRace++

One industrial session

To discover our industrial sponsors' new products: Allinea, Bull Atos Technologies, Hewlett Packard Enterprise, Intel, and Synopsys.

To know more about mission and organization of our academic partner "La Maison de la Simulation".

One Award

A simulation challenge! The team from IRMA-University of Strasbourg received an award for their work on the software Feel++

Participation

70 attendees, 5 countries: France, Italy, Slovenia, United Kingdom, USA.

Stay tuned to SimRace!

To keep up-to-date with SimRace news, send your email address to simrace2015@ifpen.fr