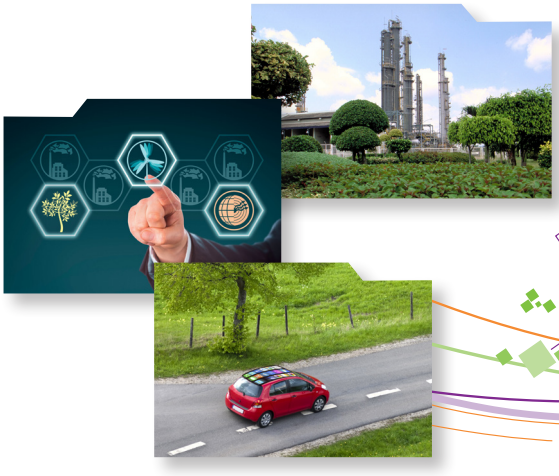


Science@ifpen

Issue 33 - June 2018

SPECIAL ISSUE
Computational performance

Numerical simulations and scientific calculations are widely used in the energy field: to manage oil and gas reserves, exploit geothermal energy and design wind farms, for example. However, these physical models are increasingly complex, involving hydraulic, mechanical, chemical and thermal couplings. Numerical methods must also be able to handle phase changes as well as heterogeneous and multiscale media, that may contain evolving discontinuities. Accordingly, the algorithms to be developed require a large amount of operations.

Thanks to parallel algorithms, combined with specific programming models, data and operations are distributed between several computing resources – processors, cores and graphics cards – making the effective communication between these entities a real challenge. To improve code performance, IFPEN has developed algorithms based on domain decomposition techniques, particularly for particle simulations and sparse linear solvers. IFPEN is also developing adaptive methods, based on multiscale approaches, as well as statistical treatments and a posteriori error estimates.

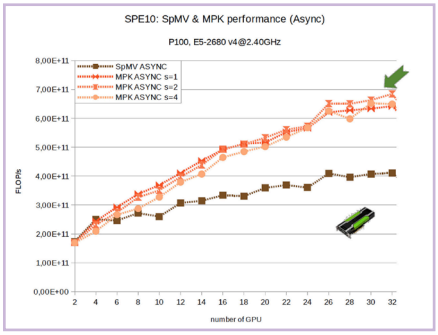
I hope you enjoy reading this issue.

Jocelyne Erhel,
Member of IFPEN's Scientific Board

Solving sparse linear systems on heterogeneous architectures

Numerical simulation is a strategic tool, complementary to experimental studies, used to gain a precise understanding of complex physical phenomena. With many simulation tools[a], performance closely depends on how effectively linear systems are solved, being the most time consuming part of the process. Exploiting the power of parallel computing, offered by the complex and heterogeneous hardware architectures[b] of current computing tools, makes it possible to obtain simulation results with the desired degree of accuracy in an acceptable period of time. However, since resolution algorithms are not capable of fully exploiting these architectures, a rapid decline in performance is observed beyond a certain number of calculation units.

Our research efforts thus focused on the design of parallel algorithms for the resolution of large-scale sparse matrices. These algorithms make use of modern hardware architectures thanks to adapted programming models. This led to the development of the MCGSolver library, containing a broad choice of pre-conditioned parallel iterative linear solvers for multi-core and multi-GPU architectures[1]. This library provides a platform for the transparent and decoupled management of numerical algorithms and various levels of parallelism, via numerous programming models[c]. MCGSolver is constantly enhanced with new methods, such as those based on communication avoiding (figure).



Performance gain obtained thanks to communication avoiding.

This library is available in IFPEN's simulation tools via the ALIEN software module, co-developed with the CEA, which provides access to a wide choice of pre-conditioned linear solvers via a single interface.

a - As for the geological storage of CO_2 or multiscale particle flows.
b - Made up of multi-core processors (x86/ARM) and accelerator cards (GPU).
c - MPI, HARTS[2], OpenMP, CUDA, SIMD.

(1) ***A. Anciaux-Sedrakian,*** *J. Eaton,* ***J-M. Gratien, T. Guignon,*** *P. Have,* ***C. Preux, O. Ricois***
DOI:10.2118/173223-MS

(2) ***A. Roussel, J-M. Gratien,*** *et* ***T. Gautier***
DOI:10.2516/ogst/2016020

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Pushing back the boundaries of parallelization

The numerical simulation and HPC[a] professions have benefited significantly from technological advances in the field of processors, particularly multi-core architectures, in recent decades.

The parallelization methods employed to enhance the performance of numerical calculation are useful but their efficiency decreases as the degree increases. To overcome this limitation, IFPEN's researchers have developed pragmatic approaches.

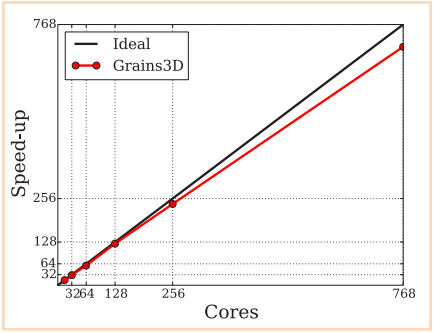
Two examples, implemented on IFPEN's Grains3D and PeliGRIFF computational codes respectively, illustrate their approach:

- The first consisted in developing specific methods (for example, applied to domain decomposition techniques[b]) aimed at optimizing the "efficiency" of HPC calculations, thereby avoiding the additional costs associated with inter-processor communications. For the biggest system studied[c], the performance obtained for 768 cores[1] (figure) was around 91% of the ideal case.

- A second method was based on a multiscale strategy[2], consisting in modeling and solving physical problems on a small scale, before transferring data filtered using statistical approaches to larger scales via cascading.

This approach was successfully used in 2015 within the context of the ANR's MORE4LESS collaborative project, dedicated to the multiscale modeling of reactive particle flows.

a - High Performance Computing.
b - Separation into coupled sub-problems, defined for smaller domains forming a division of the global domain.
c - Around 230 million fluidized particles.
d - Standardized for a complete knot of 16 cores.



Grains3D[d] parallel computing performances in fluidized bed calculations.

(1) ***A. D. Rakotonirina, A. Wachs,*** *Powder Technology, 2015, 154-172.*
DOI: 10.1016/j.powtec.2017.10.033

(2) ***A. Esteghamatian, F. Euzenat, A. Hammouti,*** *M. Lance,* ***A. Wachs,*** *International Journal of Multiphase Flow.*
DOI:10.1016/j.ijmultiphaseflow.2017.11.003

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More efficient flow simulations inspired by optimal control

Multiphase mixture (gas and liquid) flow simulation in porous media has a variety of applications in the field of geosciences[a] but also in the fields of engineering and chemical processes.

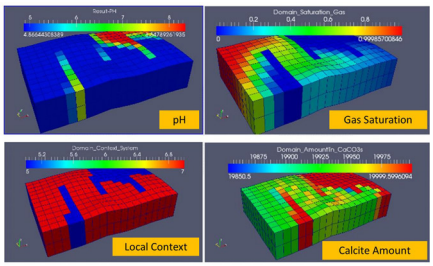
In industrial simulators, globally implicit equation formulations are crucial for ensuring calculation robustness and performance, as well as maintaining close coupling between fluid flows and thermodynamics. However, mathematical and numerical difficulties remain, such as, for example, treating the appearance and disappearance of phases simultaneously with the transport of components. The numerical methods need to be adapted to take into account the variable structure of the system of equations and solve the associated inequalities.

A variety of different innovative solutions have been proposed in recent years, via a reformulation based on "complementarity constraints"[b], used in optimization and optimal control. Drawing on these new ideas and its long-standing expertise, IFPEN has developed a unified approach and a general framework facilitating the development of algorithms and their computerization. These algorithms have been tested on prototypes[1] and then successfully deployed in operational simulators.

Using this approach, it is now possible to handle systems coupling flows with chemical[2] (figure), thermal and compaction[3] reactions.

Current research is aimed at integrating kinetic chemical reactions and adapting solvers used in the field of optimization.

a - CO_2 storage, gas storage, the exploitation of oil and gas resources, geothermal energy, ground remediation.
b - Via which the positivity of two magnitudes and the nullity of at least one of them is concisely expressed.



Example of multiphase reactive flow simulation (CO_2 storage and calcite dissolution).

(1) ***I. Ben Gharbia*** *and* ***al.,*** *SPE Reservoir Simulation Symposium 2015, 23-25 February, Houston.*
DOI: 10.2118/173249-MS

(2) ***T. Faney*** *and* ***al.,*** *Workshop "Reactive Transport Modeling in the Geological Sciences", IHP, Paris. November 17-18, 2015.*
http://www.irisa.fr/sage/RTworkshop-2015/Exposes/Faney.pdf

(3) ***C. Meiller*** *and* ***al.,*** *AAPG ACE, 100th, Houston, USA, 2-5 april 2017*
http://www.searchanddiscovery.com/abstracts/html/2017/90291ace/abstracts/2611970.html

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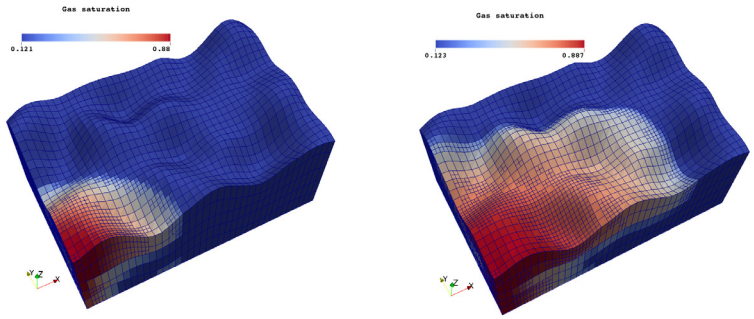
Faster and just as good: the motto of adaptive methods

In the field of numerical simulation, a sufficiently accurate representation of the data associated with physical models requires, in general, a very large numerical grid that, despite existing computing power, results in excessively long calculation times.

For example, geological models, which cover extensive geographic zones, require a fine grid that can contain hundreds of millions of grid cells. Moreover, they require several additional calculations for the calibration[a] of reservoir properties[b] from experimental data. Therefore, the process chain that follows for a single simulation can render the calculation time exorbitant.

To overcome this problem, IFPEN develops and implements acceleration strategies.

Adaptive mesh refinement is a judicious solution both in terms of saving memory resources and reducing calculation times, while maintaining results of a satisfactory quality. For this, a "fine" resolution approach is reserved for the zones where such accuracy is required and a "coarse" approach is used elsewhere. The success of such a strategy is inextricably linked to the tool used to decide which zones require a fine approach and which do not (figure).



Result of a multiphase flow calculation after 500 and 1,500 days, using an adaptive mesh.

In this respect, a posteriori error estimates [1,2], specifically developed in recent years by IFPEN, represent an extremely efficient tool for adaptive mesh refinement algorithms.

This efficiency can be explained by the mathematical rigor of the methods used, in contrast with other more heuristic tools. In addition, they have led to the formulation of stopping criteria for linear/non-linear solvers, leading to significant CPU time savings, without impacting the precision of results.

a - Adjustment process using uncertainty analysis and optimization tools.
b - Porosities, permeabilities, fluid viscosities, capillary pressures, etc.

(1) ***J.-M. Gratien, O. Ricois, S. Yousef,*** *Oil Gas Sci. Technol (2016), 71, 59. DOI: 10.2516/ogst/2016009*

(2) *M. Vohralík and* ***S. Yousef.*** *Comput. Methods Appl. Mech. Engrg. 331 (2018), 728–760. DOI: 10.1016/j.cma.2017.11.027*

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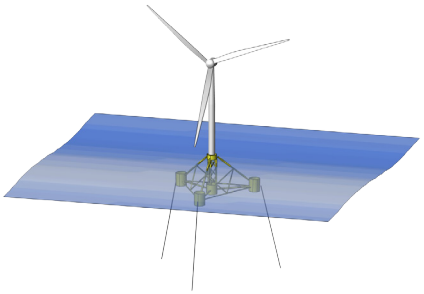
Wind turbines have the wind in their sails, thanks to GPUs

IFPEN has been carrying out research in the field of floating wind turbines for a number of years, developing, for this purpose, the DeepLines Wind™ simulation tool, in partnership with Principia[1]. The software enables the coupled calculation of hydrodynamic loads on the floating support and its mooring systems as well as the aerodynamic stresses exerted on the blades. The latter are estimated via the Wind module, recently developed by IFPEN and added to the initial DeepLines software.

The majority of aerodynamic dimensioning methods for wind turbines use analytical approaches based on the Blade Element Momentum[a] method. To validate these approaches, a vortex-type Lagrangian method was developed[2]. For this, it is necessary to solve a system of equations (N-body problem[b]), which mobilizes virtually all of the global calculation time. To reduce it, the "critical" part of the calculation was transferred to the GPUs (Graphical Processing Units) using the specific CUDA[c] language. This substantially reduced calculation times — one or two-fold — thereby rendering the code operational on a daily basis.

To pursue this optimization avenue, Fast Multipole Method-type solutions may deliver additional calculation costs savings (one-fold reduction).



Configuration of a wind turbine on the IFPEN/SBM Offshore floater for simulations with DeepLines Wind™.

a - Method based on the actuator disk law and a "blade element" approach enabling the load forces of wind turbine blades to be calculated.
b - Problem consisting in solving the interactions between N-bodies interacting according to a physical law.
c - Compute Unified Device Architecture.

(1) ***C. Le Cunff*** *and* ***al.,*** *32nd International Conference on Ocean, Offshore and Arctic Engineering, Nantes, France, 2013.*

(2) ***F. Blondel*** *and* ***al.,*** *Congrès français de mécanique (French Mechanics Conference), Lille, France, 2017.*

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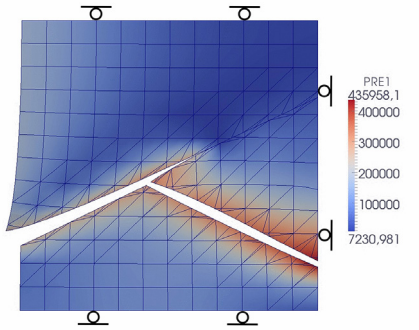
A hydro-mechanical model for underground naturally fractured rocks

Natural underground fractures in rocks provide fluids with preferential flow pathways. The resulting global permeability is exploited for energy production (geothermal energy and oil and gas recovery). However, these fractures represent a threat from the point of view of geological storage site integrity. It is therefore essential to anticipate their impact on rock properties and predict potential fracture extensions and reorientations, under the effect of in situ fluid pressure and mechanical stress existing in the rock. It is to this end that a completely coupled hydro-mechanical numerical model has been developed.

This new model[1] is based on the extended finite element method (X-FEM), making it possible to overcome problems relating to the generation of the calculation mesh in the presence of fractures and its modification consequent to their evolution[a]. Fluid flow in fractures is governed by fracture opening and by the fluid exchanges taking place with the surrounding porous medium. The mechanical behavior of the fracture is described by a cohesive zone model.

Called HM-XFEM, the hydro-mechanical model has been validated by comparison with analytical solutions and tested on synthetic cases[b], in order to verify its capacity to predict fracture behavior, incorporating the effects of mechanical stress (figure).

Examples of potential future enhancements to the model are the inclusion of multiphase flow, diffusion of chemical species and mechanical anisotropy of the porous rock.



Influence of mechanical boundary conditions and stresses on fluid flow pathways for two connected fractures[c] (fluid flow from the lower right corner).

a - Because the mesh does not need to conform to fracture geometry.
b - Not from real cases.
c - Representation of fracture opening and fluid pressure [Pa].

(1) *M. Faivre, **B. Paul,** F. Golfier, R. Giot, P. Massin, **D. Colombo,** Engineering Fracture Mechanics 2016. DOI: 10.1016/j.engfracmech.2016.03.029*

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Awards

• ***Céline Chizallet*** *was awarded the SCF (The French Chemistry Society) prize in the 2018 young researcher catalysis division for her important and original contribution in the field of the prediction of catalytic performances and the elucidation of reaction mechanisms combining quantum calculations, kinetic modeling and experiments.*

• *On 2 February,* ***Alexandra Gimbernat,*** *former PhD student at IFPEN, won the 2017 SCF thesis prize, awarded by the Union des industries chimiques (French Chemical Industries Union), in recognition of her work dedicated to the development of a new three-phase process for the direct conversion of sugars into high added-value chemical products.*

Appointment

• ***Hélène Olivier-Bourbigou,*** *Head of IFPEN's Molecular Catalysis department, has been elected a member of the Académie des technologies (French Academy of Technologies). This is further recognition of the excellence and national and international influence of her research.*

News

• ***IFPEN's Scientific Board*** *welcomes seven new members from the world of science: Janne Blichert-Toft (geosciences), Christophe Coperet (catalysis, inorganic chemistry), Marc-Olivier Coppens (chemical engineering, nanotechnology, Nature-Inspired Chemical Engineering (NICE)), Mohamed Gabsi (electrical engineering, electronics), Anke Lindner (physical chemistry, microfluidics), Jean-François Minster (geosciences, economics) and Christine Rousselle (combustion, engines, optical diagnostics).*

• ***IFPEN and ANDRA*** *have signed a four-year partnership agreement aimed at overcoming scientific challenges in the fields of geological modeling, monitoring, instrumentation and analysis, numerical simulations and steel corrosion.*

Upcoming scientific events

• *Rencontre scientifique event* ***– Trace pollutants: recent advances in chemistry, analytical and process sciences –*** *3 to 5 December 2018, Rueil-Malmaison – www.rs-trace-pollutants.com*

• *Scientific conference* ***– Large-Eddy Simulation for Internal Combustion Engine Flows (LES4ICE) –*** *11 and12 December 2018, Rueil-Malmaison – www.rs-les4ice.com*

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