High Performance Computing for Energy

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about the use of exascale computers in Oil & Gas, Wind Energy and Biogas Combustion industries

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1. Introduction

Energy needs worldwide will increase yearly until 2020 and far beyond. The International Energy Agency (IEA) 2014 report [1] estimates that the global energy demand is set to grow by 37% by 2040. Energy scarcity or inefficient usage can lead to higher prices, which will have a critical impact on the economy, as emphasized by the Energy Challenge in the Horizon 2020 work program and by the priorities of the Brazilian Ministry of Science and Technology.

During the last years, High Performance Computing (HPC) resources have undergone a dramatic transformation, with an explosion on the available parallelism and the use of special purpose processors. The number of cores in an Exaflop (10^{18} Flops) computer will be in the order of 100 million. This imposes a severe pressure to increase the parallel efficiency of the applications. At the same time this massive parallelism opens new opportunities to increase the accuracy when simulating physical phenomena.

New energy sources, if untapped, might become crucial in the mid-term. Intensive numerical simulations and prototyping are needed to assess their real value and improve their throughput. The impact of exascale HPC and data intensive algorithms in the energy industry is initially established in the U.S. Department of Energy (DOE) document "Synergistic Challenges in Data-Intensive Science and Exascale Computing" [2].

In HPC4E project we have worked on prepare applications for exascale computers in three energy industries of common interest both to EU and Brazil: Oil & Gas, Wind and Biogas combustion.

2. HPC in Oil & Gas industry

The Oil and Gas (O&G) industry has been one of the most active buyers of HPC technology in the last decades. Seismic data processing is an extremely demanding task in terms of computational demand. Its essential task is transforming seismic data records (i.e. "sound" tracks recoding the response of the Earth to external impulses) into maps of the subsurface. The reason for the constant race for larger and faster supercomputers in O&G has been driven by four main factors: on one hand, the amount of recorded data has exploded since the early 90's due to the possibility of acquiring 3D surveys rather than 2D surveys, a higher density of seismic receivers and longer, more active acquisition efforts that can last weeks of continuous data generation in some cases. The increase in raw data amounts has shown to be very effective in reducing uncertainties in exploratory efforts. On the other hand, the assumptions required to model the behavior of waves in the subsurface have been reduced from earlier ray assumptions to simple finite-frequency models in the acoustic regime, to currently full 3D viscoelastic anisotropic wave fields. This results in a huge cost increase in the wave simulation part of the imaging workflows but largely increases the fidelity of these simulations to the real world. Last but not least, the workflows developed to extract valuable information from seismic data by means of wave modelling have increased in complexity, from simple reverse-propagation principles to present-day full waveform inversion (FWI) [3] technology that involves an iterative improvement of the geological models, i.e. running hundreds or thousands of modelling runs in the process. Last but not least, processing high-frequency data results in a considerable overhead in terms of compute time, roughly increasing by a factor x16 each time we double such frequency. Frequencies are related directly to spatial resolution of subsurface images, hence the need to push towards the highest possible values.

Each of these aspects, when properly addressed, have had a positive impact in terms of returns for O&G companies, which have been able to reduce significantly the uncertainties related to exploration. The 3D acquisition effort alone resulted in a jump in exploration drilling success from 13% in 1991 to 44% in 1996 [4]. Such success would have not been possible without HPC resources devoted to its processing. But perhaps even more crucially, the existence of new technologies allowed opening areas previously thought impossible to explore into hugely successful business stories, as for example the Gulf of Mexico or the Brazilian Pre-salts. Without HPC there would have been no possibility to exploit hydrocarbons in these areas efficiently.

Europe has been a key player in these technology-driven O&G exploration efforts. Albeit the Old Continent holds a minimum percentage of the world's hydrocarbon reservoirs, its O&G companies are at the forefront of technology and their usage for an efficient and profitable extraction of hydrocarbons. BP, for example, was the first company to employ wide-azimuth towed streamers (WATS) in 2005. The huge cost of this exploration technology was first reviewed by simulating its effect on the resulting subsurface image, which showed that the returns would overshadow the initial investment. Nowadays, WATS is a standard technology worldwide in the sector. Total boasts the fastest non-public supercomputer in the world (21st in the world) and Eni the 37th fastest. Other non-EU O&G-related companies also have a strong presence in the list (e.g. PGS, SaudiAramco). Repsol has been a pioneer in using accelerator clusters for O&G exploration [5] and is still a large player in the technology sector related to HPC and hydrocarbon exploration [6].

The technology race is on worldwide. China's Tianhe-1A was 40% used in the 2010-11 period by petroleum companies [7]. At the present, Tianhe-1A is the 52nd fastest computer in the world but Tianhe-2 is 2nd and TaihuLight is 1st, all in China [8].

The future holds more need for HPC in the exploration industry. The biggest problems at this moment rely on widely adopting 3D elastic FWI, which is about x50 more expensive than its acoustic counterpart, integrating uncertainty quantification at all workflows related to geophysical imaging, which involves thousands of realizations and dimensionality reduction techniques and, finally, assessing simultaneous joint inversion of seismic, EM and gravity data which will require an extensive analysis of the cross-talk between scales and physical properties of rocks and extremely different scales. Just as it happened with the adoption of 3D seismic in the 90's and WATS together with wave-equation migration in the 2000's, the present and future developments in exploration and co-design efforts with the hardware industry [9] will lead to further cuts in costs related to exploration, an a sharp decrease in uncertainty related to drilling and the possibility of exploiting regions previously inaccessible or just too expensive to explore.

Current major hydrocarbon findings in Brazil [10], USA [11] or UK [12] are being achieved by European O&G companies employing a large amount of in-house technology. HPC is, and will remain, a cornerstone in its development. Europe has a chance to remain an HPC applications powerhouse and lead the next generation of efficient and reliable exploration technology.

3. HPC in Wind Energy industry

Wind power is the renewable source with the most successful deployment over the past two decades (1996-2016), growing from 2 GW to 490 GW of world installed capacity. This trend is expected to continue because the global demand for wind energy is still large, with a share of global energy demand foreseen to grow from 2% in 2010 up to 11% in 2030. At the present, according to the World Energy Council, the total investments in the global wind sector reached USD 109 billion over the course of 2015. However, the future prosperity of wind energy depends on technological developments and project financing improving, two aspects related to the development of new turbine prototypes, the reduction of wind farm design uncertainties, the mitigation of risks, and the reduction of the cost of wind energy in the energy supply mix. The competitiveness of wind energy can be improved with an accurate wind resource assessment, wind turbine and farm layout design and short-term micro-scale wind simulations to forecast the daily power production. All these aspects rely on numerical modelling, which has already become a pillar for industry and sector stakeholders. The increase of computational capabilities to Exascale is a must for further progress on several fronts, which at present are still hampered by current HPC resources. These include:

Wind resource assessment. Wind resource assessment is associated to the planning phase of wind energy development, a process that can last several years and includes site prospecting and wind farm design and financing. Detailed and robust information about the relative size of the wind resource across the area of interest is crucial for the commercial evaluation of a wind farm. In this regard, a key point for wind energy efficiency is the accurate characterization of the wind potential on wind farms, requiring an accurate determination of the wind velocity field (both off-shore or in complex terrains) and to account for the downwind power-loss effects of wind turbines. The accuracy of the simulation is key to predict potential energy production as a function of the turbine positions. This will determine the long-term cost effectiveness of the farm, and therefore, the viability of a given site. At present, the main industries of the sector make use of Computational Fluid dynamics (CFD) models based on the Reynolds-Averaged Navier–Stokes (RANS) approximation, typically assuming neutral atmospheric stratification and steady homogeneous boundary conditions. Wind farm models, embedded in the microscale flow solver, simulate turbine wake effects and predict the power deficit and added turbulence intensity across the wind farm. With respect to linearized models, the introduction on industry of RANS-CFDs models increased notably the accuracy of wind resource mapping. However, the wind energy community is still hampered by projects showing discrepancies between calculated and actual experienced resources and design conditions, resulting in substantial impacts on the commercial value of a wind farm. Discrepancies can be originated by a number of factors, including inaccurate RANS model physics and resolution. In this sense, the introduction of more computationally demanding transient Large Eddy Simulations (LES), still very much constrained to a research level, is promising. For example, a demonstrator test-case simulation run during the HPC4E project with an explicit WMLES model and using 9.216 CPUs on the MareNostrum-4 supercomputer took around 1 day to simulate a full diurnal cycle (one wind direction sector). Given the good performance of the method on new emerging HPC architectures, it is fair to say than WMLES-like models could be a standard for wind farm model in complex terrains in upcoming Exascale machines.

Uncertainty Quantification (UQ). Wind resource assessment and power forecasts are highly prone to uncertainties coming from natural variability of the flow model inputs (e.g. wind speed and direction, wind rose, turbulence intensity, atmospheric stability, seasonal effects, vegetation and terrain heterogeneities, etc.), lack of constrain on input data and their variability, inadequate model physics, or coarse model resolution. In order to characterize and quantify uncertainties, stochastic approaches (e.g. the polynomial chaos technique) are necessary, requiring of large code-specific and uncertain parameter-specific efforts. Exascale HPC will allow a quantification of all these aspects, thereby reducing the investment risks of a project.

Short-term power forecast. The increase in wind energy share to the global energy mix and the liberalized nature of current electricity markets require of short-term (i.e. few days ahead) wind power forecasts. In particular, forecasts are oriented to efficiently dispatch wind farm power production into the grid allowing the transmission system operator to manage the power sources. At present, a battery of methodologies (e.g. statistical downscaling, subrogate models, machine learning, etc.) is used by industry to correlate mesoscale Numerical Weather Prediction (NWP) model forecasts and expected wind farm power production. Exascale computing is foreseen to allow operational implementation of more realistic dynamical downscaling approaches, in which the whole meso-to-micro model chain runs concurrently to cover all the relevant spatial scales.

Design of wind turbines. Next generation turbines are expected to be the most significant technology innovations for off-shore wind exploitation. These imply larger rotors and a range of innovations in foundations. Today, the largest offshore wind turbine deployed on a commercial-scale wind already exceeds 150 m in rotor diameter and 8 MW. The commercialization of 10 and 15 MW turbines is expected by early 2020s and 2030s respectively. These sizes pose several challenges to manufacturers and will likely involve modular blade technologies. Optimal, efficient and reliable design of turbine components requires also of HPC, involving complex Fluid-Structure Interaction (FSI) simulations at the edge of Exascale. From the computational point of view this new wind turbines present challenges given its high Reynolds numbers and the use of thicker airfoils (i.e. the stall regime can be easily achieved, fluttering, etc.). Being LES the optimal methodology to tackle these complex physics a computational challenge arises, since the basic premise of LES that energy-containing and dynamically-important eddies must be resolved everywhere in the domain is hard to meet in the near-wall region, as the stress-producing eddies become progressively smaller toward the wall. In fact, the Reynolds number characterizing the ratio of the boundary-layer thickness to the size of such small near-wall eddies is of the order of $Re_{tau} = O(10^4)$ for next generation wind turbines, corresponding to the chord Reynolds number of Re_c =10M-20M typical of 15 MW wind turbine. The number of elements required in wall-resolved LES (WRLES) of a wind turbine is then estimated to be on the order of half a trillion [13]. Combined with around 5 million time steps integration required in wing simulations and $O(10^2)$ floating-point operations per time step and per element, the number of total floating-point operations would approach $O(10^{22})$ per one simulation. Assuming a linear scaling code, this would require a 3 orders of magnitude more computational resources than is needed with wall-modeled LES (WMLES) [16]. A typical WMLES run requires 2 MCPUh [15] in a computer with 1 Petaflops and 50.000 cores. For WRLES 2.000 MCPUh would be needed, this is 1.666 days on the full Petascale computer. In an Exascale machine this would translate into 10 days with the full computer. A WMLES simulation could be performed in only 15 minutes in an Exascale machine. Inclusion of FSI, noise prediction and UQ clearly puts this type of assessment on the Exascale domain [14].

4. HPC in Biogas Combustion industry

Reducing fossil fuel consumption and CO2 emissions have become a priority at the international level, as agreed in the Paris Agreement on December 2015 [17]. The global energy demand is expected to experience a large growth over the 28-year period from 2012 to 2040 and the transportation and power sectors being two of the largest consumers. In particular, the transportation sector represents about 25% of the share and has a growth rate of 1.4%/year [18]. In the case of road transport, increased consumption of low-carbon fuels and deployment of hybrid or electric vehicles present viable alternatives, although the majority of vehicles operating today still use conventional fuels associated with internal combustion engines (ICs). A similar situation is present in the aero sector, fastest growing transport sector with growth rate of 1.4%/year [18], where aero-derivative gas turbines (GTs) keep improving to accommodate for demands in efficiency and pollutant emission. On the other hand, in the power generation industry, the situation is also similar. Advances on alternative energy supply systems such as wind turbines, solar photovoltaic or solar concentration technologies are attractive as a real alternative forcing traditional systems based on thermal power plants to be more efficient introducing new challenges in the sector. From the total energy sources, fossil fuels are still the main portion and estimations anticipate that liquid fuels, natural gas, and coal will account for 78% of total world energy consumption by 2040 [18]. The conversion of energy from fossil fuels to power is achieved by combustion and some projections indicate that the combustion of liquid fuels will still dominate transportation and power generation industries for the next 50 years and, even longer [19]. In this scenario, further understanding of the physics and chemistry of the combustion process is fundamental to achieving improvements in fuel efficiency, reducing greenhouse gas emissions and pollutants, while transitioning to alternative fuels and greener technologies for power generation and transportation [19].

The use of advance numerical simulations has enabled to make important contributions for increasing cycle efficiency, reduction of pollutant emissions, and use of alternative fuels in practical applications [20][22]. Numerical tools are employed routinely every day to design and optimize combustion systems by aircraft, automotive or GT manufacturers. Indeed, the increase in computing power over the last years has led to transition from RANS to large-eddy simulations (LES) in the design and development process reducing the uncertainty of the models and increasing the reliability of the numerical predictions [23]. In this new era, when future exascale architectures become available, the use of LES or even DNS could transition to make a more important role on better understanding the performance of combustion systems in more complex conditions. The full characterization of practical combustion systems is a complex task and brings many challenges associated to different disciplines of engineering, chemistry, physics, computer scientist and mathematics, among others. In particular, one of the most important parts is the modelling of the reacting spray under realistic conditions, as it includes the interaction of complex physical phenomena as high-pressure liquid fuel injection, atomization, vaporization, fuel/air mixing and combustion. This interaction is not well understood and plays a major role in the overall performance of the system. With the use of future exascale architectures, the CFD codes will have to adapt to run efficiently on these machines with new algorithms and numerical methods, but will have the full potential of performing exaFLOPS operations.

One of the most demanding part of reacting spray computations, is to account for the detailed chemical kinetics of the flames. In practice, traditional hydrocarbon fuels require of the order of hundred species and more than thousands of reactions to characterize the combustion process at engine-like conditions [19][21]. In this type of problems, the resolution of the Navier-Stokes equations becomes negligible compared the chemistry calculation, and the effort is dedicated to simplify the chemistry problem. These chemical kinetics schemes become even larger with complex surrogates or blending of fuels, so this holds the investigation of alternative fuels and reduces the applicability of numerical simulations in this context [19][21]. The correct prediction of the formation and destruction of species and radicals not only requires small time steps, but also high resolution in the computational domain, as some species can have short and large life times. In practice, the emissions are controlled by slow and fast reactions, i.e. NOx is governed by low time scales, but CO coming from the partial oxidation of CO_2 is characterized by fast time scales, so both slow and fast processes are important and need to be taken into account. This means the numerical simulations will have to be run for long physical times using fine grids and small time steps. In addition, this high requirements in terms of spatial and temporal resolution is even more demanding in the case of systems operated at moderate or high pressure. Under these conditions, the reacting layers are smaller and the computational cost of the simulations increases dramatically. There are strategies to simplify the chemistry problem, like chemical reduction, chemistry tabulation, transported PDF models or conditional closures, but those are only valid for well-known regimes and conditions, and their applicability to general problems can be questionable [24][26].

Another important limitation of the current modelling technologies is associated to the atomization process of the fuel. The formation of the spray is a complex physical phenomenon characterized by the break-up process of the liquid film into droplets and its subsequent atomization stages until the droplets are vaporized achieving the gas phase. The atomization process can be divided into primary and secondary breakup with different physical dynamics and are controlled by droplet collisions, coalescence, heat transfer, phase change along with turbulent interactions between phases [27][46]. This is especially complex at the conditions of the operation of the engines, which usually have high Reynolds and Weber numbers conditions with liquid fuel injection at high speed on small nozzle diameters. There are many approaches to solve these problems, going from Lagrangian droplet methods to fully Eulerian approaches [28][29], but due to the complexity of the problem and the large resources requirements for problems of practical interest, this is out of the scope with the present computational technologies. Complex physical phenomena yet to be understood occur on the sprays at supercritical conditions, also demanding more accurate numerical simulations that can elucidate the mechanisms behind this physical process [30]. An additional problem related to the development of full engine simulations, is the characterization of the engine cooling. This is frequently developed by the existence of cooling holes in jet engines to increase the convective heat transfer or film cooling in the case of IC engines to create a film along the chamber walls protecting the metal part and reducing the local temperature of the combustion chamber. The modelling of these physical processes requires appropriate resolution in the computational domain to fully characterize the cooling jets or an appropriate modelling strategy to account for the multiphase problem at the film when using oil for cooling [31]. These are particularly demanding problems that are not feasibility with the today's modelling strategies and current computational resources at conditions of practical interest.

The third fundamental and yet unresolved fluid mechanics problem in our century is the turbulence. The effects of turbulence on these two fundamental processes, spray atomization and combustion are still to be fully understood, but it is known to have strong implications in the thermochemical and hydrodynamic processes of the spray flames. The interaction of turbulence with the reacting layer affects the structure of the flames and can have a large impact on the chemical structure, affecting the autoignition process and the flow dynamics [25][26]. Additionally to this effect, the boundary layer requirements in practical combustion systems is usually a limiting factor on full engine simulations, since the Reynolds numbers of the flow along with the resolution required for the breakup and reacting layer leads to unpractical number of computing cells with current computing technologies. Furthermore, if surface roughness wants to be taken into account, the resolution requirements for the simulations increase exponentially. This can be the situation where the predictions of the acoustics, shock waves or the heat transfer coefficients are critical for the application [32][33]. This situation, also stressed in conditions of reacting multiphase flows over complex geometries, makes the modelling of these systems unaffordable for operating conditions of practical interest.

On top of these challenges, there exist different sources of model uncertainties inherently in LES simulations. The main sources of error usually come from boundary conditions, physical models or chemical kinetics, but in general, it is difficult to separate them [34]. The use of uncertainty quantification (UQ) methods can be applied to evaluate deficiencies on these sources and becomes a powerful tool for model assessment and validation. These uncertainties can have an important impact on model predictions and must be carefully considered when compare to experimental data or when given for system design or for emissions control [35]. However, the application of UQ in the context of LES still deserves further attention and demands for large resources as LES is inherently unsteady and requires statistically converged data to obtain mean values.

In summary, the exa-scale era will provide a significant platform for making important contributions in the power and transportation sectors towards more efficient, more flexible and with low emissions systems with direct impact on public health and climate change. With the use of these new architectures and with the corresponding advances on the codes to fully exploit this new chip capabilities, the challenges on propulsion technologies and power generation systems will be conveniently addressed allowing a transition to a greener and more advance combustion systems based on alternative fuels combined with renewable energy technologies that can operate jointly.

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