

In-Situ Visualization in Fluid Mechanics using Open-Source tools: integration of Catalyst into *Code_Saturne*

Lorendeau Benjamin, Ribés Alejandro, Fournier Yvan and Jomier Julien

Abstract The volume of data produced by numerical simulations performed on high performance computers is becoming increasingly large. The visualization of these large post-generated volumes of data is currently a bottleneck for the realization of engineering and physics studies in industrial environments. In this context, Catalyst is a prototype in-situ visualization library developed by Kitware to help reduce the data post-treatment overhead. On the other side, *Code_Saturne* is a Computational Fluid Dynamics code used at EDF, one of the biggest electricity producers in Europe, for its large scale simulations. In this chapter we present a study case where Catalyst is integrated into *Code_Saturne*. We evaluate the feasibility and performance of this integration by running several use cases in one of our corporate supercomputers.

1 Introduction

Computational Fluid Dynamics (CFD) is a fundamental step for the study and optimization of electricity production. Indeed, current power plants use water as a mean of convective heat transfer. Consequently, the simulation and visualization of fluid dynamics phenomena is of great importance for the energy industry. Electricité de France (EDF), being one of the biggest

Lorendeau Benjamin
EDF R&D, Clamart, France, e-mail: benjamin.lorendeau@gmail.com

Ribés Alejandro
EDF R&D, Clamart, France e-mail: alejandro.ribes@edf.fr

Fournier Yvan
EDF R&D, Chatou, France e-mail: yvan.fournier@edf.fr

Jomier Julien
Kitware, Villeurbanne, France e-mail: julien.jomier@kitware.com

electricity producer in Europe, has developed for the past 15 years an open source CFD code named *Code_Saturne*, allowing for the solution of very large models [14]. EDF has several supercomputers that regularly run this code in order to perform analysis involving large amounts of data. In this context, the postprocessing and visualization of data becomes a critical point.

In the past, studies and improvements in scientific simulation have been mainly focused on the solver, due to being the most cycle-consuming part in the simulation process. Thus, visualization has been traditionally run sequentially on a smaller computer and at the very end of the solver computation. At the time, this was easily explained by the small need for both memory and computation resources in most of the visualization cases. Nevertheless, with the increase of our computational capabilities, we tend to use and generate much more data than what we were used to. Thus, as the scale of CFD simulation problems is getting wider, specific issues are emerging related to input/output efficiency. In particular, data generated during the solver computation and used for the visualization are the source of a worrisome overhead. Even worse, some researchers are starting to spend more time for writing and reading data than for running solvers and visualizations [12]. This new trend is asking us to design new I/O strategies and consider visualization as a part of our high-performance simulation systems.

Most fluid dynamic engineers at EDF R&D are currently visualizing lower temporal and spatial resolution versions of their simulations in order to avoid I/O issues when large quantities of data are involved. We decided to address the subject of coprocessing and *in-situ* visualization which has been proved to be an effective solution against the current limitations of this problem [6], [13]. Our aim is to provide our engineers with an operational research-oriented tool in a mid-term basis. For this, we choose to evaluate Catalyst as an industrial tool for performing In-Situ visualization. Catalyst, developed by Kitware, is a library for Paraview that implements the coprocessing, by defining the visualization process through Paraview and exploiting the VTK's parallel algorithms for the processing of the simulation data [9].

In this article, we propose a study upon the effectiveness and scalability of a prototype implementation of the coprocessing in an industrial case based on the coupling of *Code_Saturne* with Catalyst. In section 2 we discuss works related to recent visualization *in-situ* systems. We will then introduce in section 3 *Code_Saturne*, the CFD code developed at EDF R&D. In section 4 we present our integration of Catalyst into *Code_Saturne* and how it is used by the users in the framework of fluid dynamic simulations. Section 5 describes our use case and presents results on one of our corporate clusters. Finally, section 6 presents our analysis of the results and describes our on-going and future work.

2 Related Work

The size of generated data has become an important subject in high performance computing, due to the need of a better input/output efficiency in our computing system. To answer this problem, several visualization systems has been created. We can distinguish two main approaches in recent solutions. The first one is to integrate a specific *in-situ* visualization directly to our simulation code. Such an approach proved to be an efficient way to provide coprocessing for a given simulation plus visualization system as it is the case in the hurricane prediction [7] and earthquake [13] simulation systems. This method has been proved to lead to good performances but is limited to a specific implementation. Thus it does not respond to our needs.

The second approach is to provide a general postprocessing framework letting the simulation and the visualization code communicate together. EPSN which is a general coupling system, allows for the connection of M simulation nodes to N visualization nodes through a network [8]. This solution is a loosely coupled approach, requiring separate resources and data transfer through the network. This approach presents the advantage of not overloading the nodes used for computation. Thus the visualization code does not interfere with the execution of the simulation. Based on the same approach, a ParaView plugin named ICARUS [3] exists. It differs from EPSN in design by lower requirements as it only needs the use of a single HDF5 library and file driver extension. Such solutions offer tools for researchers to interact with their simulations by allowing them, first to monitor their current states but also to modify some parameters of the remaining simulation steps. Those computational steering solutions as well as the RealityGrid project [4] focus on interactivity with simulation whereas our main objective is to provide *in-situ* visualization operations to researchers while minimizing input/output overhead and disk space use.

Both built upon the well known parallel visualization algorithms library VTK, VisIt [5] and ParaView [10] provide through libsim [15] and Catalyst [9] the possibility to coprocess simulation data. Those *in-situ* solutions are tightly coupled and while they limit potential interactions with the running simulation, they also highly reduce the need of network data transfer. Thus, it contributes at circumventing the inefficiency of high performance computing input/output systems. Those solutions takes their benefits from directly accessing the simulation memory to perform visualization treatments by simply asking a pointer to the available data. One major drawback of this approach is the necessity to provide an understandable data layout to those libraries. Moreover, as this type of solution often gains from computing predetermined visualization tasks, it is not suited for results exploration. As building a steering solution for Code_Saturne is out of the scope of this case study, we do not consider these drawbacks as a limitation.

After evaluating the performances offered by Kitware [9], we choose Catalyst as our coprocessing library for our case study as it answers our visual-

ization needs while focusing on the reduce of data amount use. Ultimately, Kitware is still actively developing Catalyst, and we are optimistic that more services allowing the interactions with the running simulation will soon be available.

3 *Code_Saturne*: A Computational Fluid Dynamics code

Code_Saturne is a computational fluid dynamics software designed to solve the Navier-Stokes equations in the cases of 2D, 2D axisymmetric or 3D flows. Development started in 1997, with a first release in 2000, and the code has been released as free software under a GPL licence since 2007. Its main module is designed for the simulation of flows which may be steady or unsteady, laminar or turbulent, incompressible or potentially dilatable, isothermal or not. Scalars and turbulent fluctuations of scalars can be taken into account. The code includes specific modules, referred to as “specific physical models”, for the treatment of atmospheric flows, Lagrangian particle tracking, semi-transparent radiative transfer, gas combustion, pulverised coal combustion, electricity effects (Joule effect and electric arcs) and compressible flows. *Code_Saturne* relies on a finite volume discretisation and allows the use of various mesh types which may be hybrid (containing several kinds of elements) and may have structural non-conformities (hanging nodes). The parallelization is based on standard spatial partitioning with ghost cells that facilitate data passing between adjacent cells lying across the boundaries of disconnected parts using the Message Passing Interface. More technical details are presented in [1] and [2], and many resources are available at <http://www.code-saturne.org>. *Code_Saturne* is also used as a base for the NEPTUNE_CFD code, specialized in multiphase flows, and which uses a different time stepping scheme, but mostly the same volume discretization scheme.

As *Code_Saturne* is used for industrial cases involving complex flows, with turbulence modeling requiring sufficiently fine resolution, large meshes are often needed. In 2000, the largest meshes used for actual studies were around 1 500 000 cells; today, they have reached up to 350 000 000 million cells. More common studies use meshes about 10 times smaller than that. Meshes up to 3.2 billion cells have been tested for a few time steps, to ensure the code’s internal mechanisms work well at scale.

Code_Saturne focuses on the solver, and its uses requires external tools for the major part of the meshing and visualisation tasks, though the code itself offers major preprocessing features to make these easier, such as parallel joining of independently-built and read submeshes (whether conforming or not), and user-definable postprocessing functions. Many input mesh and visualisation output formats are supported (including the EDF and CEA MED format, and the standardized CGNS format).

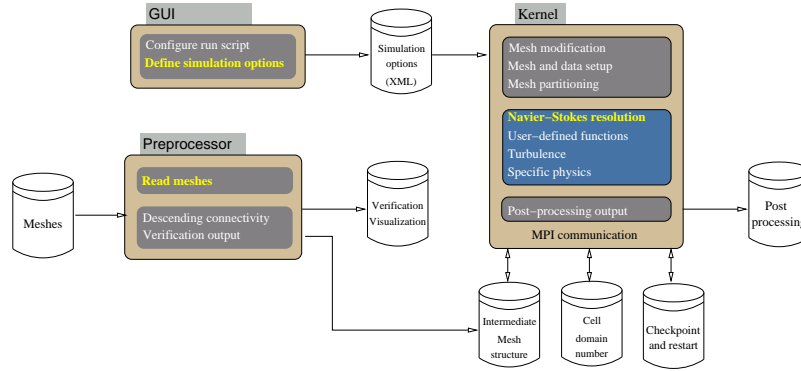


Fig. 1: *Code_Saturne* toolchain components.

The number of separate executable tools is quite reduced, with a few interactive tools and associated commands designed for data setup.

To make the use of HPC as seamless as possible, without multiplying the number of tools or requiring complex libraries or dependencies, mesh, checkpoint/restart, and postprocessing output files are partitioning independent: in addition to the connectivity of each local mesh, which is described with a local numbering, global ids are also maintained, for import and export purposes, and for ghost cell to local cell matching. Multiple ranks participate in reading and writing files using MPI-IO.

Typically, computational resource requirements are primarily determined either by the time to solution, or the size of the model. For time to solution, the number of cores may be selected in order to solve the problem in a given time. In practice, optimal performance is often obtained in a range of 30 000 to 60 000 cells per rank on a typical HPC cluster (this being the best compromise between communication latency and cache behavior). On machines with very good network/compute performance ratios, such as IBM Blue Genes or Cray X series, this range may be a bit wider.

4 Using Catalyst

Catalyst is the coprocessing library of ParaView. It has been designed to be tightly coupled with simulation codes to perform in situ analysis at run time. Catalyst leverages the Visualization Toolkit (VTK) for scalable data analysis and visualization. Furthermore, it can be coupled with the ParaView In Situ Analysis framework to perform run-time visualization of data extracts and steering of the data analysis pipeline.

Catalyst provides two sets of tools: one for simulation users and one for simulation developers. For simulation users, it is possible to create a coprocessing pipeline using two different methods. The first method does not require any

knowledge of ParaView and relies on pre-generated scripts. These predefined scripts can be written in C++ or Python and are, usually, expected to run without any configuration options. The second method uses the ParaView interface to generate a coprocessing script from scratch and intuitively adjust its parameters as needed. This method is similar to using ParaView interactively to setup desired post-processing pipelines. The goal of these pipelines is to extract post-processed information during the simulation run. Ideally one should start with a representative dataset from the simulation. It is also possible to modify directly the generated Python's scripts which have been previously created using ParaView. However, this would require a knowledge of the ParaView Python API.

For simulation developers, Catalyst provides the tools to create an adaptor between the simulation code and the visualization pipeline. The adaptor binds the simulation code and Catalyst so that both the functions of the simulation code and the general-purpose application programming interface (API) of Catalyst can be accessed. As Catalyst itself is independent of the simulation code, only the adaptor has to be developed by the designers of the solver. This flexibility is critical in order to successfully integrate external code into complex simulations usually running with different languages and packages. Catalyst is also easily extensible so that users can deploy new analysis and visualization techniques to existing coprocessing installations. Catalyst provides all the communication and synchronization routine and the pipeline mechanics necessary for coprocessing. Catalyst also provides powerful data processing capabilities through VTK filters as well as many writers and support for compositing and rendering.

Catalyst has also been developed with features to address limitations that come with pre-configuring a pipeline, but there may still be some unexpected data in the arbitrary simulation. To address these situations, the pipeline must be adjusted interactively. The Catalyst library can leverage ParaView's client server mechanism to allow an interactive ParaView client to connect to a server running inside an in situ pipeline. ParaView can then read from a Catalyst data source like it reads from a file. This offers to construct/modify a pipeline interactively in the ParaView client via this live data source. Additionally, by enabling the client-server architecture in the Catalyst library, some or all of the data analysis and visualization pipeline can offload, if desired, to a separate machine, e.g., a smaller visualization cluster with specialized graphics hardware.

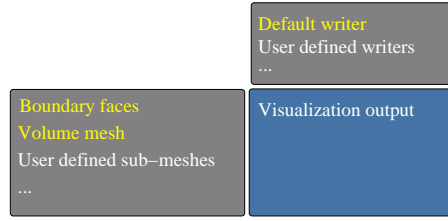


Fig. 3: *Code_Saturne* postprocessing output subsystem.

A postprocessing mesh may be any sub-mesh of the computation mesh (or even a separate auxiliary mesh in some cases), which may optionally be re-defined over time steps, while a writer is a combination of the selection of an output format (such as EnSight gold, MED, or CGNS), an output frequency, sub-directory and file name prefix, and additional metadata specifying for example whether associated meshes will be fixed or time varying (if the selected format supports it). To each postprocessing *mesh* may be associated a list of *writers* among those defined (an empty list meaning no output). By default, the global volume mesh and boundary *meshes* are associated to a main *writer*, whose default settings include the EnSight gold format and output at the last time step only. The user may modify those settings and associations, as well as define additional *meshes* and *writers*, both using the GUI and user functions (useful for more advanced cases and finer control). Using this system, output at different mesh formats, with different frequencies, and possibly different variables may be generated simultaneously, allowing fine tuning depending on the intended usage.

Code_Saturne suggests a clear separation of tasks best handled by the code or those handled by external tools. For example, although computing a gradient may be handled directly by visualization tools, it is best done in the user-defined output of the code itself, to ensure it is done in a manner consistent with the discretization, and exploiting the knowledge of prescribed boundary conditions. On the other hand, postprocessing *meshes* are defined as subsets of the computational mesh, but generation of clips and slices are not handled by the code, as it is expected visualization tools may handle those geometric operations. Both may be combined: for example, a volume sub-mesh involving cells around a clip plane may be output by *Code_Saturne*, reducing the data that needs to be handled by a visualization tool to produce that clip.

4.1.2 Adaptor implementation

When embedding Catalyst there is always a non-zero cost in terms of time, memory and the number of processors. Naively, one could simply address these issues by simply requesting a greater number of processors, but in most cases this simply is not possible or practical. Therefore, great care must be taken in the construction of the adaptors. If memory is limited, the adaptor

either uses complicated pointer manipulation or uses a smaller region of memory. If memory is not limited, then deep copy of the simulation data structures into a VTK data object doubles the resident memory, but also creates a CPU cost involved with copying data. The overriding overhead issue in embedding ParaView Catalyst in a simulation code is the memory management in an adaptor translating data structures in the running simulation.

In order to coprocess the simulation data, Catalyst must be provided with the data formatted to the VTK data object structure. To accomplish this, several solutions are possible, essentially depending on the format used for the data of the simulation code. In the case when the format of the simulation code is similar to VTK and, moreover, the simulation data can be shared at any time, then it is possible to feed Catalyst with a direct pointer to the simulation memory. This option is indeed preferred, when possible, as it allows to decrease the memory footprint. Another option is to fully or partially copy the data from the simulation into a VTK object, and then send this object to Catalyst.

As users of *Code_Saturne* are provided with several output formats and as the data structure in our simulation differs from the VTK data object structure, feeding Catalyst with a direct pointer to the simulation memory is not possible. Thus, in this configuration data is copied from the simulation into a VTK data object. In fact, we allocate a `vtkDoubleArray` data structure to store our data for Catalyst. Furthermore, we provide a pointer of this VTK data structure to *Code_Saturne* so it can transform its simulation data and then fill the VTK data object.

The memory cost increase of our solution can be alleviated by using more machines. The CPU cost of the copy is in a range similar to the one needed when adapting simulation data to a specific output format. This cost is largely affordable comparatively to the time to write data to disk when storing time step specific outputs.

4.1.3 Pipeline configuration

From the point of view of an engineer performing a fluid mechanics simulation using *Code_Saturne*, the workflow of a coprocessing-simulation is 1) to define a ParaView pipeline describing what the user wants to study and 2) to run the simulation. Since users are already familiar with fluid mechanics simulations, defining the pipeline for the coprocessing remains the main sticking point. Thus this new process should be done in an efficient way and should not become a cumbersome bottleneck. This point is of great importance, especially in an industrial environment like ours.

As we have explained in the previous section, the definition of a Catalyst pipeline can be achieved either programmatically or via the ParaView interface. In our industrial context, the former was considered too complicated and time consuming for the end user, especially when setting camera pa-

rameters is needed, as no visualization feedback is provided. Therefore, the Catalyst pipeline has been created using the ParaView user’s interface. This solution appears to be much easier as one can simply interact with ParaView in the same way he/she uses to when visualizing the results a posteriori. This solution is also easier to deploy with ParaView using the its companion coprocessing plugin.

Indeed, using ParaView to define the coprocessing requires a representative input dataset. One could use the available resources on a large cluster in order to setup the pipeline. However we chose to provide a simplified or under-sampled version of the large geometry to define the pipeline. In fact, this strategy is possible in ParaView but some characteristics of the initial geometry must be present in its simplified version; more importantly the name of the data fields must remain the same, as they are part of the definition of the pipeline.

The generation of the coprocessing pipeline implies several steps. First of all, the users start with a CAD (Computer Aided Design) version of the geometry which is parametrized. This parametric representation can generate meshes at different resolution levels. In our case, this is performed inside the open-source SALOME [11] platform for numerical simulation.

We then generate two different meshes, one at high resolution (up to 204M hexahedrals in the current use cases) that will be used for the CFD simulation and one with a lower resolution to define the pipeline (700 000 hexahedrals in our use cases). The lowest resolution mesh is fed into *Code_Saturne* to perform a short simulation. This allows ParaView to obtain a representation containing not only the geometry but also the result fields. This is the data that is then used to define the pipeline. The different processing pipelines are presented next.

5 Results

5.1 Required User Interactions for Coprocessing

Before presenting our results we briefly describe how the user interactions was performed. The following steps were necessary in order to use the developed coprocessing technology:

- 1) The user generates a “light version” of the mesh. This step has already been discussed in section 4.1.2. Indeed, the user possess a CAD (Computer Aided Design) version of the geometry that is parametrized, it is then possible to obtain meshes at different spatial resolutions. A “light mesh” of small size in memory and representative of the CAD geometry is obtained. Figure 4a represents the “light version” of the mesh used in our experiments.

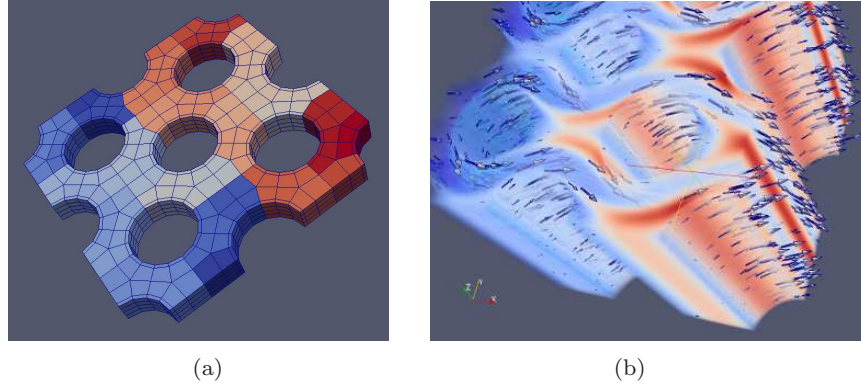


Fig. 4: (a) original geometry of our use case
(b) a final coprocessed picture of our simulation

2) We run a short simulation (normally just a few seconds on a local machine) on the “light mesh”. This obtains the informations about the result fields we need to create a visualisation pipeline in ParaView (e.g. temperature, pressure, velocity). We could then say that we obtain an “augmented light mesh”.

3) The mesh and the fields obtained at the end of step 2 are read in ParaView and the user can define her/his visualisation pipeline. At the end of this step a simple click in the ParaView interface will create a Python file that programmatically defines the visualisation operations that will be performed *in-situ*.

4) Finally the real simulation is ran using a full resolution size mesh. The coprocessing part of the simulation reads the python script containing the definition of the visualisation pipeline. This step is expected to be time-consuming.

5.2 Use Cases

Our simulations have been run on Ivanoe, an EDF corporate supercomputer, composed of 1382 nodes, each node having 12 cores for a total of 16584 cores. In these simulations we associate one process by core and we use from 720 cores up to 3600 cores. We include two use cases that were run on this supercomputer. The choice of the cases is motivated by two main factors: the size of the mesh and the complexity of the visualization pipeline. Let us define in more detail why these two factors:

1) Mesh size. We chose to use two meshes representing the same geometry but at different resolutions, one made of 51M hexahedral elements and another

of 204M hexahedrals. In our industrial environment at EDF most simulation engineers use meshes composed by less than 51M of element, then we choose this mesh size to be representative of the work performed by an average engineer in his work routine. Furthermore, a 51M elements mesh more than doubles the size used in the results presented in [9] for the PHASTA adaptor. On the other side, when researcher oriented simulations are performed at EDF, they currently contain around 200M elements. We choose then this size as a research oriented or “heavy mesh” kind of simulation.

2) Pipeline complexity. We define two pipelines aimed to be representative of two different situations: users just performing simple and light visualization operations (mainly some slices in a volume) and another using very time-consuming visualization tasks (mainly performing a volume rendering).

Table 1: Description of our two use cases.

USE CASES SUM UP			
NAME	SIZE	PIPELINE	FIGURES
<i>CASE_A</i>	51M hexahedrals, industrial size case	heavy : volume rendering, celldatatopointdata and glyphs	3,4,5
<i>CASE_B</i>	204M hexahedrals, research size case	light : 9 slices, celldatatopointdata	6,7,8

In the following we name our uses cases: *CASE_A*, use case using an average mesh size of 51M hexahedrals and a visualization pipeline including volume rendering which aims to be very time-consuming. *CASE_B*, our second use case, contains a light visualization pipeline simply performing some slices but on a large mesh of 204M hexahedrals.

Table 1 summarizes the composition of these use cases. In all our use cases we run a simulation consisting in a fluid with physical properties identical to water passing through the mesh. Then the output is generated at each step, for a total of 10 coprocessed visualization images.

5.3 Results

Figure 4b presents an image obtained from one of our *in-situ* simulations with *CASE_A*. We see the flux of water moving around the vertical cylinders, the glyphs being attached to the velocity vectorial field. The color of the volume rendering represents the turbulent viscosity of the fluid. Figure 5a shows two graphs of *CASE_A*: in red the execution time versus the number of cores, in blue the execution time without the coprocessing overload. We are satisfied by this overload that is contained between 20 and 30% of the total execution time. It looks like this overload is reducing with the increase in

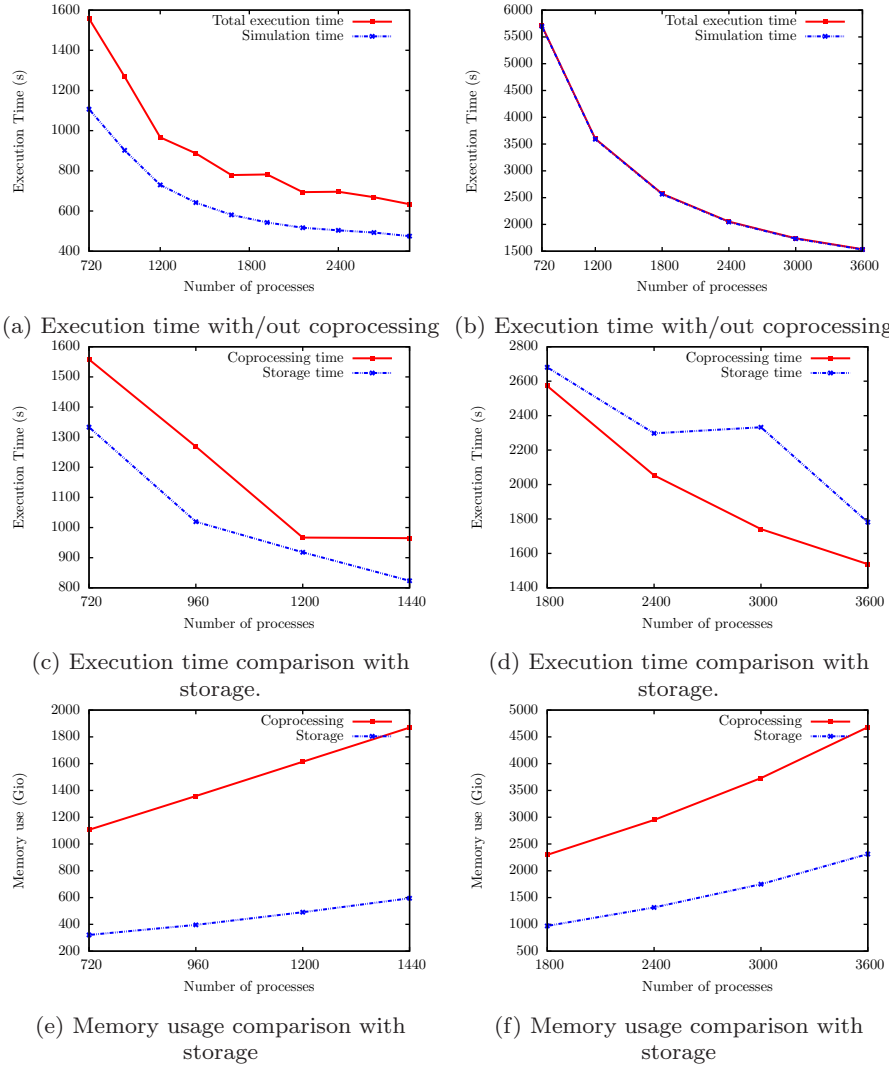


Fig. 5: CASE_A (left) and CASE_B (right) results

number of cores. Figure 5b shows the exact same behavior but with *CASE_B*. Both graphs are difficult to distinguish as the time needed for coprocessing is circumscribed between 6 and 10 seconds, the overload is lesser than one percent of the total execution time.

We also decided to compare the Catalyst overhead with a non VTK based storage strategy that performs no visualization operations. Figure 5c and 5d, show the comparison of the global execution time with Catalyst coprocessing versus the simple Ensight Gold format storage. Figure 5c presents our im-

plementation results with *CASE_A*. This compares positively for Catalyst as the overhead is approximately 10% and looks decreasing when the number of cores increase. Figure 5d presents our results for *CASE_B*. Here we can see the potential of Catalyst when lighter and more relevant visualization tasks are processed. Indeed, there is no more overhead as we gain an average of 10% of execution time while freeing ourselves from storage issues (indeed, we evaluate the execution time peak of 3000 processes as a result of concurrent accesses on our supercomputer storage disks). To emphasize this, table 2 shows how much data each solution generates, namely a basic storage in Enight Gold format versus our coprocessing implementation using Catalyst. These informations are those of our *CASE_B* when performing a 10 steps simulation. Both size are expected to grow proportionally to the size of the mesh input, and the number of steps. Therefore, we expect the gain provided by the use of coprocessing to be increasingly interesting when moving forward in use case size.

Finally, we also show the total memory use when running *in-situ* visualization compared to writing simulation results in Enight Gold format in figure 5e and 5f. We observe that memory consumption is increased by an approximate factor varying from 2 to 3. This can be explained by both our first naive memory management approach and also by a natural increase in memory consumption when visualization operations are to be performed. Indeed, our memory management implies a consumption increased by more than 2, as we need to translate data for Catalyst but still need the former data to pursue our simulation. Finally it may also be taken into account the actual memory consumption of the chosen visualization tasks.

Table 2: *CASE_B* comparison between the size of processed results and simple storage. The simulation was run on 10 steps, with 10 pictures coprocessed.

*PROCESSING SIZE COMPARISON	
STORAGE	COPROCESSING
57Gio	1,3Mio

6 Conclusion

We have successfully integrated Catalyst into Code_Saturne (a computational fluid dynamics code developed at EDF R&D). After testing the prototype in our corporate supercomputer Ivanoe, we find Catalyst to be a relevant solution to provide Code_Saturne users with visualization coprocessing. Catalyst proved to allow a simple and fast implementation of an adaptor. We use D3 (a filter originally performing a redistribution of the data among MPI pro-

cesses) as a ghost cell handler. We feel that the code responsible for the ghost cells management in D3 could be integrated directly into ParaView/Catalyst since applying D3 can be time consuming.

Our preliminary results are based on a 51M and a 204M elements mesh, which is above the average size case used by EDF engineers in our industrial environment. We plan to perform simulation on at least 400M elements meshes in the near future. We have also performed simulation up to 300 nodes and are currently planning not using more in this cluster. This is due to the typical simulation node size being around 150 nodes for our engineers. We also plan to work on another of our corporate supercomputers, an IBM BG/Q with 65k cores. In that case, we will test on a much bigger number of cores. The increase of memory use found in the results section indicates that memory optimizations are to be performed before running on the IBM BG/Q. We did not in this study perform any delicate memory tweaking in order to reduce the memory consumption. We are currently working on this point, experimenting new VTK *in-situ* data structures that may highly reduce this overhead.

We are mostly satisfied with the integration of Catalyst in Code_Saturne. Our first version of our integration will be most probably released in September 2013 as part of a new version of this open-source software.

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