ExaQUte

Exascale Quantification of Uncertainties for Technology and Science Simulation

D8.4 Report on dissemination activities

Document information table

Contract number:	800898
Project acronym:	ExaQUte
Project Coordinator:	CIMNE
Document Responsible Partner:	CIMNE
Deliverable Type:	Report
Dissemination Level:	PUblic
Related WP & Task:	WP 8 Task 8.1
Status:	Final version

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No **800898**

Prepared by:				
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Change Log

Versions	Modifications	Comments
1	Very first version	First version with structure for partners to include their input
2	Add partners inputs	Include partners information
3- Final	Final version	Definitive

Approval

Approved by:				
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Announcement

In Deliverable D8.1 (M18) we presented a first version of the Dissemination Plan for the ExaQUte project. The present document, prepared during the 2nd (and last) review period of the project, represents the updated version of the Dissemination Plan of ExaQUte, and therefore builds on the aforementioned deliverable. This document, thus, focuses on the new activities that have been undertaken from M18 to M42 regarding the dissemination activities.

It should be mentioned that the pandemic situation that started in Mach 2020 (actually, in Spain we were sent to confine to our houses the day after the celebration of the First Review meeting of this project) has had an impact in our life, and in our project, particularly in the dissemination actions.

The lockdown made impossible most of the activities related to dissemination (travels, conferences, consortium meetings…). But we reinvented our work and found different ways to do things and fulfil pour obligations. Still, in this deliverable, you will find indeed a difference between the type of action that we carried on up to M18 and our activities after M18.

1 Aim of the dissemination Plan in ExaQUte

Dissemination and exploitation of an H2020 project involves various activities that **will bring research outcomes to the attention of as many relevant people as possible**. Communication about European research projects should aim to demonstrate the ways in which research is contributing to Europe's leadership in innovation, science and technology. At the same time, it is a useful tool to account for public spending, by providing tangible proof that a collaborative research EU-funded project contributes to relevant results solving scientific and societal challenges.

Dissemination activities in ExaQUte are included in WP8 and are designed through a dissemination plan to be prepared during the first months of the project. The dissemination phase will start at the on-set of the project and will evolve as the different milestones are achieved. All partners will collaborate in the dissemination of the results among the different audiences (academic, industrial, administration, general public). All these activities will be agreed by the consortium.

The project will plan activities adequately resourced devoted to dissemination for specialized constituencies and general public, in particular for awareness and educational purposes. The dissemination plan deliverable has to consider adequate messages about the objectives of the project and its societal and economic impact.

The tools to be used should include web-based communication, press releases, brochures, multimedia material, use of social media etc. The dissemination material should be regularly updated to provide the latest version of the project status and objectives. Electronic and/or paper versions of this 'dissemination material' will be made available to the Project Officer beforehand for consultation and upon its final release.

The following table summarizes some of the reasons why dissemination activities are important for successful completion of ExaQUte.

Table 1*Importance of dissemination actions*

WHY ARE DISSEMINATION ACTIVITIES IMPORTANT IN ExaQUte?
To **make visible** scientific progress
To **get feedback** for future improvements and directions, define priorities attending to end-users and other research works
To **share knowledge** and results and take better profit from third party's results
To **attract industrial partners and investment**
To **match common needs with potential solutions**
To have better knowledge of the **potential market**

To maintain and **improve international reputation**
To **facilitate exploitation** through licensees
To **increase market demand** of extreme-scale applications (surveys about trends, etc.)
To ensure **continuity of the research** line (importance in a timeline and within an international context)

It is important to note that CIMNE has its own in-house specialized publication and congresses Departments, formed by a group of professionals with communication skills that will be involved in the ExaQUte dissemination and outreach activities. CIMNE also counts with a Network of Joint labs in Latin America (The CIMNE Classrooms Network) for cooperation in education and RTD activities, which can be used for dissemination overseas of the outcomes of ExaQUte through in-situ initiatives (details in www.cimne.com).

Different Audiences require different languages

Dissemination of the project results will consist on the communication of the outcome of the project. The particular nature of this proposal and its ultimate application to the industrial world and its potential societal impact leads to the development of a multiple dissemination technical plan, targeted to different audiences.

The identified targeted audiences of ExaQUte include:

- Specific HPC scientific exascale community, (i.e., calls FET-HPC and CoE and the rest of the European Exascale Projects Community researchers and PRACE people)
- Other scientific community, non HPC experts (end-users and application people, such as biomedical researchers, climate change researchers and so on)
- Industry (potential customers and end-users, such as aeronautic or civil engineering companies, etc.). Some of them have been already identified and participate in the ExaQUte User Panel.
- Universities (for training purposes, talented students and scientists, talking about what universities are doing in simulation and the growing interest of this field, how CAD/CAE is gaining weight in teaching)
- Government and decision-maker's agents. Due to the strategic intrinsic character that the HPC field has in the framework of the European Digital Agenda, it is important to make decision-makers aware of the outcomes of ExaQUte to ensure follow-up and better use of the results. (Crucial to adopt, for example, software-based solutions for climate change related problems, disasters, etc.)
- General Public. Communication to a lay audience should also be accomplished, mostly through communication of the main results of the project and its societal implications

1.1. Main features of the Dissemination Plan

Scientific achievement in ExQUte is disseminated using the standardized communication tools used in science and technology, such as:

- Attendance to scientific and technical conferences, forums and workshop by scientist and researchers. The conference and workshop are selected according to the availability and type of results. Communication to international conferences organized by Scientific Societies on Numerical methods and HPC related conferences, to which the groups of ExaQUte regularly contribute, such as:
  - IACM (International Association for Computational Mechanics),
  - ECCOMAS (European Community on Computational Methods in Applied Sciences),
  - SEMNI (Spanish Association for Numerical Methods in Engineering),
  - ERCOFTAC (European Research Community in Flow, Turbulence and Combustion).

- PARCFD (parallel Computational Fluid Dynamic)
- HPCC IEEE International Conference on High Performance Computing and Communications
- HiPC (*IEEE International Conference on High Performance Computing)*
- ISC High Performance, the International Supercomputing Conference
- *PRACE Scientific Conference and User Forum*
- The bi-annual series of SIAM conference on Geometric Design
- Conferences on Isogeometric analysis, IGA
- bi- annual series of SIAM conference on Uncertainty Quantification
    - PASC (Platform for Advanced Scientific Computing Conference)
- SC The International Conference for High Performance Computing, Networking, Storage and Analysis
- IEEE Cluster Conference (Cluster)
- IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGRID)

— The project is actively participate in the concentration activities and meetings related with HPC and/or the e-Infrastructures area. The objective is to encourage synergies between projects and promote activities of common interest. The coordinators of ExaQUte and other ExaQUte partners have been involved in previous HPC project and have been/are already participating in coordination actions with the European Exascale Projects community.

— Organization of a specific session on HPC Adaptive meshing and evolving geometry and simulations in the framework of the ECCOMAS-European Research Community of Computational Methods in Applied Sciences (CIMNE belongs to the organizing committee of these conferences), in which some of the partners belong to the organization committees. It will represent an opportunity to put together a think-tank on this field with the involvement of world-class experts.

— Publication of scientific and technical papers in relevant scientific journals is a cornerstone of the results of the project. The publication of the project outcomes in peer-reviewed journal is also a way to give confidence to potential users and to demonstrate the soundness of the work, supported by the scientific community.

- SIAM Journal on Scientific Computing
- International Journal of High Performance Computing Applications
- IEEE Transactions on Parallel and Distributed Systems
- Future Generation Computing Systems
- Parallel Computing
- Concurrency and Computation
- Journal of Grid Computing
- Archives of Computational Methods in Engineering
- Computer Methods in Applied Mechanics and Engineering
- International Journal for Numerical Methods in Engineering
- Computational Mechanics
- Journal of Wind Engineering and Industrial Aerodynamics
- International Journal for Numerical Methods in Fluids

— Training sessions for partners and other scientists and code developers.
— Presentation of results of the project in form of dissemination material and practical demos at the SC and ISC-HPC events where BSC holds a booth.

— Final ExaQUte Workshop with participation of ExaQUte User Panel and other relevant stakeholders.

Regarding this last issue (training), examples of the actions to be implemented in the framework of ExaQUte are the GiD and KRATOS conferences regularly organized by CIMNE every two years. They represent an opportunity to bring together users and developers of the platforms in order to exchange ideas and experience, and receive direct feedback from users. The meeting is organized in a conference format including oral presentations and discussion on advances in the development and applications of GiD and KRATOS to different fields in engineering and science and to identify future directions for research and practice. Also, BSC organizes a regular yearly training on the PyCOMPSs/COMPSs programming model at the PRACE Advanced Training Center (PATC).

It is crystal clear that the specific outputs of the ExaQUte project (codes and know-how) are not of direct use for a general audience, and not even for a general scientific community (although the tools will for sure be used in the framework of very different fields of research, and its general impact, as described in the previous section, can be huge when applied to solve critical societal challenging problems).

Tentative users of the type of tools to be developed in the framework of this project are highly specialized modelers that have a chance to perform research and run their development in the top-rated supercomputing facilities in Europe (or elsewhere).

Regarding specific communication issues between users of the new tools developed in ExaQUte, it is worth to highlight here the experience of CIMNE with the KRATOS and GiD community. GiD and KRATOS developers, together with their users, are a very active community in terms of collaborating and exchanging knowledge and experiences in their field, in the form of web-pages, mailing lists and wiki pages (as examples of this kind of communication, visit KRATOS's wikipage at: http://kratos-wiki.cimne.upc.edu and GiD mailing list repository at http://www.gidhome.com/support/mailing-list). In these spaces, users of the codes exchange communications about encountered troubles, "tricks" or needs.

This type of feedback is very valuable to the software developers, since they keep them updated of the necessities raised by users and helps them to improve their codes. Following the successful KRATOS and GiD dissemination philosophy, ExaQUte uses similar tools to ensure best spreading and tuning of the outputs of the project, ensuring its extension and continuity after the end of the project.

General communication of the projects' results to the **non-scientific audience** will be pursued by adapting the contents to the audience towards it is intended. Some of the envisaged actions, especially dedicated to the uptake of the outcomes of the project by the industrial sector, are the following:

- Public presentation events to potential users and industries. The consortium will organize public events where the new tools will be presented;
- Publications in trade press and presentations in industrial fairs;
- Market-oriented publications in magazines and marketing material produced by partners' press office;
- Contact with Administrations and policy-makers (either at the regional/national/European level) involved in decision-making related to the efforts carried out to implement and exploit HPC infrastructures;

1.2. Publications and Open Access:

Regarding the publication policy to be adopted, the project targets journals of good quality (first quartile) and Open-Access publishing will be favored whenever possible. All published results arising from the research funded under ExaQUte are openly accessible, in accordance with Horizon 2020's mandate on open access to all publications. These include all peer-reviewed publications and also any resulting monographs, books, conference proceedings, slides, grey literature, etc. Green open access is fostered among partners, where post prints or publishers' PDFs of the research publications will be made available through one or more of the partners' institutional repositories, at no charge, and after an embargo period of between zero and six months has elapsed, depending on publisher policy. A strict self-archiving policy has been adopted, using open channels (for example Research Gate, university webpage, etc.).

ExaQUte embraces the initiatives of the European Commission to promote the open access to research data, aiming to improve and maximize access to and re-use of research data generated by Horizon 2020 projects. The main platform (project repository) to be used to publish and grant open access to the research data will be Scipedia (www.scipedia.com). Scipedia is an innovative scientific and technical digital publisher platform and professional social network promoted by the coordinator CIMNE. In this platform, a specific collection will be created for the project. This collection will gather the different research reports, published papers, along with the rest of the data generated in the project and selected to be openly available according to the DMP. Scipedia will ensure that the published content of the project is harvested by OpenAIRE aggregator, as a way to ensure compliance with the EC's policies on Open Access. The published data can optionally be additionally stored in the repositories of the project partners.

Aligned with those initiatives, a Data Management Plan (DMP) has been designed for ExaQUte project. A first version of this plan has been produced at the beginning of the projects as a deliverable released (D8.1) on M6 of the project, which can be updated during the project if necessary.

PU documents related to this project will be uploaded to the ExaQUte customized repository created under the Open Science Platform Scipedia, available at `https://www.scipedia.com/institution/exaqute.eu`, a snapshot of which is shown in Fig. (1).

Figure 1: *Scipedia repository to share open documents*

2 Dissemination activities

2.1. General dissemination tools and materials

2.1.1 ExaQUte webpage and Twitter account

The main dissemination tool of the ExaQUte project is it website www.ExaQUte.eu, created and made public a few weeks after the onset of the project. A snapshot of its home page is show in Fig.2&3.

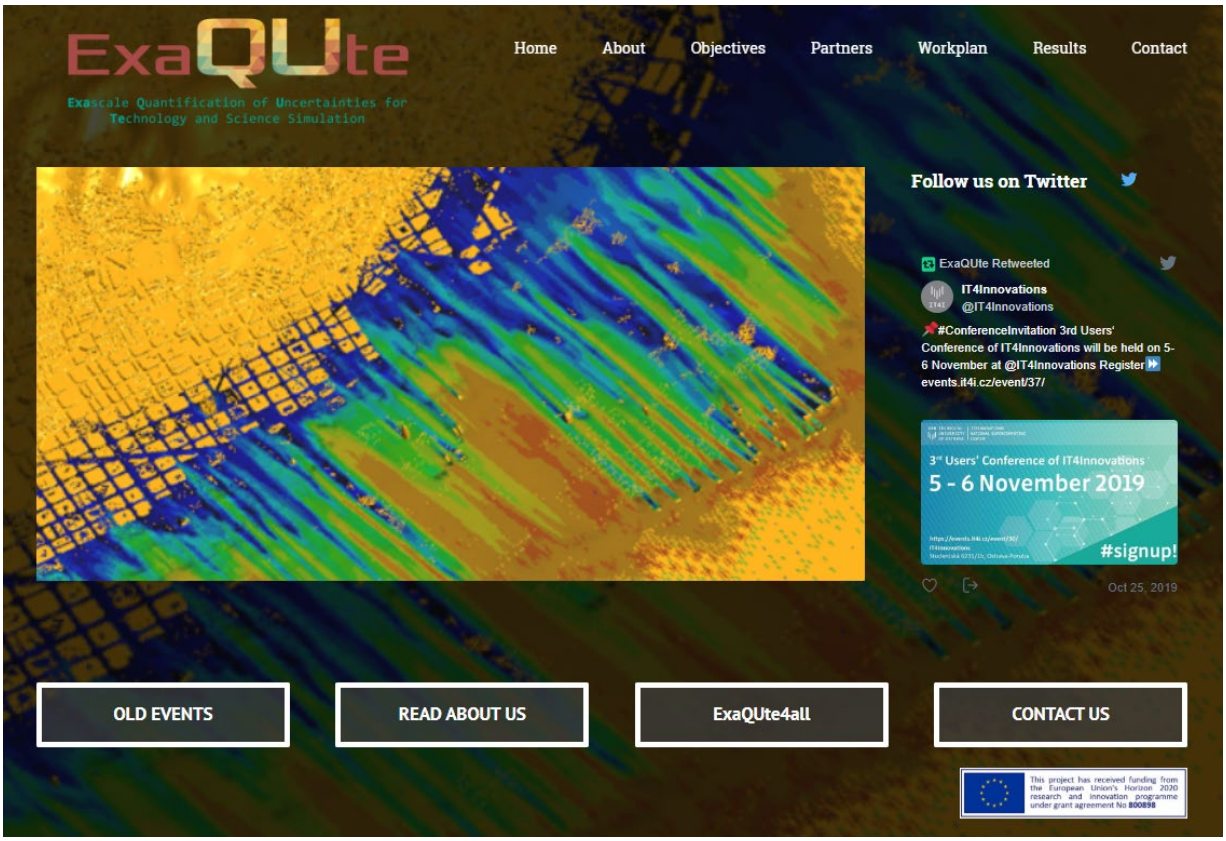


Figure 2 *ExaQUte main webpage*

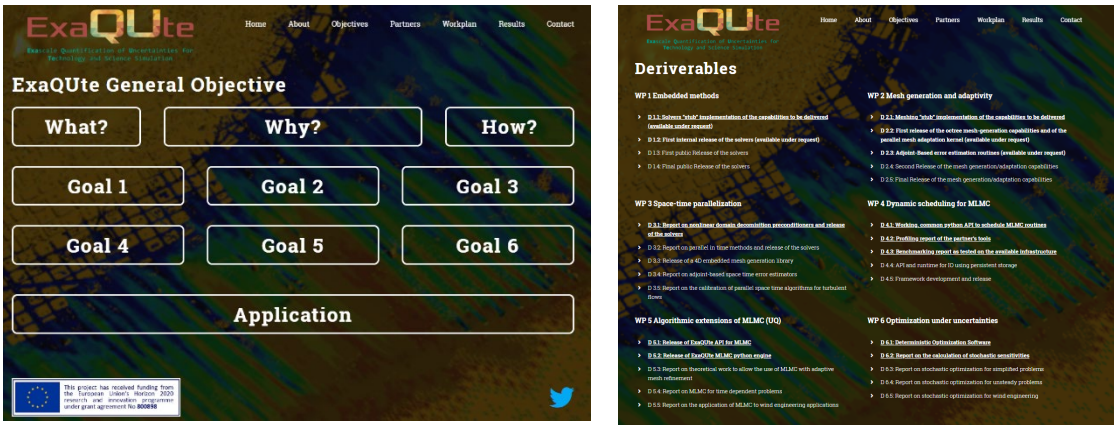


Figure 3 *Snapshots of ExaQUte webpage*

In parallel, a twitter account (@ExaQUteEU) was created to announce in a more dynamic way activities of the project or information relevant for people interested in HPC research.

Figure 4. *ExaQUte titter account*

2.1.2 ExaQUte logo

A “corporative” logo was also created for ExaQUte, whose design, more than just images and words, had to be able to tell a story about our project: what we do and what the project stands for.

Professionals at CIMNE’s Publications Department were able to extract the very essence of ExaQUte from a short summary of the projects and a list of keywords, and summarized the key objective of NUMEXAS in one of its main tasks: SIMULATION.

The materialized visualization of this top feature of ExaQute was represented in the created logo through a simulation mesh symbol, which was integrated in the project’s name by its use as the filling of the capital letters UQ, which stand for Quantification and Uncertainties, key issues in the project. The result of this conceptualization work is a new logo (Fig.5), self-contained in the project acronym/name, which was quickly accepted by the whole consortium.

Figure 5 *ExaQUte logo*

2.1.3 ExaQUte leaflet

A leaflet diptych was also produce to have some physical support to be handled to visitors of the different participating institutions or as take-away material to be used in conferences/workshops/seminars or any other type of event.

The leaflet (Fig. 6 a,b) has been designed to be attractive to all type of audiences, highlighting the main objectives of the project, its structure and its application outcomes. Project's facts and Contact information is included, encouraging more specialized audiences to address their enquires and get more information.

***Figure 6a**. External pages of ExaQUte's Diptych*

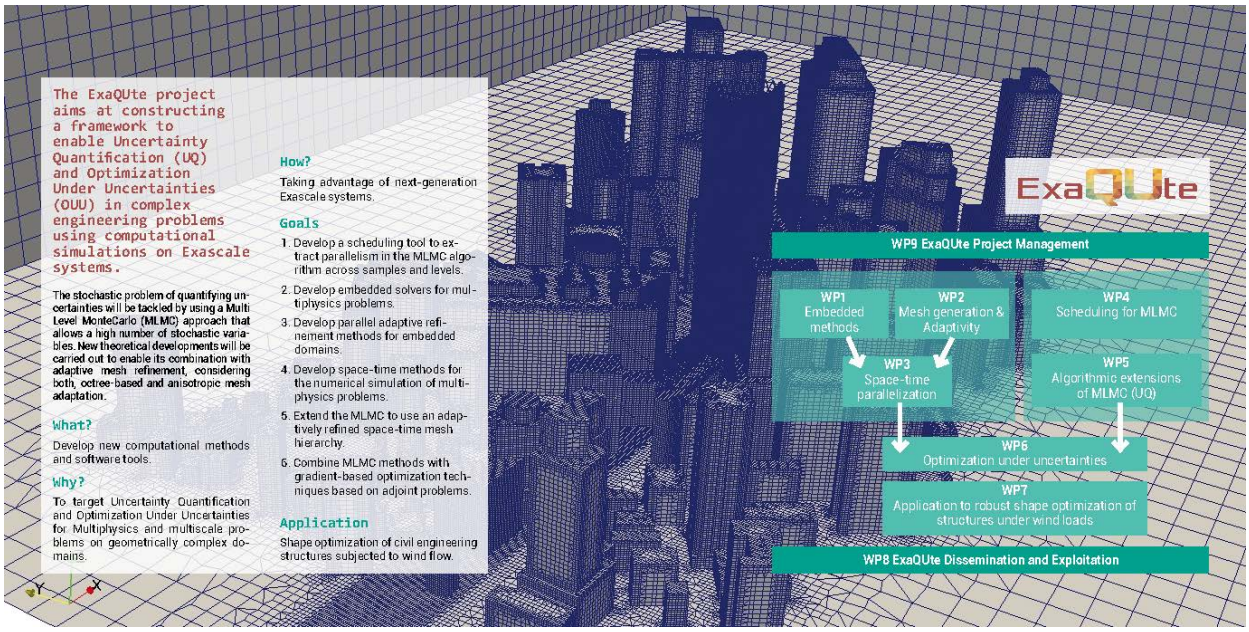
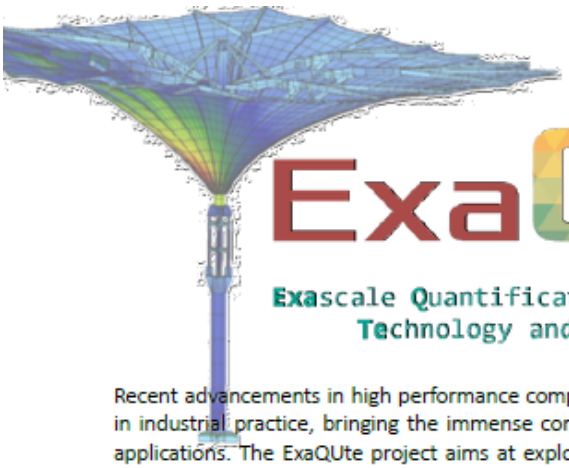


***Figure 6b**. Internal pages of ExaQUte's Diptych*

2.1.4 ExaQUte Description for the general people

Since different audiences require different dissemination material, we have produced a document describing the goals of ExaQUte in a comprehensive way for non-scientific



www.exaqute.eu

ExaQUte

Exascale Quantification of Uncertainties for Technology and Science Simulation

Recent advancements in high performance computing (HPC) will soon allow for the use of exascale systems in industrial practice, bringing the immense computational power of today's machines to real engineering applications. The ExaQUte project aims at exploiting such systems, pushing our current physics simulation capabilities by performing Uncertainty Quantification (UQ) and Optimization Under Uncertainties (UQO).

If we analyze the performance of current simulation tools, nowadays we can use numerical methods to accurately simulate and predict the behavior of a real phenomenon (for instance the interaction of structures and fluids, such as a building and the wind), provided that the values of relevant parameters at the initial state from external contributions to the system are known beforehand. This type of analysis can be costly for large and accurate cases, such a whole high-rise building, but it is still doable with our current technology.

Why dealing with uncertainty?

Uncertainty comes into play when some of the input parameters of our problem are not exactly known a priori. Then, since the inputs for the simulation are not exact, the solution of the problem we are simulating

Tossing a coin

A way to visualize the concepts of uncertainty and parallelism is by thinking of the example of tossing a coin. In an ideal set up, when tossing a coin a set number of times, and always in the same exact way, it would land on the same side every single time. However, in reality, there are many factors that are uncertain, such as the action of the air when the coin is moving, or shaking the hand. This leads to a certain proportion of heads and tails that will depend on all the external factors that contribute to the system. To obtain these exact percentages, one should think that the more throws, the more accurate the result.

For the sake of argument, consider that a hundred throws are enough to fully describe this behavior. In case you are asked to do this experiment by yourself, it will take you some time to toss the coin repeatedly until reaching the 100th experiment. If instead, 99 colleagues come to help you, you will have the analysis finished in one single go. This is the concept of parallelism.

Following the coin example, ExaQUte aims at understanding the relation between the uncertainty (shaking of the hand, action of air) and final result (head or tail), in the smallest possible amount of time (parallelism).

Optimize the simulation results while taking into account uncertainty

Moreover, provided that we are able to model an uncertain phenomenon such as wind, in the same way as the coin example, how can we use this knowledge in engineering? How can we exploit the uncertain solution? Is it possible to use this result to optimize the shape of buildings accordingly?

ExaQUte will answer this final question by combining the concept of uncertainties with optimization. Typically, optimization is used to find the optimal design that yields the best performance for a given analysis with a specific set of inputs and parameters. This, however, may result in fragile designs that are only adequate for the set of conditions they were conceived for. In this regard, the information given by uncertainty quantification allows us to converge to a final robust design which takes into account a wide range of different and uncertain conditions.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 800898

2.1.5 ExaQUte Video

We have produced a video to explain the goals of ExaQUte.

The link to the video is the following: What is ExaQUte? - YouTube

2.2. Common dissemination activities with EC Exascale research projects

As we learn from CIMNES's former exascale project NUMEXAS, specific emphasis was put by the EC to develop coordinated actions (both form the scientific and the dissemination point of view) with the rest of on-going EC projects in the areas of exascale computing.

Following this recommendation, still encouraged by the European Commission, ExaQUte joined the joint dissemination group of all the EUROPEAN EXASCALE PROJECTS AND INFRASTRUCTURE, composed of all the EC projects awarded in EC exascale calls.

The group has created a joint landing page to have access to all the participating projects https://www.montblanc-project.eu/euroexascale

Find below the projects that participate in this initiative

As members of the joint European exascale projects and infrastructure coordination and dissemination group, representatives of ExaQUte have attended the teleconferences that the group holds every other week.

Since ExaQUte joined the group, we have been actively participating in the joint conference calls and activities of the group, the main on which had to do with the preparation of Joint activities related to conference, workshop and training

2.2.1. EuroHPC Summit Week 2019 Poznan (Poland) 13-17 May 2019

ExaQute was present at EuroHPC Summit Week 2019 held in Poznan (Poland) on 13-17 May 2018.

In this event, an ExaQUte poster was displayed and Rosa M Badia (BSC) was one of the presenters in the plenary on Wednesday, covering PyCOMPSs programming model aspects related to the project.

Figure 7. *Microfiber cloth for screens and bookmark for all EC Exascale Projects 2019*

2.2.2. ISC Conference 2019 (Frankfurt 17-19 June)

ExaQUte was present at ISC Conference 2019 in Frankfurt and joint the booth with other EC exascale projects.

The booth was attended by ExaQUte partners that were able to present initial project results and network with other ISC participants. BSC also participated in that event with its own booth, where general dissemination about the project was delivered, as well as PyCOMPSs demonstrations

Figure 8 *Common European Exascale Projects booth at ISC Conference 2019*

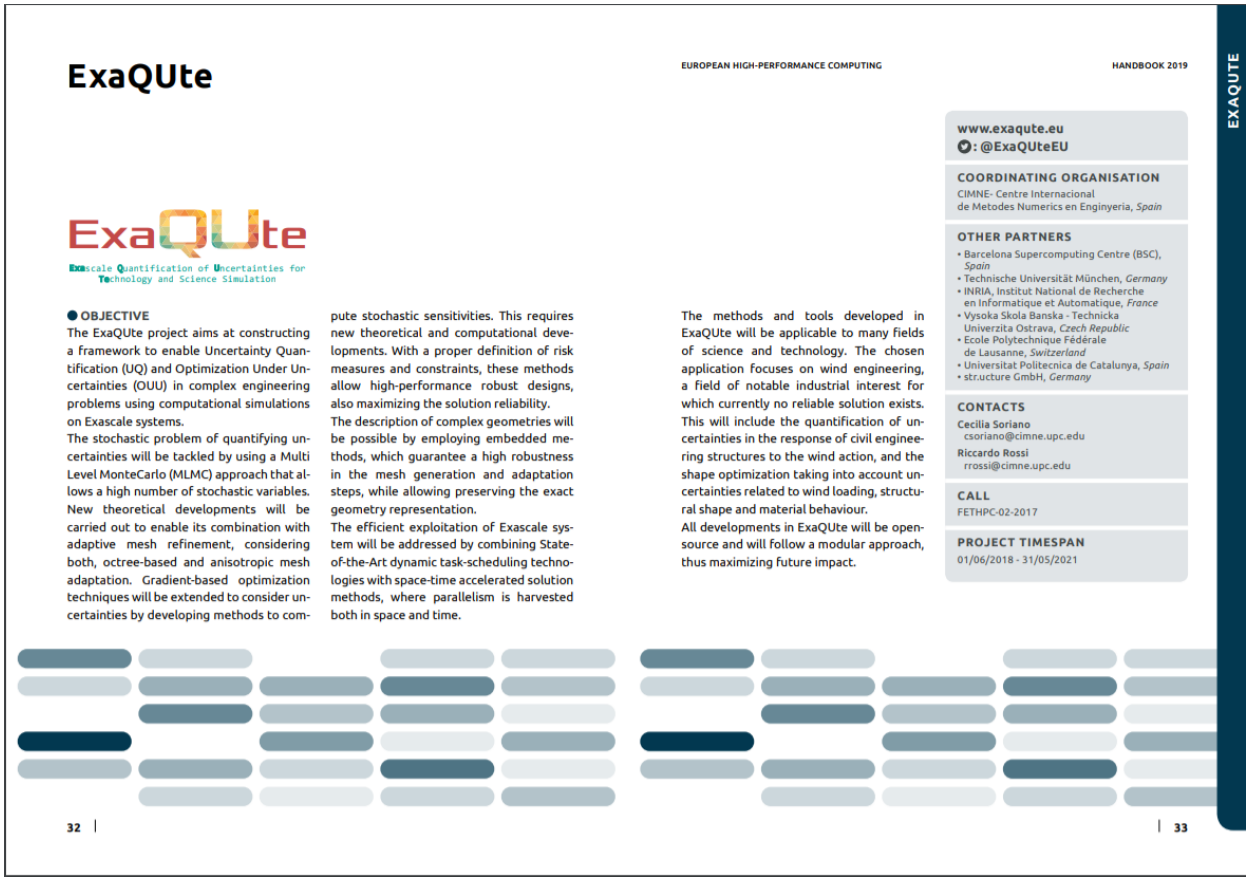
2.2.3. European HPC Handbook

ExaQUte has been included in the European HPC Handbook, 2018 and 2019 Edition *https://www.etp4hpc.eu/pujades/files/ETP4HPC_Handbook_2019_web.pdf*

The Handbook, that is updated every year, is an overview of the European HPC projects. Its increasing size is a sign of the vitality of the European HPC landscape. The Handbook now includes, besides the traditional projects financed by HPC cPPP-related calls, other projects

closely related to HPC, such as HPC and Big Data testbeds, international cooperations, and naturally the European Processor Initiative(EPI).

https://www.etp4hpc.eu/pujades/files/ETP4HPC_Handbook_2019_web.pdf



ExaQUte

EUROPEAN HIGH-PERFORMANCE COMPUTING HANDBOOK 2019

EXAQUTE

ExaQUte

Exascale Quantification of Uncertainties for Technology and Science Simulation

OBJECTIVE

The ExaQUte project aims at constructing a framework to enable Uncertainty Quantification (UQ) and Optimization Under Uncertainties (OUU) in complex engineering problems using computational simulations on Exascale systems.

The stochastic problem of quantifying uncertainties will be tackled by using a Multi Level MonteCarlo (MLMC) approach that allows a high number of stochastic variables. New theoretical developments will be carried out to enable its combination with adaptive mesh refinement, considering both, octree-based and anisotropic mesh adaptation. Gradient-based optimization techniques will be extended to consider uncertainties by developing methods to compute stochastic sensitivities. This requires new theoretical and computational developments. With a proper definition of risk measures and constraints, these methods allow high-performance robust designs, also maximizing the solution reliability.

The description of complex geometries will be possible by employing embedded methods, which guarantee a high robustness in the mesh generation and adaptation steps, while allowing preserving the exact geometry representation.

The efficient exploitation of Exascale system will be addressed by combining State-of-the-Art dynamic task-scheduling technologies with space-time accelerated solution methods, where parallelism is harvested both in space and time.

The methods and tools developed in ExaQUte will be applicable to many fields of science and technology. The chosen application focuses on wind engineering, a field of notable industrial interest for which currently no reliable solution exists. This will include the quantification of uncertainties in the response of civil engineering structures to the wind action, and the shape optimization taking into account uncertainties related to wind loading, structural shape and material behaviour.

All developments in ExaQUte will be open-source and will follow a modular approach, thus maximizing future impact.

www.exaqute.eu
: @ExaQUteEU

COORDINATING ORGANISATION

CIMNE- Centre Internacional de Metodes Numerics en Enginyeria, *Spain*

OTHER PARTNERS

- Barcelona Supercomputing Centre (BSC), *Spain*
- Technische Universität München, *Germany*
- INRIA, Institut National de Recherche en Informatique et Automatique, *France*
- Vysoka Skola Banska - Technicka Univerzita Ostrava, *Czech Republic*
- Ecole Polytechnique Fédérale de Lausanne, *Switzerland*
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CALL

FETHPC-02-2017

PROJECT TIMESPAN

01/06/2018 - 31/05/2021

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Again ExaQUte has been included in the European HPC Handbook 2021 Edition :

https://www.etp4hpc.eu/pujades/files/European%20HPC%20Handbook%202021%20final.pdf

ExaQUte

ExaQUte - EXAscale Quantification of Uncertainties for Technology and Science Simulation

ExaQUte

Exascale Quantification of Uncertainties for Technology and Science Simulation

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Transition to Exascale Computing

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CALL
FETHPC-02-2017

PROJECT TIMESPAN
01/06/2018 - 31/05/2021

2.2.4. SC 2019

ExaQUte will be present at the SC Conference Series. SC19 will be held **from Nov. 17-22 in Denver**, www.supercomputing.org sharing the booth of the European Exascale project and Infrastructures group. The booth will be attended by project partners. BSC will also have its own booth where additional dissemination will be performed, as well as PyCOMPSs demonstrations. (photo booth #2215)

Figure 9 *Common European Exascale Projects booth at ISC Conference 2019*

2.2.5. Dr. Rosa Badia receives the ICT Woman Award

The researcher of the Barcelona Supercomputing Center (BSC) Rosa M. Badia, and researcher of ExaQUte, has received the ICT Woman Award in the Academic / Researcher category granted by the Department of Digital Policies and Public Administration of the Generalitat de Catalunya.

This award recognizes the international projection of Badia's research work in the area of parallel programming models and its contribution to the promotion of women's participation in the ICT.

CONGRATULATIONS Rosa!

Figure 10 *Rosa Badia (ExaQUte/BSC) receives the ICT Woman Award granted by the Department of Digital Policies and Public Administration of the Generalitat de Catalunya*

2.2.6. BSC researcher Rosa M. Badia receives the HPDC Achievement Award 2021r. Award

Rosa M. Badia (Leader of WP 4 in ExaQUte) is the first researcher to carry out her work in Europe recognized by this award.

Rosa M. Badia, the Workflows and distributed computing group manager at the Barcelona Supercomputing Center (BSC) and coordinator of the EuroHPC project eFlows4HPC, has received the HPDC Achievement Award 2021 for her innovations in parallel task-based programming models, workflow applications and systems, and leadership in the high performance computing research community.

The International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC) recognizes with this prize an individual who has made long-lasting, influential contributions to the foundations or practice of the field of high-performance parallel and distributed computing (HPDC).

Congratulation Rosa!

It has been a pleasure to work with you in ExaQUte.

She is the first researcher to carry out her work in Europe recognized by this award.

Rosa M. Badia, the Workflows and distributed computing group manager at the Barcelona Supercomputing Center (BSC) and coordinator of the EuroHPC project eFlows4HPC, has received the HPDC Achievement Award 2021 for her innovations in parallel task-based programming models, workflow applications and systems, and leadership in the high performance computing research community.

The International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC) recognizes with this prize an individual who has made long-lasting, influential contributions to the foundations or practice of the field of high-performance parallel and distributed computing (HPDC).

Badia is the first researcher to carry out her work in Europe recognized by these awards: "I am very pleased to receive this award for the achievements in my research on parallel programming models for distributed computing, as well as for my community activities. This is for the first time given to a European-based researcher and encourages me to continue my activities in making easier the development of applications for complex computing platforms, as we are doing in the eFlows4HPC project", says Rosa M. Badia.

Figure 10.2 *Rosa Badia (ExaQUte/BSC) Rosa M. Badia receives the HPDC Achievement Award 2021.*

3 Open Source

The ExaQUte project aims at constructing a framework to enable Uncertainty Quantification (UQ) and Optimization Under Uncertainties (OUU) in complex engineering problems, using computational simulations on Exascale systems. The methods and simulation tools developed in ExaQUte will be applicable to many fields of science and technology.

In particular, the chosen application focuses on **wind engineering**, a field of notable industrial interest. The problem to be solved has to do with the quantification of uncertainties in the simulation of the **response of civil engineering structures to the wind action**, and the shape optimization taking into account uncertainties related to wind loading, structural shape and material behavior.

The project entails the numerical simulations of heavy real engineering problems trhough the use of different codes and solvers that, given some input data, produce a file including the values of the relevant parameters that describe the results of the simulation of the original.

First, ExaQUte has created an intranet, organized under a GitLab repository at https://gitlab.com/principe/exaqute, a snapshot of which is shown in Fig. 11. This repository is used to share all working-in-progress documents and deliverables for the European Commission. All source files of all deliverables are contained in this repository. The final version of each deliverable is also published online at https://www.scipedia.com/sj/exaqute-deliverables.

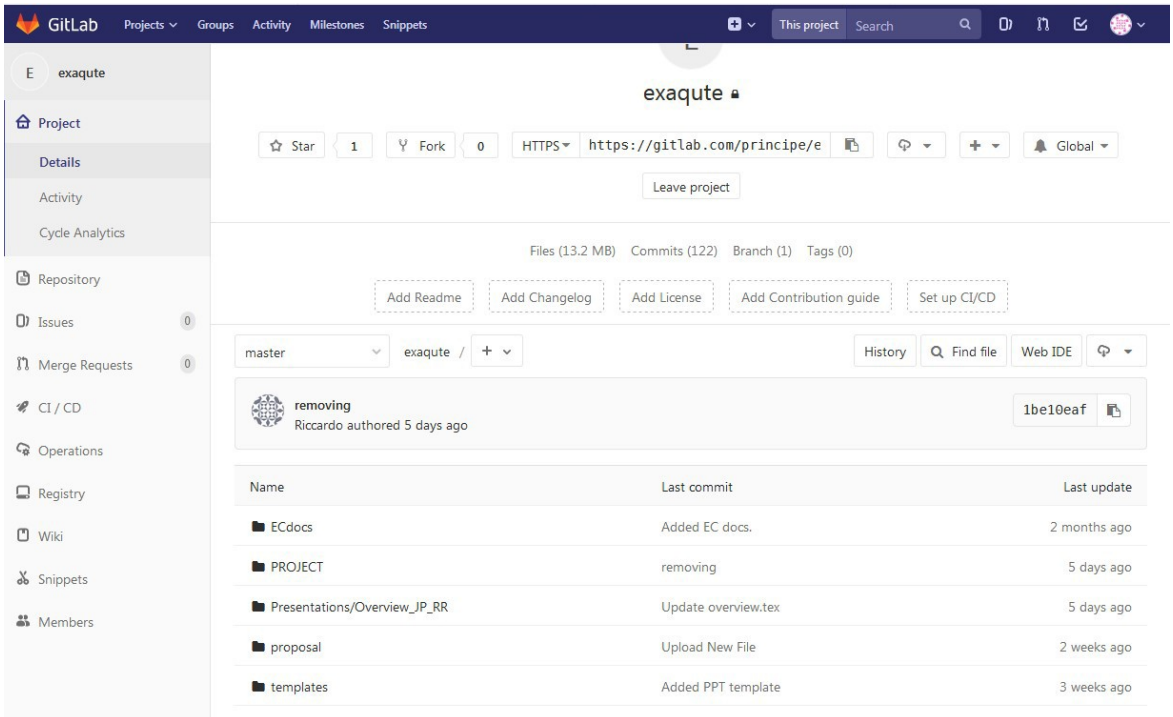


Figure 11: *Git repository to share documents between partners*

At the same time, all the developments on fluid dynamics, uncertainty quantification, optimization and high performance computing of ExaQUte are integrated in the GitHub page

of the Kratos Multiphysics software: https://github.com/KratosMultiphysics/Kratos (Fig. 12). This GitHub repository includes a detailed wiki with the documentation of the project. On this platform, all the developments of ExaQUte will be integrated.

Kratos adopts open standards for input and output formats, thus simplifying the exchange of data. In particular, a JSON (Java Script Object Notation) format is employed in the definition of the parameters defining the simulation. Simulation results can be stored either in proprietary "post.bin" format (which can be opened by the GiD software) or in HDF5 format.

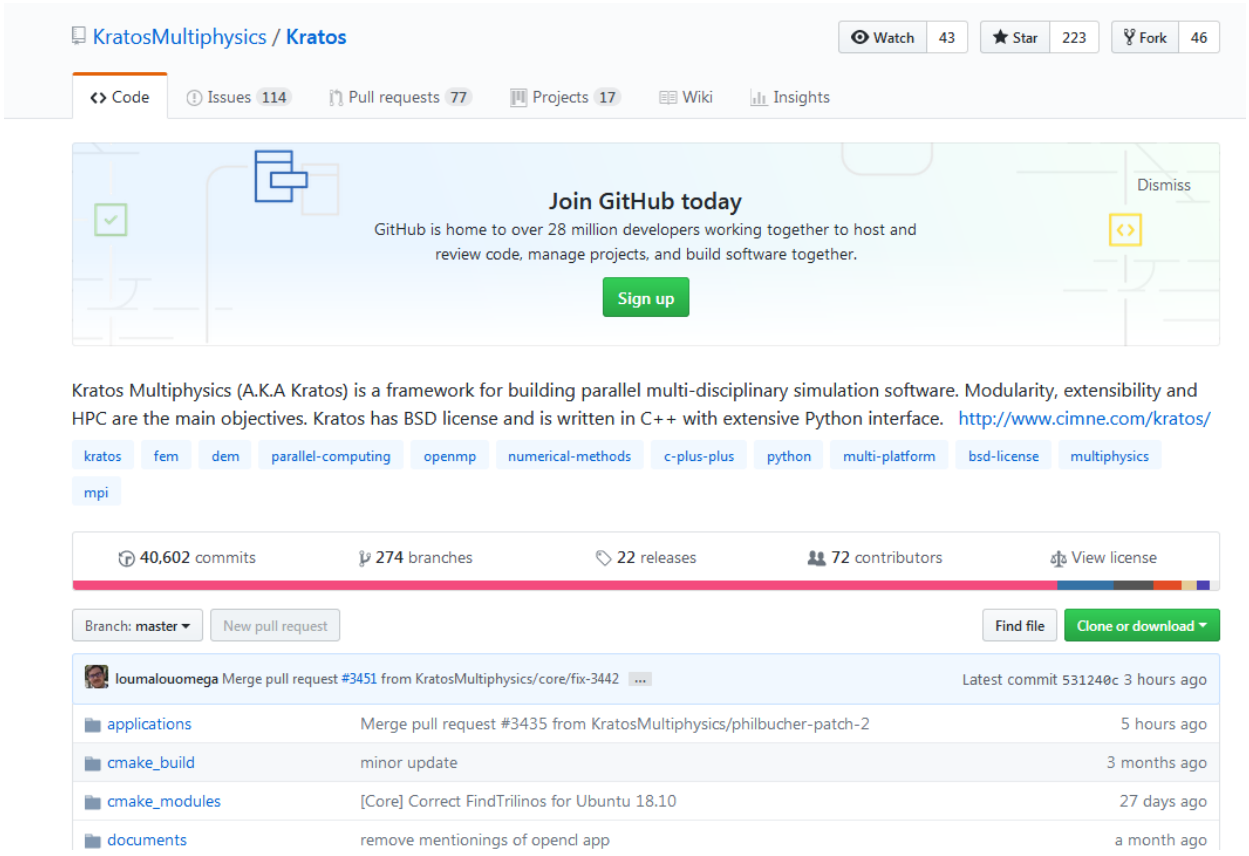


Figure 12: *Snapshot of the Kratos Multiphysics software GitHub repository*

Time parallelization is under development on the FEMPAR solver, which is publicly available in https://gitlab.com/fempar/fempar, and shown in Fig. 13.

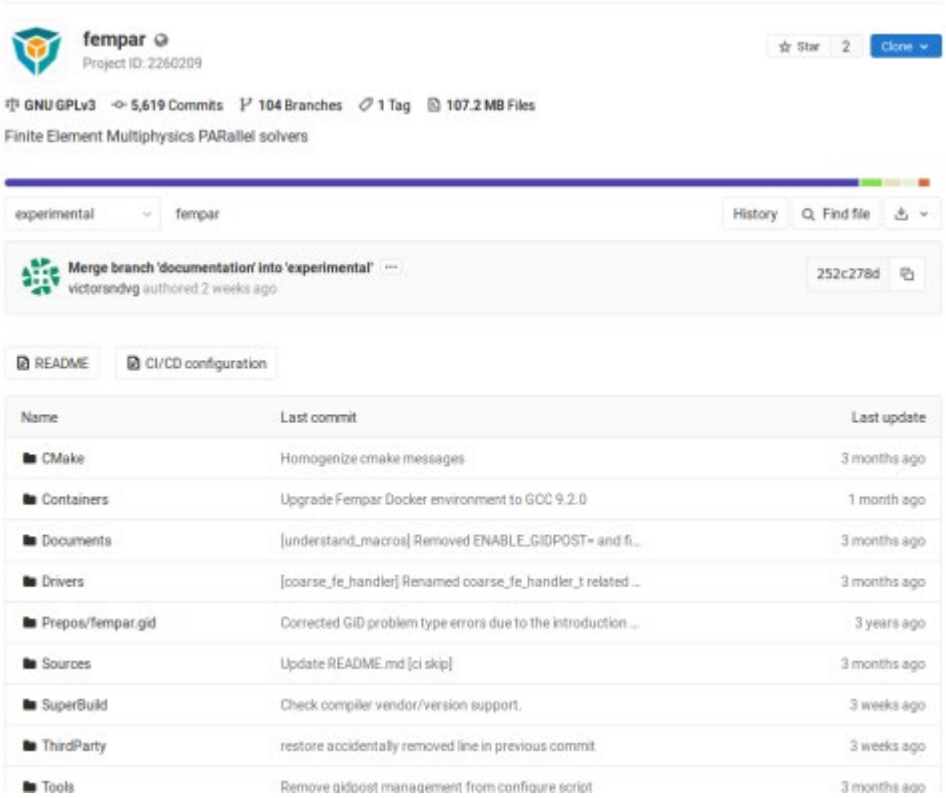


Figure 13: *Snapshot of the FemPar software GitLab repository*

In the project, a new collaborative library to develop hierarchical Monte Carlo algorithms to perform Uncertainty Quantification has been created. This library is called XMC, it is open-source with BSD license and available at https://gitlab.com/RiccardoRossi/exaqute-xmc. The aim of this library is to contain all the capabilities to run Monte Carlo analysis on distributed environments. As a first approach, XMC uses Kratos as its main solver, but it is designed to be exploited in the future by any other solver. This library is under-development by BSC, CIMNE, EPFL.

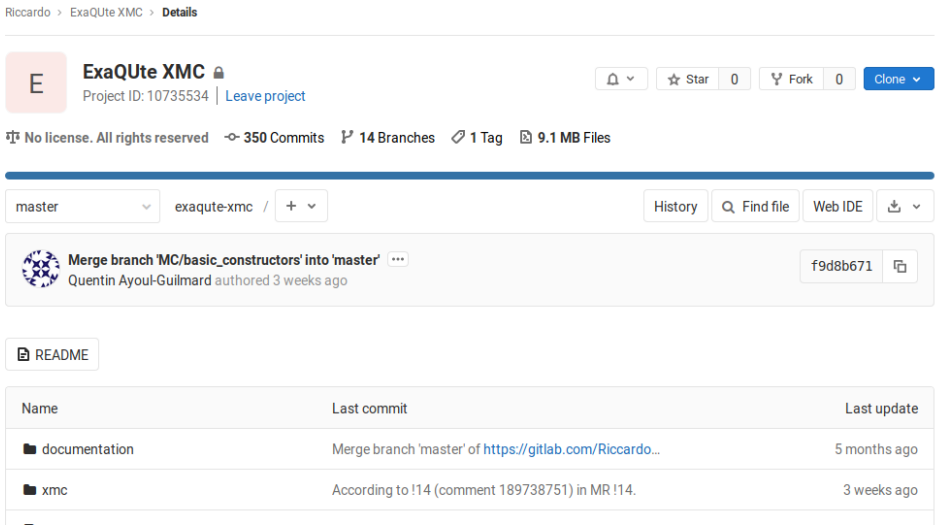


Figure 14: *Snapshot of the XMC library GitLab repository*

In addition, parallel computing is performed by using workflow management tools that allow to run multiple analyses in large scale environments. The workflow management tools used in the project are PyCOMPSs (https://github.com/bsc-wdc/compss), from BSC, and HyperLoom/Quake from IT4i. The former is available at https://github.com/It4innovations/HyperLoom, while the latter at https://code.it4i.cz/boh126/quake). Both are publicly available in their respective repositories.

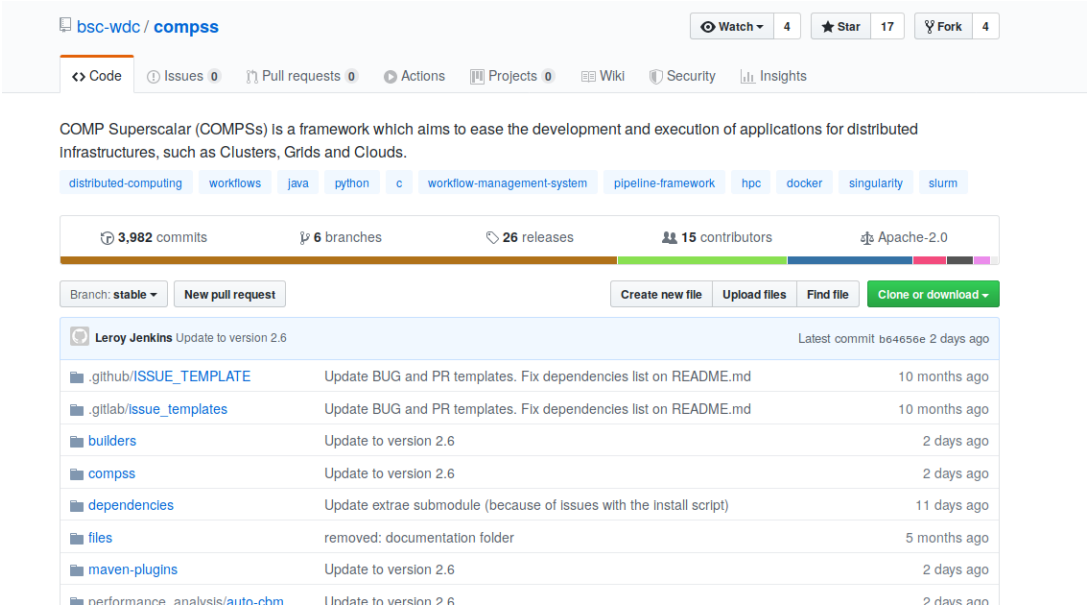


Figure 15: *Snapshot of the PyCOMPSs framework GitHub repository*

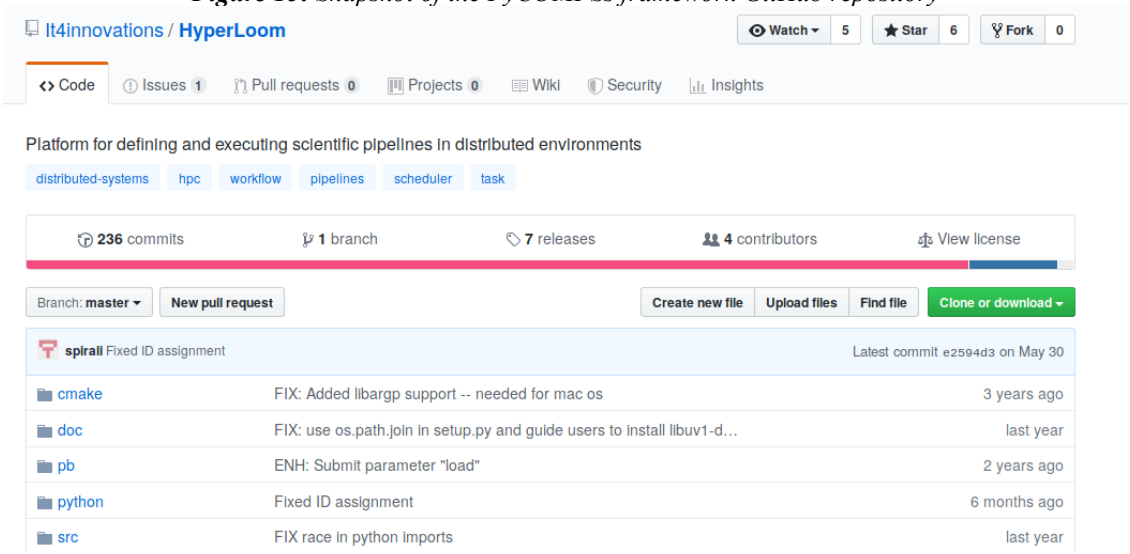


Figure 16: *Snapshot of the HyperLoom framework GitHub repository*

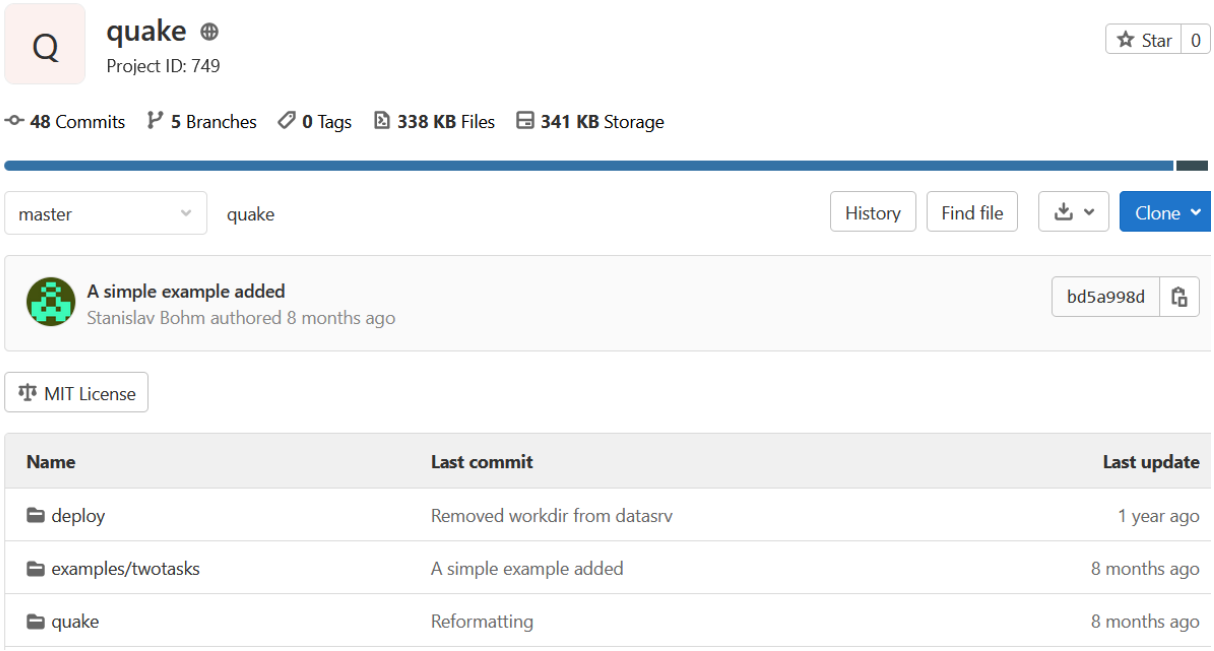


Figure 17: *Snapshot of the Quake framework GitLab repository*

To integrate the distributed computing frameworks (PyCOMPSs, HyperLoom/Quake) with the Kratos Multiphysics software and the XMC library, a common API was defined. We refer for example to WP4 for details. The API is defined in the open-source repository https://github.com/ExaQUte-project/exaqute-api. Three different workflows can be called, using the same API: local, PyCOMPSs and Quake. A snapshot of the GitHub repository is shown in Fig. 18.

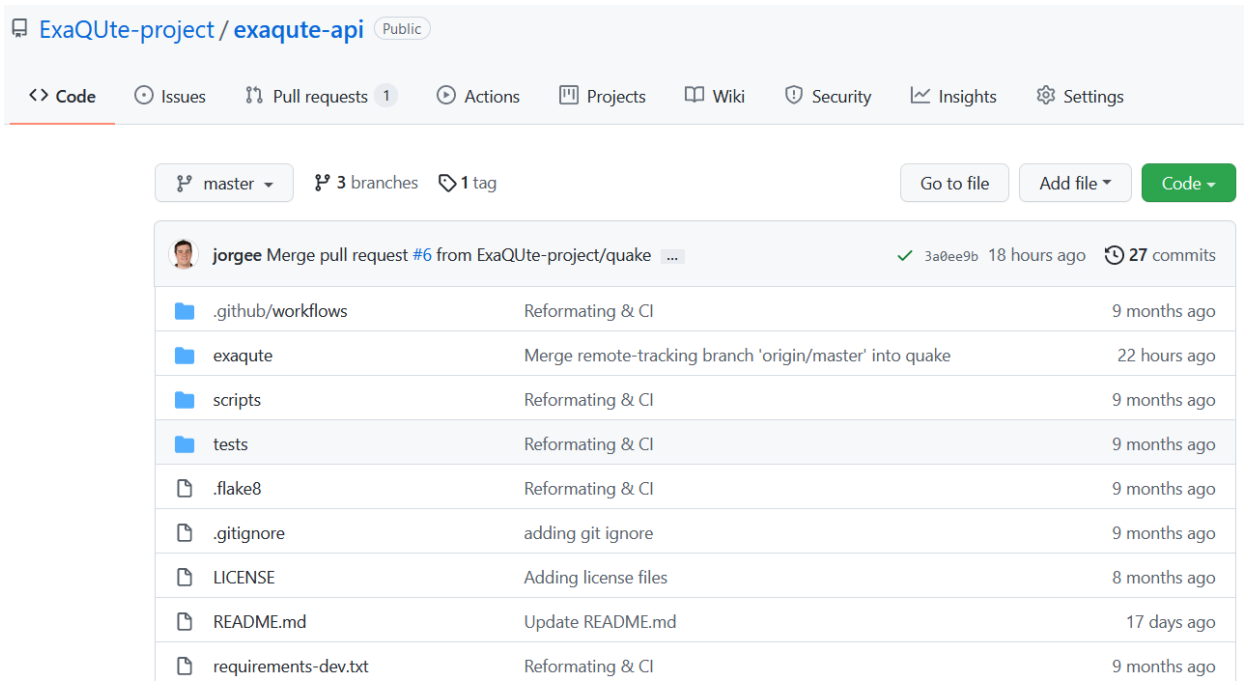


Figure 18: *Snapshot of the ExaQUte API GitHub repository*

As known from WP2, the remeshing library Mmg and its MPI parallel version ParMmg have been extensively used during the ExaQUte project. The two remeshing libraries are open-acces and available at https://github.com/MmgTools/mmg (v5.6.0) and https://github.com/MmgTools/ParMmg (v1.4.0), respectively. A snapshot of the Mmg repository is shown in Fig. 19 and a snapshot of the ParMmg repository is shown in Fig. 20.

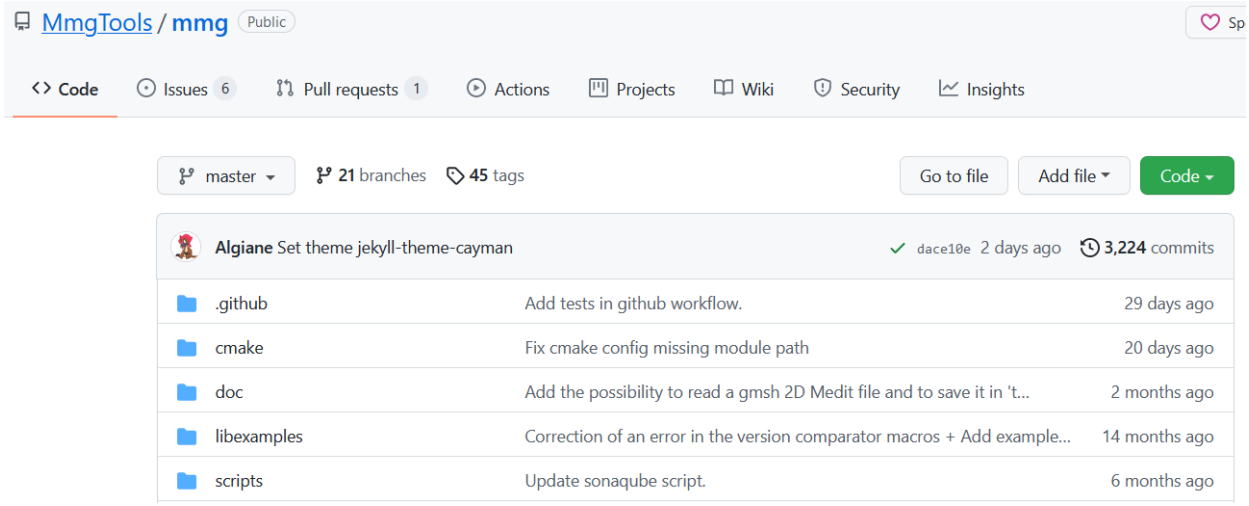


Figure 19: *Snapshot of the Mmg library GitHub repository*

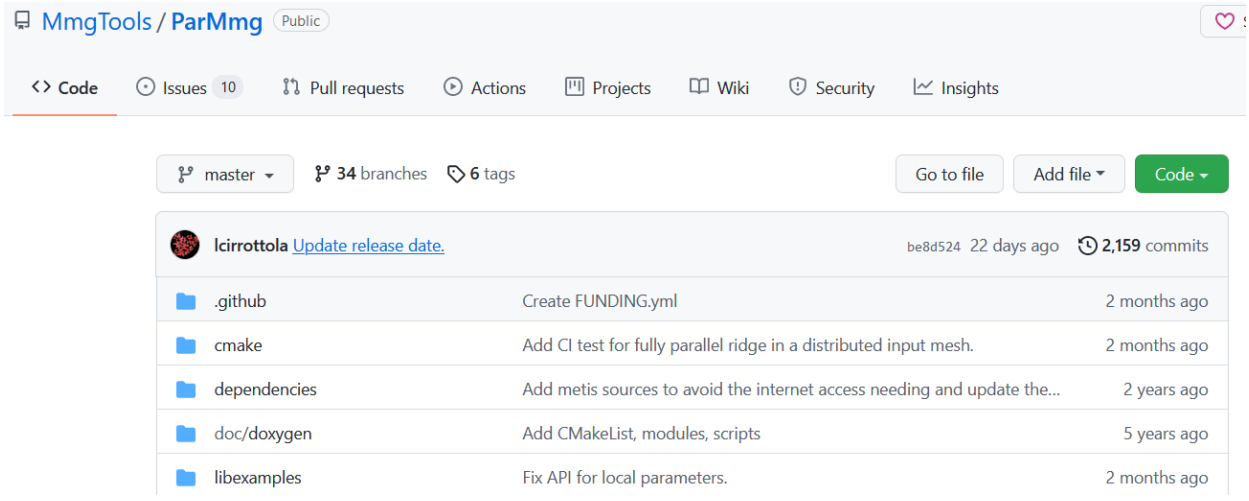


Figure 20: *Snapshot of the ParMmg library GitHub repository*

As commented for example in deliverable 1.4, many different applications have been run using a combination of all of these libraries and software mentioned above. First, simple examples were designed to validate the overall workflow. Then, applications of wind engineering interest were designed and run. The systems executed during the ExaQUte project are available in the open-source Kratos Multiphysics Examples GitHub repository https://github.com/KratosMultiphysics/Examples, see Fig. 21.

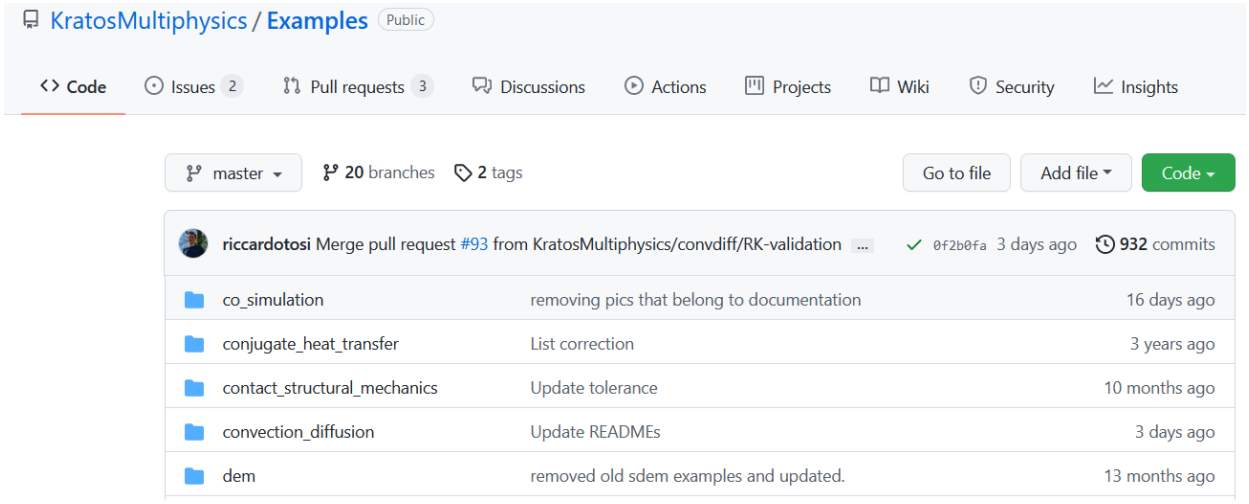


Figure 21: *Snapshot of the Kratos Multiphysics Examples GitHub repository*

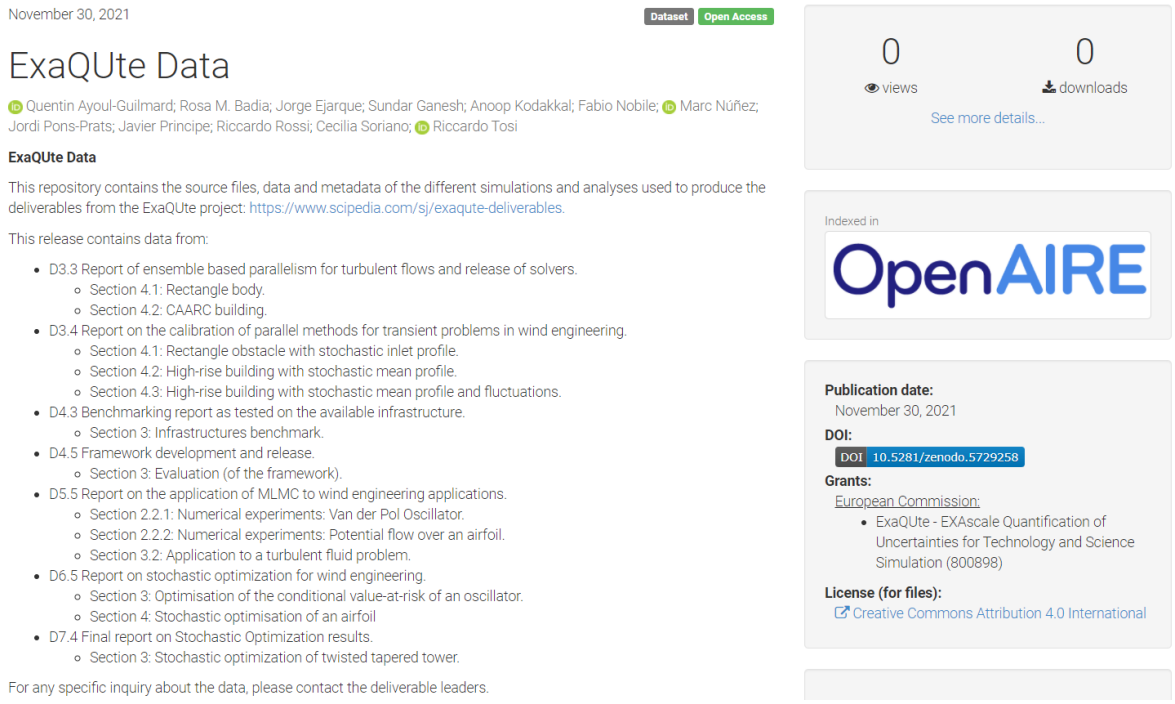
3.1 Data summary

As described in deliverable 8.1, research data are findable, accessible, interoperable and re-usable, as required by the FAIR standards, to ensure it is soundly managed.

Documents and Dissemination material All the deliverables are open-source (with some exceptions) and available in the Scipedia platform https://www.scipedia.com/sj/exaqute-deliverables. Scientific publications connected with the ExaQUte project are available at https://www.scipedia.com/sj/exaqute. Source files of all deliverables are published at https://gitlab.com/principe/exaqute and are available under request.

Data related to the geometry of the structure to be simulated Simulation geometries are prepared using GiD and are available in the open-source repository Kratos Multiphysics Examples (https://github.com/KratosMultiphysics/Examples). Both mesh discretizations and simulation settings (written in json format) are available in the repository.

Data produced as outcome of the numerical simulation As commented in section 1.3 of deliverable 8.1, intermediate results of uncertainty quantification and optimization under uncertainties analyses are never stored, since they are analyzed on the fly. On the other hand, simulation results are stored and post-processed. The most relevant data are open-source and available at https://doi.org/10.5281/zenodo.5729257. We remark that this is a selection data. If someone is interested in all of the data generated during the project, they can be made available under request, writing to the principal investigators (rrossi@cimne.upc.edu and principe@cimne.upc.edu).



November 30, 2021

Dataset Open Access

ExaQUte Data

Quentin Ayoul-Guilmard; Rosa M. Badia; Jorge Ejarque; Sundar Ganesh; Anoop Kodakkal; Fabio Nobile; Marc Núñez; Jordi Pons-Prats; Javier Principe; Riccardo Rossi; Cecilia Soriano; Riccardo Tosi

ExaQUte Data

This repository contains the source files, data and metadata of the different simulations and analyses used to produce the deliverables from the ExaQUte project: https://www.scipedia.com/sj/exaqute-deliverables.

This release contains data from:

- D3.3 Report of ensemble based parallelism for turbulent flows and release of solvers.
  - Section 4.1: Rectangle body.
  - Section 4.2: CAARC building.
- D3.4 Report on the calibration of parallel methods for transient problems in wind engineering.
  - Section 4.1: Rectangle obstacle with stochastic inlet profile.
  - Section 4.2: High-rise building with stochastic mean profile.
  - Section 4.3: High-rise building with stochastic mean profile and fluctuations.
- D4.3 Benchmarking report as tested on the available infrastructure.
  - Section 3: Infrastructures benchmark.
- D4.5 Framework development and release.
  - Section 3: Evaluation (of the framework).
- D5.5 Report on the application of MLMC to wind engineering applications.
  - Section 2.2.1: Numerical experiments: Van der Pol Oscillator.
  - Section 2.2.2: Numerical experiments: Potential flow over an airfoil.
  - Section 3.2: Application to a turbulent fluid problem.
- D6.5 Report on stochastic optimization for wind engineering.
  - Section 3: Optimisation of the conditional value-at-risk of an oscillator.
  - Section 4: Stochastic optimisation of an airfoil
- D7.4 Final report on Stochastic Optimization results.
  - Section 3: Stochastic optimization of twisted tapered tower.

For any specific inquiry about the data, please contact the deliverable leaders.

0 views 0 downloads

See more details...

Indexed in OpenAIRE

Publication date:
November 30, 2021

DOI:
DOI 10.5281/zenodo.5729258

Grants:
European Commission:
- ExaQUte - EXAscale Quantification of Uncertainties for Technology and Science Simulation (800898)

License (for files):
Creative Commons Attribution 4.0 International

Figure 22: *Snapshot of the ExaQUte Data Zenodo release.*

Data for validation of the simulations To validate the implementations and the tools used to solve the problems of interest, validation examples are first run to assess the accuracy of the methods and of the software. Typically, each software is validated independently and we refer to their repository for details. The validation of the workflow consisting of the integration between multiple software (for example Kratos Multiphysics, XMC, PyCOMPSs/HyperLoom/Quake, Mmg/ParMmg, ExaQUte API) is open source and available at https://gitlab.com/RiccardoRossi/exaqute-xmc/-/tree/master/tests or at https://github.com/KratosMultiphysics/Examples.

Software As commented above, all ExaQUte related software are open-source and available online.

4 Research Outcomes

4.1 Workshops and trainings

4.1.1. PATC training,

PRACE, the Partnership for Advanced Computing in Europe appointed BSC as one of the PRACE Advanced Training Centre (PATC)

In this framework a training activity was delivered by the Workflows and Distributed Computing group at BSC (Barcelona, **29-30 January 2019**) on the development of applications using the PyCOMPSs/COMPSs programming model.

The training is yearly organized under the PATC program. In this edition, the training was attended by multiple ExaQUte partners: EPFL, CIMNE, TUM, and BSC.

Figure 13: *Training sessions on development of applications using the PyCOMPSs/COMPSs programming model*

4.1.2. 5th Kratos Workshop

The fifth edition of the Kratos Workshop took place at the Technical University of Munich from the **25th to the 27th of March 2019**.

The Kratos Workshop is the main meeting of users and developers of the Kratos Multiphysics open-source framework. Its goal is to bring together developers, industrial users and researchers to present new features in the code and discuss new and potential applications.

The main objectives of the workshop were:

- Give an overview on the open-source Multiphysics software project for potential future users and contributors.
- Provide forum for recent and (potential) future users and developers in research and industry.
- Improve the common knowledge of developers by presenting the latest features of the Kratos and solutions based on Kratos.
- Team building.
- In person discussions and contacts.
- Take advantage of round tables to discuss important issues and features.
- Dissemination of Kratos capabilities to local research centers and industries.

The workshop included Presentations about Kratos Multiphysics and its use in industrial and research applications, Discussion roundtables focusing on code design and development of new features, and a Hands-on Kratos Course. Siemens and Altair participated in the sessions dedicated to industrial Applications with Kratos SIEMENS Altair

In addition, different talks were given to beginner users, to help them getting familiar with the software. Many ExaQUte members attended the workshop, and we took the chance to organize a progress meeting on the days following the workshop.

Figure 14: *ExaQUte participants at the consortium meeting at TUM (Munich, Germany)*

4.1.3. EuroHPC Summit Week 2019 Poznan (Poland) 13-17 May 2019

ExaQute was present at EuroHPC Summit Week 2019 held in Poznan (Poland) on 13-17 May 2018.

In this event, an ExaQUte poster was displayed and Rosa M Badia (BSC) was one of the presenters in the plenary on Wednesday, covering PyCOMPSs programming model aspects related to the project.

4.1.4. ISC Conference 2019 (Frankfurt 17-19 June)

ISC High Performance
The HPC Event.

ExaQUte was present at ISC Conference 2019 in Frankfurt and joint the booth with other EC exascale projects.

The booth was attended by ExaQUte partners that were able to present initial project results and network with other ISC participants.

BSC also participated in that event with its own booth, where general dissemination about the project was delivered, as well as PyCOMPSs demonstrations

Figure 15: *ExaQUte at the joint the booth EC exascale projects at ISC19*

4.1.5. International Congress on Industrial and Applied Mathematics (ICIAM)

International Congress on Industrial and Applied Mathematics (ICIAM) **Valencia (SPAIN), 15-19 July 2019**

Fabio Nobile (EPFL) gave a presentation featuring ExaQUte in the mini-symposium 'Multifidelity methods for uncertainty quantification and optimization in complex systems', titled 'Accurate statistical estimators by continuation MLMC for engineering'.

4.1.6. US National Congress on Computational Mechanics (USNCCM)

US National Congress on Computational Mechanics (USNCCM) **Austin, TX, USA, Jul 28 – August 1**

Brendan Keith (TUM) resented research on risk-averse stochastic shape optimization of tall buildings; work done in collaboration with the ExaQUte partners at TUM and CIMNE. He gave an invited lecture at a minisymposium in honor of Professor Mary Wheeler.

Figure 16: *Brendan Keith (TUM) at USNCCM*

4.1.7. Workshop FrontUQ

3nd workshop FrontUQ (https://frontuq19.com/) Frontiers of Uncertainty Quantification in Fluid Dynamics. Held in Pisa (Italy) – 11-13 September 2019.

Participation of BSC, CIMNE, EPFL and TUM at the FrontUQ conference with three talks touching different ExaQUte topics.

- EPFL's talk centered on accurate statistical estimators for uncertain variables.
- CIMNE/BSC discussed and showed results of a recently-developed Monte Carlo method, designed for improving the computational cost improvement of when running in supercomputers.
- TUM/CIMNE's presentation focused on the parametric stochastic optimization of civil engineering buildings, influenced by the random behavior of wind.

Figure 17: *ExaQUte participants at the the FrontUQ Workshop*

4.1.8. RICAM Special Semester of Optimization

RICAM
JOHANN · RADON · INSTITUTE
FOR COMPUTATIONAL AND APPLIED MATHEMATICS

SPECIAL SEMESTER
Optimization
Linz, October 14-December 11, 2019

The RICAM (Radon Institute for Computational and Applied Mathematic) special semester on "Optimization" covers various aspects of optimization. Besides more classical themes like PDE-constrained and non-smooth optimization or feedback control the activities during the semester put a special focus on new trends and developments in this field like e.g. numerical methods for data science, influence of uncertainties, nonlocal effects or conic and copositive optimization

Quentin Ayoul-Guilmard (EPFL) presented a poster featuring ExaQUte, titled 'Multi-level Monte Carlo estimators for gradient-based optimization in engineering'.

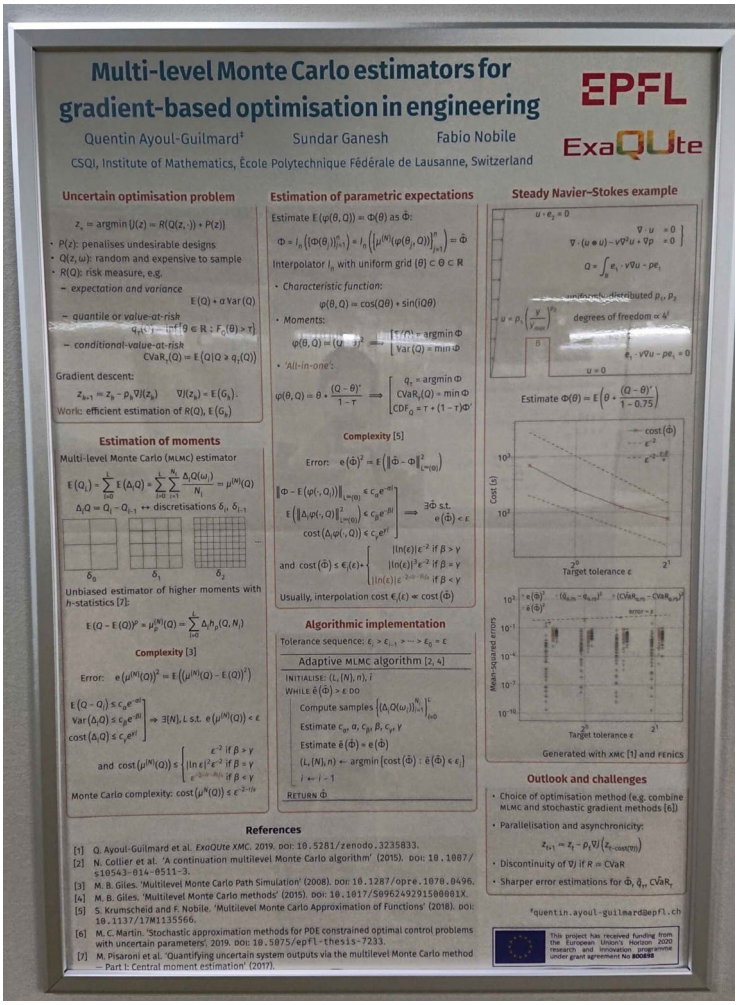


Figure 18: *Poster at RICAM featuring ExaQUte*

4.1.9. CIMNE Coffee Talks

During the whole year CIMNE organizes coffee talks where researches have the chance to present their research developments.

On November 2019, Riccardo Tosi (CIMNE) presented research on workflow design of asynchronous Monte Carlo algorithms; work done in collaboration with the ExaQUte partners at BSC.

Figure 19: *Riccardo Tosi (CIMNE) at CIMNE coffee talks*

4.1.10. After the Pandemic

- PRACE, the Partnership for Advanced Computing in Europe appointed BSC as one of the PRACE Advanced Training Centre (PATC (BSC (Barcelona, 29-30 January 2019)
- 5th Kratos Workshop, Technical University of Munich from the 25th to the 27th of March 2019
- EuroHPC Summit Week 2019 Poznan (Poland) 13-17 May 2019
- ISC Conference 2019 (Frankfurt 17-19 June)
- International Congress on Industrial and Applied Mathematics Valencia (SPAIN), 15-19 July 2019 (ICIAM).
- US National Congress on Computational Mechanics (USNCCM) TX, USA, Jul 28 – August 1.
- Workshop FrontUQ, Pisa (Italy) – 11-13 September 2019

- RICAM Special Semester of Optimization
- CIMNE cofee talk November 2019.
- RICAM Special Semester of Optimization
- CIMNE cofee talk November 2019.
- ExaQUte workshop October 2021
- Mini symposium organization (B. Keith, U. Khristenko): SIAM CSE21, MS: Numerical methods for fractional PDEs.
- 2021-06-15: intervention by Fabio Nobile and Quentin Ayoul-Guilmard at summer school on numerical analysis by CEA–EDF–INRIA; Paris, France (programme).
- Programming Distributed Computing Platforms with COMPSs", PRACE Advanced Training course (PATC), Jan 2019, Jan 2020, Jan 2021.
- Rosa M Badia, "Programming parallel codes with PyCOMPSs", ACM Europe Summer School on HPC Computer Architectures for AI and Dedicated Applications, 30 August - 3 September 2021
- Workshops: Stanislav Bohm presented „Quake: Multi-node scheduling "at ExaQUte Workshop on 8 Oct 2021

4.1.11. ExaQUte Workshop

The ExaQUte Workshop took place in Barcelona on the 8th of October 2021. Importunely, the pandemic situation did not allow the presence of the partners of the full ExaQUte consortium but this did not prevent it from being a busy meeting with interesting discussions.

The workshop was announced in CIMNE's website and by all members:
https://www.cimne.com/vnews/11442/exaqute-workshop-(end-of-project)
and was distributed though Google Meet Video call link: https://meet.google.com/ibh-vmcq-kng.
It was also shared in social media:
https://twitter.com/ExaQUteEU/status/1446381057612394526.

The main purpose of this workshop is to bring the main contributions and work-in-progress of the different partners to the scientific community in an informal configuration. Since the workshop was carried out in virtual format, the sessions were recorded, and they are available to the general public in the following link:
ExaQUte project - YouTube.

The workshop featured talks from each of the partners. Riccardo Rossi from CIMNE opened the session with the advances of the use of uncertainty quantification methods in wind engineering. Luca Cirrotola followed with the description of their adaptive refinement software using distributed memory parallelization. Javier Principe described the use of embedded multilevel Monte Carlo methods to perform Uncertainty Quantification with complex geometries. Stanislav Bohm and Rosa Badia introduced the programming models developed by IT4i and BSC used in the project, respectively. Quentin Ayoul-Guilmard

explained the methodology applied to solve multilevel Monte Carlo algorithms for parametric expectations. Khristenko Ustim described the method used in the project to synthetically generate wind for the simulations. Finally, Anoop Kodakkal closed the session with an optimization under uncertainty workflow applied to wind engineering problems.

ExaQUte
Exascale Quantification of Uncertainties for Technology and Science Simulation

ExaQUte Workshop (End of Project)

Friday 8th October 2021, CIMNE, Barcelona, Spain
C/Gran Capitán, s/n; Edifici C-1, Campus Nord UPC
08034 Barcelona, Spain. O.C.Zienkiewicz Room

Face to face and Online

09:30 - 10:15 Towards UQ in wind engineering (Riccardo Rossi, CIMNE)
Authors: R.Tosi, M.Nuñez, J.Principe,R.Rossi

10:15 - 11:00 Distributed memory parallelization of unstructured mesh adaptation (Algian Froehly, INRIA)
Authors: H.Beaugendre, L.Cirrottola, A.Froehly M.Ricchiuto

11:00 - 11:30 Break

11:30 - 12:15 Embedded multilevel Monte Carlo for UQ in complex geometries (Javier Principe, UPC) Authors: S.Badia, J.Hampton, J. Principe

12:15 - 13:00 Quake: Multi-node scheduling (Stanislav Bohm, IT4i)
Authors: Stanislav Bohm, Tomas Karasek

13:00 - 14:30 Break

14:30 - 15:15 Extensions to PyCOMPSs to better support the ExaQUte requirements, (Rosa Badia, BSC)
Authors: Rosa Badia, Jorge Ejarte

15:15 - 16:00 Efficient multi-level Monte Carlo algorithms for robust engineering design (Sundar Ganesh, EPFL)
Authors: Sundar Ganesh, Quentin Ayoul-Guilmard Fabio Nobile

16:00 - 16:30 Break

16:30 - 17:15 Stochastic optimization in wind engineering applications (Anoop Kodakkal/Ustim Khristenko, TUM)Authors: A.Kodakkal, U.Khristenko, B.Keith, R.Wüchner, K.U. Bletzinger, B. Wohlmuth

17:15 - 18:00 "Perspectives of commercial CFD application in urban city planning (A.Bider/ A. Michalski / A. Michalski, Struc-uture)
Authors: A.Bider/ A, Michalski / A. Michalski)

18:00 - 18:30 Closing

ExaQUte Workshop agenda

4.2 Publications in journals and communications in conferences

Scientific achievement in ExaQUte is planned to be disseminated using the standardized communication tools used in science and technology, mainly through publication of scientific and technical papers in relevant scientific journals and books

The publication of the project outcomes in peer-reviewed journal is a way to give confidence to potential users and to demonstrate the soundness of the work, supported by the scientific community.

As project coordinator, CIMNE has given instructions to all partners to remember to communicate always to the coordinator any publication related to the outcomes of the project and to always acknowledge the EC as a source of funding in their publications.

1.1.1. Journals

- Riccardo Tosi, Ramon Amela, Rosa M. Badia, Riccardo Rossi: "*Scalable Dynamic asynchronous framework for Monte Carlo algorithms*." SIAM Journal on Scientific Computing , 2019 (under review), https://www.siam.org/publications/journals/related/journal-policies/detail/open-access
- Cristian Ramon-Cortes, Ramon Amela, Jorge Ejarque, Philippe Clauss, Rosa M. Badia "*AutoParallel: Automatic parallelisation and distributed execution of affine loop nests in Python.* " IEEE Transactions On Parallel and Distributed Systems, 2019 (under review),
- D Drzisga, B Keith, B Wohlmuth "*The surrogate matrix methodology: a priori error estimation*." SIAM Journal on Scientific Computing 2019 (in print)
- D Drzisga, B Keith, B Wohlmuth "*The surrogate matrix methodology: Low-cost assembly for isogeometric analysis.*". Computer Methods in Applied Mechanics and Engineering. 2019
- D Drzisga, B Keith, B Wohlmuth: *The surrogate matrix methodology: A reference implementation for low-cost assembly in isogeometric analysis*. MethoX 2019 (under review), (https://www.elsevier.com/journals/methodsx/2215-0161/open-access-journal)
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