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Data driven Computational Mechanics at EXascale

DCoMEX

Data driven Computational Mechanics at EXascale

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COMMUNICATION, DISSEMINATION AND EXPLOITATION REPORT

DELIVERABLE D9.3

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http://www.dcomex.eu/
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1. Executive Summary

DCoMEX is a large-scale European project that aims to provide unprecedented advances to the field of computational mechanics by developing novel numerical methods enhanced by artificial intelligence algorithms. The key innovation of this project is the development of a novel scalable library of AI-enhanced algorithms for the solution of large scale sparse linear systems of equations that lay at the core of computational mechanics. The potential of the DCoMEX computational framework will be demonstrated by detailed simulations in two case studies: (i) patient-specific optimization of cancer immunotherapy treatment, and (ii) design of advanced composite materials and structures at multiple scales. Both these case studies are representative of a family of computational mechanics problems that necessitate peta- and exascale computations.

The present document (D9.3) provides a report on the communication, dissemination, and exploitation activities undertaken by the consortium members during the first 18 months of the DCoMEX project, and those planned for the forthcoming period.

Chapter two is devoted to the topic of dissemination and the reader will get an overview of the conferences DCoMEX researchers have attended to date and the status of the project in terms of scientific publications. Additionally, a roadmap on future disseminations activities is provided pertaining to the forthcoming project period. Chapter three is similarly structured, summarizing first part activities in communication and then moving on to plans for the forthcoming months, while chapter four is dedicated to the topic of exploitation. Chapter five summarizes again the key points and restates the main directions in communication, dissemination, and exploitation activities.

2. Dissemination Activities

The dissemination activities are expected to spread the scientific and technological knowledge created in the context of the DCoMEX project, aiming to raise the awareness of respective user communities and IT experts in the objectives and expected results of the project. This will be heavily supported by the communication activities, outlined in the following section. **DCoMEX** will follow a dual dissemination strategy including publications in highly acclaimed international journals and conferences and by providing open-access (with the green open access model) to the project results.

2.1. Past activities

During the past 18 months dissemination activities focused on maximizing the DCoMEX outreach in target audiences, disseminate the scientific and technological knowledge generated in the project and establish links with other relevant projects and initiatives.

To reach these objectives, DCoMEX researchers participated actively in 4 conferences/workshops, covering different topics in the field of computational science and high-performance computing. Table 1 provides an overview of all participations until September 2022, Given the fact that the project's results weren't mature enough until month 12, as well as the mobility issues caused by the pandemic, we consider this participation as satisfactory. Through their presence in these conference/workshops, DCoMEX researchers established links with other researchers from the HPC community, along with other EU projects that on the topic of computational mechanics.

Type of Dissemination	Date	Title	Presenter	Title of Conference/Workshop
Conference	9.06.2022	Large deformation multi-scale analysis of thin nanocomposite shell structures	G. Sotiropoulos	ECCOMAS 2022, Oslo
Workshop	14-15.06.2022		G. Stavroulakis	Teratec Forum, The European meeting for Experts in Digital technologies Simulation, Paris
Conference	29.09.2022	Data Driven Material Design at Exascale	V. Papadopoulos	International Symposium on Polymer Nanocomposites (ISPN 2022), France
Workshop			G. Stavroulakis	First EuroHPC19 Projects collaboration workshop. Madrid

Table 1: Overview of participations in conferences/workshops

In addition to the above, as of today, 3 publications with acknowledgement of DCoMEX in peer-reviewed scientific journals can be reported and 3 are currently under review. Table 2 provides an overview of all scientific publications until September 2022.

Type of Dissemination	Status	Title	Authors	Journal
Journal article	published	Machine learning	S. Nikolopoulos,	Engineering Structures

		accelerated transient analysis of stochastic nonlinear structures	I. Kalogeris, V. Papadopoulos	
Journal article	published	Domain Decomposition Methods for 3D crack propagation using XFEM	S. Bakalakos, M. Georgioudakis, M. Papadrakakis	Computer Methods in Applied Mechanics and Engineering
Journal article	published	A computational framework for the indirect estimation of the interface thermal resistance of composite materials using XPINNs	L. Papadopoulos, S. Bakalakos, S. Nikolopoulos, I. Kalogeris, V. Papadopoulos	International Journal of Heat and Mass Transfer
Journal article	under review	AI-enhanced iterative solvers for accelerating the solution of large-scale parameterized systems	S. Nikolopoulos, I. Kalogeris, G. Stavroulakis, V. Papadopoulos	(preprint available at arXiv:2207.02543v3)
Journal article	Under review	Multiscale analysis of nonlinear systems using a hierarchy of deep neural networks	S. Pyrialakos, I. Kalogeris, V. Papadopoulos	(preprint available at https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4221631)
Journal article	Under review	The stress-free state of human erythrocytes: data driven inference of a transferable RBC model	L. Amoudruz, A. Economides, G. Arampatzis, P. Koumoutsakos	

Table 2: Overview of scientific publications and papers

2.2. Planned activities

The activities for the dissemination of the project's results will continue until the end of the project and beyond that. As the project grows more mature and more tangible results have been accomplished, it is expected that the number of dissemination activities will increase. In this direction, efforts will intensify in the forthcoming months to diffuse the project's results, engage wider audiences, and attract potential users in accordance with the DCoMEX's exploitation strategy. Some concrete activities planned for the near future include 4 presentations in the upcoming UNCEMP/COMPDYN (https://2023.uncecomp.org/) conference, which will be held in Athens in June, and the participation in the HiPEAC workshop in January 2023. In addition, project partners work towards a series of scientific publications of their project results before the project ends.

3. Communication activities

The goals of the communication are: (i) to raise awareness within different target communities and the general public, (ii) to demonstrate progressively the project's concept and system functionalities to key stakeholders at European level, (iii) to manage the attendance to relevant conferences and the production of publications in order to attain maximum effectiveness, (iv) to involve new end-user communities and IT providers and (v) to pave the way for exploitation of project results. To achieve this goal a rich set of diverse activities were outlined in deliverable D9.2.

3.1. Past activities

In the past 18 months the following communication activities took place:

Project's website

The project's website was established early in the project, and it can be found at: http://www.dcomex.eu/

Project's portfolio

The project's portfolio was created, which contained the project's logo, illustrative images, presentations, project flyers and brochures. This material is being regularly updated.

Use of WEB 2.0

A social media channel was established using the Facebook platform (https://www.facebook.com/dcomex.eu).

A DCoMEX community was created on Zenodo (https://zenodo.org/communities/dcomex/) to share freely the project's results among interested researchers and third parties.

In addition, a project specific github repository was created with free access to the code implementations of the project (https://github.com/DComEX/dcomex-prototype), which is regularly updated.

Press releases

A press release was distributed to Prometheas, the newspaper of the National Technical University of Athens and a second one to the EuroHPC JU site.

Organization of meetings/workshops/conferences

Members of the DCoMEX' s consortium organized a workshop titled "**Quantum Computing and its synergy with High Performance Computing in Engineering Sciences and Applications**" on July 2. This event was attended by thirty participants with physical presence and more than fifty people attended virtually.

Clustering activities

To consortium participated in two clustering meetings aiming to establish horizontal collaborations with other HPC-related projects. In particular, DCoMEX explored potential synergies with SparCity project. in the following topics:

a. With respect to Task 3.1: Domain Decomposition Method (DDM), we will explore alternative Partitioning schemes for sparse matrices and Graphs with application to DCoMEX use cases.
b. With respect to Task 3.3: Inexact block-iterative solvers for scalability and error resilience, we will explore additional mixed precision schemes with application to DCoMEX iterative solvers.

Based on these, a collaboration has been initiated with the SparCity project towards the following objectives:

Objective 1: Optimization of Sparse Matrix Vector Multiplication (SpMV), Objective 2: Partitioning of Sparse Matrices, Objective 3: Use-cases. These objectives are described in detail in D9.6.

In this first period of the project, two preparatory meetings have been arranged in order to exchange project description and app description, identify common objectives and proceed with the preparation of the collaboration plan. A common working group has been established to further develop our synergy, identify Tasks and explore the potential of achieving the Objectives.

In addition to the above, we participated in the first First EuroHPC19 Projects Collaboration Workshop, Madrid 2022, where we initiated discussions for further collaborations with other projects as well.

Educational activities

The project's results enabled the enrichment of the educational material for the following NTUA courses "Parallel Processing Systems", "Advanced Distributed Systems", "Nonlinear finite element methods" and "Stochastic finite element methods".

3.2 Planned activities

The first phase (M1-M18) of the project was mainly about raising awareness for the project on target communities and the public. As we now enter the second phase, communication activities will focus on informing target audiences about developments in the project and interacting with stakeholders. In this current phase we try to extend the reach of our channels, by setting up a stronger media presence. Furthermore, events & conferences play an important role in this phase of the project as they help us to interact with the scientific and the HPC community, and get their feedback on developments in the DCoMEX project. Following the strategy outlined in deliverable 9.2, the next steps regarding the communication activities involve:

- Intensify our social media presence.
- Organization of more workshops and minisymposia on international conferences.
- Increase clustering efforts with the HPC community and initiate industrial clustering activities.
- Arrange quarterly meetings with the working group on the SparCity project collaboration to update each other on the project progress.
- A seminar in HPC and programming will be held in NTUA under the auspices of the DCoMEX project.
- Possibilities to present the project at conferences in booths are constantly evaluated based on the cost-benefit principle.

4. Exploitation activities

This exploitation activities for the project's results were elaborated on deliverable 9.2. These were targeted towards increasing the project's visibility among stakeholders at an EU level and globally, attracting investors for the productization of software and solutions based on the DCoMEX results and promoting a business culture to each partner.

Regarding the period M1-M18, project partners report to be on track with the work involved in their assets. However, it is yet too early to demonstrate tangible exploitation activities, as these depend on the completion of the ongoing development work. Regarding the second half (M19-36) of the project, the following exploitation activities are planned.

4.1 Planned activities

For the second phase of the project (M19-M36), the members of the consortium with their diverse and complementary Research and Business contexts and capabilities will provide all potential exploitation modalities and routes to bring DCOMEX results successfully and in a sustainable manner to all targeted user communities. The exploitation strategy of the project will follow a stepwise approach and will be based on the combination of activities that will span throughout the project's duration but will vary in intensity based on the amount of information that can be made available and the produced results during the project's lifetime. The project's key exploitable assets were outlined in deliverable 9.2 "Communication, Dissemination and Exploitation Plan" and are also included in the report.

Result	Partner responsible	IPR model	Targeted end-users
R1: UQ-aware image pre-processing engine	TUM	Open source	Industrial users, supercomputing centers
R2: CPU and GPU-enabled Msolve multiscale/Multiphysics solver	NTUA	Open source	Researchers on algorithms relevant to stochastic multiscale optimisation
R3: Adaptive UQ and Bayesian analysis Korali engines	ETHZ/CSElab	Open source	Researchers on algorithms relevant to stochastic multiscale optimisation
R4: AI-Solve library	NTUA	Open source	Industrial users, supercomputing centers, academic researchers
R5: The **DCOMEX** HPC framework	CSCS	Open source	Industrial users, supercomputing centers, researchers
R6: The **DCOMEX-BIO** software for cancer immunotherapy optimisation	UCY	Patent protected	Software development and medical systems companies, hospitals, cancer research centers, clinical oncologists
R7: The **DCOMEX-MAT** software for material design	NTUA	Patent protected	Software development and material companies, academic and research centers, automotive, aerospace, building industries

Table 3: Overview of DCOMEX's key exploitable results

The consortium members responsible for each asset will be tasked with promoting it to relevant stakeholders, SMEs, academic institutions, and other research groups in the HPC ecosystem. The following concrete steps will be undertaken to accomplish this:

1. All members will take actions towards the establishment of tactical alliances with other industrial or research organizations that hold the potential of promoting the DCOMEX results.
2. The partners responsible for R6 (UCY) and R7 (NTUA), are committed to the development of demonstrators for **DCOMEX-BIO** and **DCOMEX-MAT.** An in-person sales model will be adopted and the capabilities of both software will be presented to SMEs in the fields of medicine and material design in the effort to attract private investments.

3. Following the successful deployment of the DCOMEX HPC framework (**R5**) in the Piz Daint and Aris HPC centers, efforts will be focused towards promoting the installation of this framework and its related constituents (**R1** and **R4)** to other supercomputing centers.
4. The assets **R2**, **R3** and **R4** are expected to have a strong academic impact and therefore these results will be communicated to researchers through journal publications and conference presentations, aiming to establish long-term collaborations.
5. The AI-Solve library (**R4**) will be exploited as a standalone software library for accelerating scientific computations that can be incorporated into any commercial software. Therefore, in-person demonstrations will be pursued by NTUA to companies developing simulation software (Dassault, Ansys etc.) to advertise its capabilities and seek product sales and/or co-development.

5. Summary

The scope of this document was to provide a report on the dissemination, communication and exploitation activities performed during the first 18 months of the DCoMEX project, and those planned for the forthcoming period. These three areas are considered crucial in DCoMEX and each one has been addressed individually, outlining past activities, and planning our future steps. At this stage, there are no major deviations to be reported with regards to the initial strategy in D9.2, and activities in all three areas are on track. The roadmap for the second half of the project is clear and efforts will be intensified in all three areas, following the growing maturity of the project's results.

Closing this final section, we would like to outline the general directions for these three fields:

Dissemination: DCoMEX researchers will continue with the dissemination of the research outcomes in scientific journal publications and conference presentations. The second part of the project is expected to bring an increase in the number of dissemination activities, as the development work carried by each member of the consortium approaches its completion.

Communication: All members of the consortium will contribute on creating new content with the project's results and make dedicated efforts to broaden the community around the project.

Exploitation: Project partners have identified their exploitable assets in D9.2 and devised an exploitation strategy that will take the next steps as soon as possible.