

Data driven Computational Mechanics at EXascale



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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 purpose of the present document (D9.2) is to outline the planning of the communication, dissemination and exploitation (CDE) activities undertaken by the consortium members in order to maximize the project's outreach and visibility, raise awareness over the project's actions and share its results with all interested third parties. This document illustrates the strategy and implementation steps followed by each partner to achieve these goals along with a general timeline.

The main principles of communication, dissemination and exploitation as set out in the definitions of the European Commission will be respected and detailed in this plan:

Communication starts at the outset of the project and continues throughout its entire life. It shall be resourceful, creative and its activities shall be outreaching in nature. All partners will align to carry the same message and work towards adapting it accordingly to target audiences that go beyond the project's own community.

Dissemination activities will be undertaken by all project partners to assure the wide diffusion of the project's results and the largest possible visibility through the means defined in this plan. All partners will be committed to provide information on their dissemination activities to the dissemination manager at regular intervals.

Exploitation activities will focus on 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. These actions will help in shaping the sustainable futures for each of the project's results, either as single partner or as a whole.

The CDE plan is a living document to be updated as the implementation of the project progresses and when significant changes occur.



2. Communication Activities

The communication means together with the appropriate mechanisms to monitor their impact are detailed herein. The goals 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 will be implemented, as outlined in the forthcoming subsections.

According to the impact of communication activities, the partners will update the communication strategy appropriately.

2.1. Project website

The project's website can be found at: http://www.dcomex.eu/



About

Fig 1: DCoMEX site

This site will be the main channel for the consortium members to collect and distribute information through announcements, blogs, presentations and publications and allow everyone outside the consortium to get in touch



with the **DCoMEX** partners for feedback, questions etc. It will also hold (or link to) a code repository for **DCoMEX**'s open-source results and open data.

The metric to assess the impact of this activity will be the annual number of visitors and the number of content downloads.

2.2. Project Portfolio

The project's portfolio will include the project's logo (shown in figure 2), illustrative images, presentations, videos, project flyers, brochures, the project results and any other suitable information. The material will be regularly updated throughout the project and will serve as a marketing opportunity to arouse the interest of relevant target user groups' communities.

The metric to assess the impact of this activity will be the number recipients (flyers, brochures etc.).



Fig 2: DCoMEX logo

2.3. Use of Web 2.0

DCoMEX partners will be committed to sharing new findings, thoughts and any interesting related work using social media such as Twitter (https://twitter.com/EuroHPC_JU/status/1433713950236028944?s=20), LinkedIn (https://www.linkedin.com/feed/update/urn:li:activity:6839479556399742976/), ResearchGate, Facebook (https://www.facebook.com/dcomex.eu). These channels will also be used to announce press releases, event participations, software release availability and the progress of the testbed building.

The metric to assess the impact of this activity will be the size of the network and the frequency of posts and updates.

2.4. Press Releases & Newsletters

General press releases to newspapers, including popular science and other public interest publications, will be prepared and distributed by the partners. Furthermore, electronic newsletters will be circulated in order to report the project's progress to other researchers, stakeholders and the general public. To communicate our research with the public and cancer patients, a series of outreach activities will be scheduled including talks in universities and high schools, appearance in the media and press releases in collaboration with the university press offices.

The metric to assess the impact of this activity will be the number of press releases and subscribers to newsletters.

2.5. Meetings, Workshops, Conferences

DCoMEX partners will actively participate in various fairs, conferences and workshops relevant to supercomputing, resource management and green computing (e.g., Supercomputing, ISC, European HPC Summit Week). **DCoMEX** will

also organise an annual workshop to communicate the intermediate and final project results and receive valuable feedback from the industry sector and academic participants. Candidate conferences to host the **DCoMEX** workshop include ISC, SC, IEEE CLUSTER, IPDPS, CCGrid, HiPEAC, ECCS, WCCM, UNCECOMP and others. **DCoMEX** will aim for joint activities with other related projects on a national and European level to allow a larger number of events by reducing the individual work per project for the preparation. Joint activities are also expected to increase the impact of workshops visibility at relevant conferences. The consortium will also organise an Open Day to present the project to the public.

The metric to assess the impact of this activity will be the number of organized events and the number of participants.

2.6. Clustering

DCoMEX will be communicated via current and new Coordination and Collaboration Actions, Cluster or Clustering meetings, as set up under the EC's Framework Programme. The consortium will be represented at such events by at one partner, requested by the EC. Furthermore, through least as participating dissemination/communication activities, DCoMEX will build communication and collaboration channels with relevant projects in order to establish a bidirectional transfer of knowledge. The participation of several **DCoMEX** partners in key H2020 research projects will be particularly leveraged to receive input on their progress as well as to communicate DCoMEX results to them. Examples of such projects include among others EuroEXA, (NTUA is the EuroEXA coordinator) DEEP-EST, and the Centers of Excellence EoCoE, NoMaD, MAX, ECAM, CoEGSS and POP.

The metric to assess the impact of this activity will be the number of events.

2.7. Policy makers

DCoMEX aims to establish close contact with key policymakers at national and European level by participating in relevant events organised by public authorities and organisations to raise the awareness on **DCoMEX**'s vision and results to wider audiences.

The metric to assess the impact of this activity will be the number of meetings organised.

2.8. Standardisation bodies

The **DCoMEX** partners, according to their expertise, will participate and attempt to influence the activities of standardisation processes, task forces and groups setting standards for future HPC systems.

The metric to assess the impact of this activity will be the number of meetings and events organised.

2.9. Educational activities

Curricula of graduate courses offered by the academic partners will be enriched with **DCoMEX** results. The project's advancements will support material for the courses "Parallel Processing Systems", "Advanced Distributed Systems" (NTUA) and "Computational Mechanics". At ETHZ, two MSc students are currently employed part time in the development of Korali and will integrate new material and expertise into Korali. Direct research on **DCoMEX** and will allow the supervision of a number of MSc dissertation projects to both engage students with the project and enable further research, orthogonal to the main project work to be investigated.

The metric to assess the impact of this activity will be the number of lectures in the associated curricula and the number of dissertations supervised by partners of the consortium.





2.10. Plans for further collaborations with other EuroHPC projects

The following future milestones are discussed between the coordinators of the EuroHPC-JU projects:

- A joint newsletter to update on the progress of the different projects.
- The organization of joint sessions.
- The organization of a joint workshop between the EuroHPC-JU projects.



3. Dissemination Activities

The dissemination efforts will initially concentrate on raising 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 previous section. The dissemination strategy after the first year of the project and until its end will evolve more aggressively towards the spreading of the project results, the formulation of active user communities and potential HPC vendors and IT customers. **DCoMEX** will follow a dual dissemination strategy including publication in highly acclaimed international journals and conferences and by providing open-access (with the green open access model) to the project results.

3.1. Participation in Conferences - Scientific jounals

The dissemination of **DCoMEX** algorithms and methodologies will be properly and timely presented in renowned international conferences, forums, exhibitions and events including (but not limited to) a number of European Community in Computational Methods in Applied Sciences (ECCOMAS) Conferences such as ECCS and WCCM, IEEE Supercomputing and International Supercomputing conferences, publication of **DCoMEX** results in journals with very high impact including IEEE Transactions on Parallel and Distributed Systems, Mathematical Programming, SIAM Journal on Optimisation, Journal of Machine Learning Research, ACM Transactions on Parallel Computing, ACM Transactions on Experimental Algorithmics, ACM Transactions on Mathematical Software, Journal of Computational Physics, Computer Physics Communications, Computer Methods in Applied Mechanics and Engineering (CMAME), International Journal on Numerical Methods in Engineering (IJNME) and others. We will also engage with the European and International communities in relevant areas, such as through HiPEAC meetings, with presentations to PRACE meetings, with workshops for application scientists on utilising the tools we produce.

3.2. Open access

The **DCoMEX** consortium is heavily committed to providing unrestricted access to the project results. Towards this direction, in parallel with the publication in highly acclaimed conferences and journals, **DCoMEX** results will also be made available with the green open access model, i.e., by self-archiving the project results in the **DCoMEX** website, in order to gain the visibility of the scientific research and industrial communities. At the occasion of conflict with publishing agencies, the consortium will prioritise unrestricted access to the project results.

Beyond algorithmic methodologies and software modules, the consortium maintains the same philosophy of open access for other Research Data that will be produced during the implementation of the project, including models, validation results, experimental results These will be deposited in a research data repository and the consortium will take measures to make it possible for third parties to access, mine, exploit, reproduce and disseminate - free of charge for any user. Details on the data management policies are provided in the Data Management Plan (Deliverable D9.5).



4. Exploitation Activities

This section presents the activities that will be carried out in order to increase the project's visibility among stakeholders at an EU level and globally, attract investors for the productization of software and solutions based on the DCoMEX results and promote a business culture to each partner. These actions will help in shaping the sustainable futures for each of the project's results, either as single partner or as a whole. A joint exploitation plan will be developed on the basis of a comparative analysis with respect to other potential competitors based on the current market trends and perspectives.

4.1. Exploitation of DCoMEX project results

The following table summarizes the initial exploitation strategy for the software results of DCoMEX.

Result 1: UQ-aware image pre-processing engine

Responsible partner: TUM **IPR model:** Open-source.

Targeted end-users: Industrial users, supercomputing centres.

Integration with: MSolve, Korali platform

Result 2: CPU+GPU-enabled MSolve multiscale/multiphysics solver

Responsible partner: NTUA. **IPR model:** Open-source.

Targeted end-users: Researchers on algorithms relevant to stochastic multiscale optimisation.

Integration with: Korali

Result 3: Adaptive UQ and Bayesian analysis Korali engines

Responsible partner: ETHZ/CSELab

IPR model: Open-source.

Targeted end-users: Researchers on algorithms relevant to the stochastic multiscale analysis.

Integration with: MSolve

Result 4: AI-Solve library

Responsible partner: NTUA **IPR model:** Open-source

Targeted end-users: Industrial users, supercomputing centres, academic researchers.

Potential integration with: Co-design of future GPUs with NVIDIA as to the optimal ratio between tensor and CUDA cores. Integration with existing HPC environments, future Cray Shasta platform and the EuroHPC pre-

exascale LUMI system.

Result 5: The DCoMEX HPC framework

Responsible partner: CSCS IPR model: Open-source

Targeted end-users: Industrial users, supercomputing centres, researchers

Potential integration with: OpenPower software stack and libraries.

Result 6: DCoMEX-BIO software for cancer immunotherapy optimisation



Responsible partner: UCY IPR model: Patent protected

Targeted end-users: Software development and medical systems companies, hospitals, cancer research

centres, clinical oncologists.

Potential integration with: Currently available cancer modelling software at COMSOL

Result 7: DCoMEX-MAT software for material design

Responsible partner: NTUA IPR model: Patent protected

Targeted end-users: Software development and material companies, academic and research centres,

automotive, aerospace, building industries

Potential integration with: MATERIALIZE, a commercial material design software developed by NCOMP PC

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4.2. Exploitation plan per partner

4.2.1. NTUA exploitation plan

NTUA plans to integrate **DCoMEX** codes by fusing the Al-Solve library with MSolve and Korali platforms, provided by NTUA and ETHZ, respectively. The resulting framework will be customised to target specific bioengineering application in order to derive optimal routes for cancer immunotherapy. Besides this, NTUA will exploit the new platform for advanced composite materials analysis and design. The exploitation actions of NTUA technological results will be heavily based on the release of DCoMEX tool in the industry. The software produced herein will be directed to a wide marker including software companies, automotive, aerospace, industrial and housing applications. The exploitation plan starts with a market evaluation and market trend analysis. An analysis of the strong and weak points of the new exascale solver and its capabilities over conventional ones will follow, and a business plan of a startup Company is planned. Next, efforts will be pursued to increase product visibility by presentations in relevant scientific conferences in the domain (ECCOMAS Congress, EuroMech, UNCECOMP). The access to the open-source models and their use will be made public within networks of companies working in the health sciences and composites and materials community. NTUA has extensive links with automotive and transport companies working either in the supply chain or as main developers and integrators of components (TWT, Daimler), or even users of future secondary airframe structures made by sustainable materials (Airbus Innovation Works and GKN Aerospace plc). NTUA will also liaise with modelling and simulation networks dedicated to computational materials science like M-ERA.net and ECMI (European Consortium for Mathematics in Industry), as well as European Centers of Excellence in multiscale modelling (MAX and NoMaD), to maximise the visibility of the **DCoMEX** results. In addition, NTUA in collaboration with UCY will coordinate actions for invading health industrial sector (see UCY exploitation plan for more details).

4.2.2. ETHZ/CSELab exploitation plan

As a result of the **DCoMEX** project, ETHZ/CSELab's own project for extreme-scale Bayesian UQ and optimisation, Korali, will be highly optimised, documented, and disseminated. We expect to develop continuous improvements to the framework to both support the **DCoMEX** project and our own users' research. Several researchers within ETHZ/CSELab are currently using Korali for their own research and will benefit from the developments of this project. We expect to organise Korali/**DCoMEX**-specific symposia for industry and academic users at ETHZ/CSELab to educate and disseminate their use among the larger community. We will also publish regular updates and continue developing Korali's webpage and social media sites.

4.2.3 UCY exploitation plan

A central exploitation task of the project results from UCY will be the communication of the project results and the software capabilities of **DCoMEX** framework and its corresponding customisation **DCoMEX-BIO** to the medical industry. UCY team plans to visit and present the **DCoMEX-BIO** product to international investors (i.e. Venture Capital funds) and software/medical systems companies to attract their interest with the aim to establish commercial agreements or even licensing or co-developing the product with them.

4.2.4 TUM exploitation plan

DCoMEX will offer unprecedented means for making advanced tumour simulation methods available in a clinical setting, and to test various tumour growth and treatment response models on real clinical data. This aligns with the translational research ambitions of the Image-based Biomedical Modelling group and current research activities in brain tumour image analysis. At the same time, the TUM group is highly visible in the field of tumour image segmentation, for example, from the BRATS benchmark, and they will extend their work towards benchmarking UQ aware segmentation algorithms. This allows them to generate standardised medical image segmentation algorithms in different biomedical image processing tasks, and they will integrate them with the **DCoMEX** pre-processing workflow to foster exchange and quantitative evaluations of mathematical disease models.