Data driven Computational Mechanics at EXascale

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MANAGEMENT

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Period (30.3.2023-30.9.2024)

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1. Explanation of the work carried out by the beneficiaries and Overview of the progress

The purpose of the present deliverable is to outline management and progress of the project in the final period (30.3.2023-30.9.2024) of the project. These include coordination of the project, reporting supervision and intra-consortium communication support. More specifically, the report provides information about the activities carried out by the consortium, the progress overview towards the project objectives, milestones and deliverables, the problems encountered, and corrective actions taken, actual usage of resources and claim costs. The project also describes the progress of the management activities carried out during this reporting period.

1.1 DCoMEX results achieved with respect to Objectives

<u>SO1: Construction of AI-Solve an AI-enhanced linear algebra library</u> **Results** of the

project with respect to this objective:

- We have developed two sets of ML methodologies for dimensionality reduction and surrogate modelling, which include the Diffusion Maps Algorithm (DMAP) and Convolutional Autoencoders (CAEs) (See Deliverable D 2.1).
- We have developed and tested the AI-Solve library (D32. And D3.3) fusing data-driven methods and surrogate models with efficient block-iterative sparse linear system solvers. The proof of concept for this library has been published in ref [4] for linear systems and in ref [xx] for nonlinear systems. Moreover, AI-Solve library has been implemented for the solution pipeline of the DCoMEX-MAT and DCoMEX-BIO use cases in WP7 (See deliverables 7.1 and 7.2)

<u>SO2: Exascale deployment of MSolve and Korali software engines</u>

Results of the project with respect to this objective:

- We have developed MSolve to fully utilise the combined CPU and GPU potential of modern supercomputers (Piz Daint, ARIS and MELUXINA). We demonstrated software capabilities by providing performance and correctness test on physics-based computational models (See D6.4, D8.1, D8.2).
- We extended, upgraded and tested Korali engine to include state of the art sampling algorithms that harness extreme computation architectures and integrated it to DCoMEX framework (See D4.4, D 6.4).

<u>SO3: Pre-processing of experimental image data</u>

Results of the project with respect to this objective:

- We have developed 3D image and data processing routines that extract geometries together with estimates of their uncertainties that can be propagated to predictive simulators (See D5.1 and 5.2). We also developed and tested the post-processing final software (See D5.3 and 5.4)

<u>SO4: Integration of the DCoMEX framework, application and performance evaluation.</u>

Results of the project with respect to this objective:

- The combined Korali and MSolve/AI-Solve machinery has been successfully integrated and tested in Piz Daint HPC platform (See D6.1)
- We produced the baseline frameworks DCoMEX-BIO and DCoMEX-MAT for the applications of WP7 (See D7.1 and 7.2)
- We are continuously monitoring and evaluating the software in terms of scalability, parallel efficiency, energy efficiency, and data locality as well as energy efficiency as reported in D8.1 and D8.2.

- We developed DCoMEX platform as a modular and customisable software that can be used by the broader scientific community as well as by SMEs (See section 1.2.9- Exhibitions)

SO5: Scientific contributions and dissemination.

Results of the project with respect to this objective:

- We have applied the DCoMEX framework in multiscale material design applications and presented the results in corresponding Journal Papers and Conferences (See section 1.2.9)
- We have prepared dissemination material (Posters, leaflets and videos) and presented in DCoMEX platform as novel approach applicable to engineering problems to corresponding exhibitions (See section 1.2.9)

1.2 Explanation of the work carried per WP

1.2.1 Work Package 1

The Consortium Agreement Management actions of the project coordinator (PC) conducted in the second year of the project includes: i) Research coordination actions, i.e. Work Package and Task coordination, including software development and integration actions, ii) Data management actions coordination, iii) Administrative coordination of documents and reports delivered in the EU (i.e. deliverables) in relation to the project objectives and milestones, iv) Contractual and administrative issues and possible project amendments and, finally, v) actions for the horizontal collaboration plan and the Consortium agreement signed by all relevant project participants, vi) Preparation actions for the midterm 18M project review and vii) actions stemming from the reviewers ERS, vii) coordination of the annual meetings of the DCoMEX partners, including the presentation of the project results in a dedicated Workshop at the end of the project (Athens, 2-3 Sept 2024) viii) Coordination of partners and preparation of the final review meeting.

Project management and coordination

The following Committees and corresponding persons in charge continue their actions in the second year of the project:

The Exploitation Manager (EM): The Exploitation Management was initially assigned to ETH. However, after the review meeting it has been decided to boost the exploitation efforts and this role has been reassigned to NTUA. Towards, this direction, a number of actions have been organized as described in section 3 as well as in the amendment request that is being prepared.

The Communication Manager (CM): The CM George Stavroulakis (NTUA) designed and implemented the DCoMEX website and enriched it according to the ERS comments. Furthermore, all data produced are gathered in ZENODO and all software is in github (see section 1.2.1)

The DCoMEX Steering Committee (SC): The Project SC has been assembled in the frame of the first global DCoMEX and consists of V. Papadopoulos (NTUA), P. Koumoutsakos (ETH), T. Stylianopoulos (UCY), I. Ezhov (TUM) and. I. Hantzakis (GRNET). The SC was re-assembled in 27/05/2022 and decided unanimously for the changes that should be incorporated in the amendment request (see below). After Prof. Koumoutsakos leave, ETH was represented in the SC by Prof. Eleni Chatzi.

The DCoMEX Advisory Board (AB) was assembled, and feedback was given including comments for the final project results. These were mainly comments regarding the construction and further improvement of the AI-Solve library.

Monitoring of Software codes under development

The following software codes were developed and integrated in the framework of the DCoMEX project.

● Software module that implements the diffusion maps algorithm and the convolutional auto-encoders neural network architecture. Both these implementations are related to deliverables D2.1-D2.3 and were integrated in the Korali and MSolve open access software (NTUA)

● AI-Solve. An AI-enhanced linear algebra library with exascale capabilities for tackling extreme-scale problems. The AI-Solve library was developed (NTUA) as described in deliverables D3.1-D3.3 and integrated in MSolve in D6.4 (ETHZ).

● Software module for UQ aware image segmentation were prepared and used for the purposes of 3D geometry reconstruction from 3D images and image-based estimation of geometric uncertainties according to deliverables D5.1-D5.4 (TUM).

● DCoMEX-BIO, a customized version of MSOLVE/KORALI integration for cancer immunotherapy optimization related to D7.1. (NTUA/ETHZ/TUM/UCY).

● DCoMEX-MAT, a customized version of MSOLVE/KORALI integrated for optimum design of advanced materials related to D7.2 (NTUA/ETHZ).

This procedure is an integral part of the DCoMEX and was closely monitored in the corresponding Tasks by the Task and WP leaders and coordinated by the PC.

● Resources allocated so far

- Local NTUA GPU Cluster for code development and testing
- CSCS Piz Daint Supercomputer: 50.000 node hours per semester to conduct preliminary scaling experiments.
- ARIS SC at GRNET
- MELUXINA (As suggested by the Evaluation Summary Report (ESR))

Global Consortium assemblies

Two global Consortium assembly meetings were conducted during this period. The fifth global meeting was conducted on 3rd July 2024 as a remote meeting. The sixth and final Global Assembly meeting took place in the final DCoMEX workshop at 2-3 September 2024 in Athens. The Consortium will be reassmbeled before the final review meeting for wrapping up preparation.

5th preparatory meeting (3 July 2024 remotely) summary Participants: NTUA: V. Papadopoulos, George Stavroulakis, George Goumas, I. Kalogeris, ETH:, Sergey Litvinov, Sebastian Kaltenbach, UCY: Triantafyllos Stylianopoulos, Vasileios Vavourakis, TUM: Ivan Ezhov, Bjorn Menze (UZurich), Giles Tetteh (TUM), GRNET: Ilias Hatzakis , Dimitris Dellis.

6th final meeting (2-3 Sep 2024 in person) summary Participants: NTUA: V. Papadopoulos, Yiannis Kalogeris, Gerasimos Sotiropoulos, Stefanos Pyrialakos, George Goumas (NTUA), ETH:, Sergey Litvinov, Sebastian Kaltenbach, UCY: Triantafyllos Stylianopoulos (remotely), TUM: Ivan Ezhov, Bjorn Menze (UZurich), GRNET: Ilias Hatzakis

Working groups

The following working were active in the final year of the project.

1. (WG1) NTUA/UCY/ETH/TUM. This group developed DCoMEX-BIO software. NTUA/UCY developed the mathematical framework of the tumor growth model, implemented and tested it in MSolve and validated the DCoMEX-BIO results against results from COMSOL software. The TUM/NTUA/UCY/ETHZ team integrated the image pre and post processing in the DCoMEX-BIO framework.
3. (WG2) NTUA/ GRNET. This working group has been established for the integration of DCoMEX-BIO and DCoMEX-MAT at ARIS and MELUXINA for testing, benchmarking and performance evaluation

The two groups had regular weekly meetings and reported directly to the PC.

<u>Deliverables and Milestones monitoring</u>

An internal peer review is always performed for the main project deliverables to guarantee the deliverable is developed with a high level of quality and a common format has been implemented. Each WP leader submitted the produced documents to another partner assigned as internal reviewer to check for the quality of the documents produced. The project data will remain re-usable for at least 1 year after the project ends.

All deliverables were delivered on time with small deviations, while some of the Deliverables were amended. Specifically (the Deliverables of this period are marked in blue):

No	Name	Lead	Nature	level	Est Del.	Delivered
D1.1	First year progress periodic report	NTUA	R	CO	31.3.2022	27.6.2022
D1.2	Second year progress periodic report	NTUA	R	CO	31.3.2023	2.6.2023
D1.3	Third year progress periodic report	NTUA	R	CO	30.9.2024	30.9.2024
D2.1	DMAP algorithm prototype	NTUA	O	PU	30.11.2021	24.1.2022
D2.2	DMAP and CAE surrogate model	NTUA	R	PU	31.11.2022	12.5.2023
D2.3	DMAP and CAE implementation and validation	NTUA	R	PU	31.3.2023	3.10.2023
D4.1	A novel method for the sampling of Bayesian graphs for the inference of parameters in computationally demanding models, published in a refereed journal	ETHZ	O	PU	31.3.2022	22.6.2022
D4.2:	Creation, integration, and documentation of a new Korali module based on the methods developed in the previous item	ETHZ	O	PU	M20 (delivered)	28.4.2023 (Resubmitted after ERS comments)
D4.3	A novel load-balanced TMCMC-based method for scalable sampling	ETHZ	O	PU	31.3.2022	29.08.23

D4.4	Incremental versions of Korali	ETHZ	O	PU	30.11.2023	13.12.23
D5.1	UQ aware image segmentation software Prototype	TUM	O	PU	30.11.2021	11.2.2022
D5.2	UQ aware image segmentation final software	TUM	O	PU	31.3.2022	24.6.2022
D5.3	Post-processing final software (software module)	TUM	O	PU	31.3.2024	12.7.2024
D5.4	Data processing software final evaluation and documentation	TUM	R	PU	31.3.2024	12.7.2024
D6.1	System requirements, design and architecture	ETHZ	R	PU	31.9.2021	5.10.2021
D6.2	DCoMEX codes baseline prototype	ETHZ	O	PU	31.9.2021	5.11.2022
D6.3	DCoMEX codes baseline prototype	ETHZ	R	PU	31.9.2021	5.11.2022
D6.4	DCoMEX modules integrated in MSolve/Korali	ETHZ	O	PU	31.9.2021	5.11.2022
D7.1	DCoMEX-BIO v1.0	UCY	O	PU	31.12.2023	18.2.2024
D7.2	DCoMEX-BIO v1.0	UCY	R	PU	31.12.2023	18.2.2024
D7.3	DCoMEX-MAT v2.0	UCY	O	PU	31.12.2023	18.2.2024
D7.4	DCoMEX-MAT v2.0	UCY	O	PU	31.12.2023	18.2.2024
D7.5	Protocols of optimum cancer immunotherapy treatment	UCY	O	PU	30.9.2024	30.9.2024
D7.6	Optimum material compositions for CNT reinforced concrete applications	UCY	O	PU	30.9.2024	30.9.2024
D7.7	DCoMEX-BIO and DCoMEX-MAT commercialization plan	UCY	O	PU	30.9.2024	30.9.2024
D8.1	Performance evaluation of DCoMEX-BIO	GRNET	O	PU	31.7.2024	30.9.2024
D8.2	Performance evaluation of DCoMEX-MAT	GRNET	O	PU	31.7.2024	30.9.2024
D9.1	DCoMEX Website	ETHZ	DEC	PU	30.6.2021	30.9.2021
D9.2	Communication, dissemination and exploitation plan	ETHZ	R	PU	30.9.2021	2.11.2021
D9.3	Communication, dissemination and exploitation plan	ETHZ	R	PU	3.11.2022	3.11.2022

D9.4	Communication, dissemination and exploitation plan	ETHZ	R	PU	30.09.2024	30.09.2024
D9.5	Data Management Plan	ETHZ	ORPD	PU	30.9.2021	18.10.2021
D9.6	Collaboration Plan	NTUA	R	PU	30.9.2021	28.9.2021

All Milestones have been met and verified according to the following table (the Milestones met in this final period are marked in blue):

Mileston e No.	Milestone name	WP	Due date	Verified by
1	Project start	1	M1	Kick-off meeting
2	Communication, dissemination and exploitation plan produced	9	M6	Documentation
3	UQ aware image segmentation final software (software module)	5	M12	Software released and validated
4	First year Progress Periodic Report	1	M12	Documentation
5	DMAP and CAE implementation and validation Report	2	M26	Software released and validated,
6	Second year Progress Periodic Report	1	M24	Documentation
7	AI-Solve performance evaluation (report)	3	**M33**	Documentation
8	Incremental versions of Korali	4	**M33**	Software released and validated
9	DCoMEX-MAT and DCoMEX-BIO developed	7	**M33**	Software prototypes released and
10	Protocols for optimum cancer immunotherapy treatment	7	**M42**	Documentation
11	Optimal material composition for reinforced concrete applications	7	**M42**	Documentation
12	Post-processing methodology Report	5	**M42**	Documentation
13	Data processing software final evaluation and documentation (report)	5	**M42**	Documentation

14	Performance evaluation of DCoMEX-MAT and DCoMEX-BIO prototypes	8	**M42**	Software released, validated, evaluated and
15	Third year Progress Final Report	1	**M42**	Documentation
16	Project end	1	**M42**	Documentation

1.2.2 Work package 2

Task 2.1: Implementation of the data-informed sampling scheme (M12-M18)

The Transitional Markov chain Monte Carlo (TMCMC) was used to sample the Bayesian posterior of a transferable Red Blood cell model. A data-driven neural network was employed which successfully reduced the computational costs of the sampling.

Task 2.2: DMAP surrogate implementation (M2-M16).
This Task has been completed. However, as reported in the minutes of the 2nd project meeting, we decided to implement Convolutional Auto-encoders surrogates in addition to the Diffusion Maps described originally in the proposal. The reasons for this change have been clearly explained by the WP Leader (V. Papadopoulos) and were analytically reported in the corresponding deliverable D2.1. Some extra PMs are planned as well as an extension to the end month of the deliverable from M8 to M16. This extra time is required for the transition from DMAP to CAE. This change along with other project adjustments, was included in the first amendment request.

Task 2.3 DMAP and CAE implementation and validation Report (M9-M24)
This Task has been completed. Due to the delay in Task 2.2 this task was also delayed and finished M24.

Task 2.4, Implementation of the surrogate refinement strategy (M17-M24):
This Task has been completed. Due to the delay in Task 2.2 this task was also delayed and finished M24.

Task 2.5, Implementation of a surrogate validation strategy (M21-M26):
This Task is progressing according to the schedule. Due to the delay in Task 2.2 this task was also delayed and finished M24.

1.2.3 Work package 3

Task 3.1 DDM preconditioners for exascale systems (M1-M10)
This task has been completed as scheduled.

Task 3.2 Surrogate models for preconditioning and coarse problem solution(M1-M20)
This task has been completed as scheduled.

Tasks 3.3 Inexact Solvers for scalability end error resilience (M5-M24)
This task has been completed as scheduled.

Tasks 3.4 Sparse Computations (M5-M24)
This task has been completed as scheduled.

Tasks 3.5, 3.6 and 3.7

The Tasks 3.5 “Communication Optimization” (M5-M36), 3.6 “Fault Tolerant- Energy aware operation” (M5-M36) and 3.7 “Algorithmic Implementation of AI-Solve exascale considerations” (M7-M36), have been completed succesfully.

1.2.4 Work package 4

Task 4.1 Development of a novel hierarchical Bayesian sampling method (M2-M10)

This Task has been accomplished as scheduled. A novel methodology for the sampling of complex Bayesian graphs was developed in this task and reported in the Journal Publication of Deliverable D4.1.

Task 4.2 Extension of the Korali for the description of general Bayesian direct acyclic graphs (M2-M10)
This Task has been accomplished as scheduled. The descriptive language of Korali will be extended in order to accommodate the description of complex Bayesian problems. To this extend the results of Task 4.1 have been integrated into the Korali framework to be used in the integration process with MSolve in WP6 and used in the applications of WP7.

Task 4.3 Reducing the cost of evaluating the likelihood function using surrogate models **(M2-M26)**

The ETH/CSELab team tried to develop the load-balanced scalable sampling algorithm described in the Task 4.3. However, their efforts were not successful, and this Task cannot be met. An alternative strategy was pursued and a novel load-balanced TMCMC-based method for scalable sampling was proposed (D4.3). However, this shift resulted in a delay of delivering this Task (form M10 to M26)

Task 4.4, Integration of the new methods in the Korali framework (M12-M26)

This Task has been completed resulting in an optimized and functional Korali software (See D4.4). Due to the delay in the Tasks 4.2 and 4.3 this was also delayed and completed M26.

1.2.5 Work package 5

Task 5.1 Algorithms for 3D geometry reconstruction from 3D images (M1-M10)

A prototype of the UQ aware image processing model has been constructed and reported in Deliverable D5.1. It makes algorithms for 3D geometry reconstruction from 3D images available. Standard image processing and deep learning algorithms have been further employed for the processing of arbitrary 3D images. Data are exported in the form of meshes and FEM discretizations are generated and fed to MSolve. WG3 is working in a weekly basis integrating this software to MSolve and preparing for the applications in WP7.

Task 5.2 Image-based estimation of geometric uncertainties (M1- 12)

In this Task the final additions to the UQ aware image processing model and software tool were implemented. As reported in the Deliverable D5.2, this extension includes algorithms for 3D geometry reconstruction from 3D images. The D5.1 report contains the specifications of Task 5.2 and describes the image-based estimation of geometric uncertainties that has now been added to the image segmentation software tool.

Task 5.3: Post-processing and visualising simulation results (M36)
The tools for enabling the post-processing and result data analytics were be provided and further optimised for the application cases studies. This Task was completed successfully.

1.2.6 Work package 6

Tasks 6.1, 6.2 and 6.3

Tasks 6.1 "Software and hardware requirements" (M1-M6), 6.2 "System design and architecture" (M2-M4) and 6.3 "Software engineering framework" (M1-M6), have been completed. These outcomes are described in detail in the Deliverable D6.1 report.

Task 6.4 Integration (M7-M24)

This central task of the DCoMEX software product has been accomplished. For the development of the MSolve/Korali platform integration, WG3 was created. First the MGroup and ETHZ-CSELab integrated MSolve and Korali and tested their combined functionality with a use case that uses Korali to perform parameter inference for a relatively simple heat transfer model implemented in MSolve. The integrated model was implemented with the assistance of ETHZ-CSCS in a containerised environment with CI/CD. With this, target of having the DCoMEX prototype deployed in Piz Daint by M15 was met successfully.

DCoMEX software framework has been fully tested and deployed on CSCS' Alps system with the following key tasks accomplished:

- Integration of the AISolve module.
- Implement a generic API for running user-provided models and inference.
- Test a prototype of DCoMEX-BIO model in the framework.
- Comprehensive online documentation for users of the Framework.

Task 6.5 Low level code optimization (M7-M36)

Task 6.5 focusses on low-level code optimisation of the modules – namely MSolve, AISolve and Korali – when running in the integrated DCoMEX framework on representative HPC systems. In order to perform this work two components are required: first, the integrated framework developed in Task 6.4; and second, a representative model that has computational complexity on the same order as the final DCoMEX-BIO and DCOMEX-MAT use cases. This work was completed M36 since the first prototype version of DCoMEX-BIO was available on M28 (the final prototypes were delivered in M33 (D7.1 and D7.2).

Work on code optimization was performed by the partners in WG1 responsible for each software module, NTUA for MSolve/AISolve and ETHZ-CSELab for Korali, This Task was amended and delivered M36 instead of M24 initially planned.

Task 6.6 Testing and benchmarking (M13-M36)

The framework for testing and deploying the DCoMEX Framework has been prioritized - given the complexity requirements of the software modules. CSCS took the lead on this work to: i) provide a containerized environment that supports MPI, CUDA, Python and .NET runtimes ii) implement separate CI/CD workflows for MSolve and Korali iii) implement a CI/CD pipeline for the integrated framework that tests and deploys the framework on the Piz Daint system at CSCS, iv) provide continuous improvement to the CI/CD tooling and support to the partners. In parallel, GRNET has independently tested the DCoMEX software modules on the ARIS system, both bare-metal and in Singularity containers. A detailed description of the testing framework, CI/CD workflow and its open-source implementation are described in the report for the M15 deliverable D6.2, and the open-source prototype is available on GitHub.

Similarly, to the optimization work in T6.5, benchmarking of the DCoMEX framework requires the DCoMEX-BIO and DCoMEX-MAT prototype to perform benchmarks on representative workloads. Early implementation of representative benchmarks was performed by NTUA with the assistance of CSELab in M20. However, since the first versions of the prototypes were available in M28, this Task was amended as well and completed M36 instead of M24 initially planned.

1.2.7 Work package 7

Task 7.1: Development and integration of the mathematical and computational model into the DCoMEX framework Participants: NTUA, ETHZ/CSELab, UCY, TUM Duration: M5-M42

For this Task, UCY developed the mathematical framework of a tumour growth model and worked together with MGroup (NTUA) for the implementation of the equations in the MSolve software platform. This way, a prototype of the DCoMEX-BIO software platform was created and tested against simple advection-diffusion-reaction equations. DCoMEX-BIO was then extended to include the total parameters and equations of the tumor growth model and the immunotherapy treatment (injections) and validate the results with results from corresponding models run in COMSOL software.

Task 7.1.1 Verification and model validation with preclinical and clinical data (M5-M42)

DCoMEX-BIO was informed with pre- clinical data obtained from the UCY team for both treated and non-treated cases, using Bayesian inference. As a final stage, the MSolve/Korali framework of DCoMEX-BIO was applied in order to optimize the cancer immunotherapy treatment. A final validated and tested prototype version of the DCoMEX-BIO software has been launched.

Task 7.1.2: Derivation of protocols for optimized use of immunotherapy, Participants: NTUA, ETHZ/CSELab, UCY, TUM Duration: M24-M42

Multiple simulations were repeated varying, within the physiological/pathophysiological range, the values of the key model parameters identified by task 7.1.1 to affect the solution of the model. Also, the parameters of the tumour microenvironment were varied to correspond to different tumour types and stages of progression. From the model predictions, a map was constructed to depict the optimum therapeutic outcome (i.e., extent of tumour shrinkage) as a function of the model parameters. A detailed report is provided in D.7.5

Task 7.2: Multiscale modelling of CNT reinforced concrete structures, Participants: NTUA, ETHZ/CSELab, UCY, TUM Duration: M5-M42

A multiscale modelling framework for structures made up of concrete reinforced with carbon nanomaterials was developed. First, isolated fillers (GRF, CNT/G) were modelled at the nanoscale. Random mesoscale RVEs were then generated. A macroscale nested FE2 solution scheme was constructed for the structure, which encompasses all scales and delivers the overall mechanical properties of the system. An initial dataset of these off-line calculations will be used to construct DNN surrogate as the AI-Solve solver for this application.

Task 7.2.1: Verification and model validation, Participants: NTUA, ETHZ/CSELab, UCY, TUM Duration: M5-M42

The results of the numerical simulations obtained in Task 7.2.1 were systematically compared with experimental data in all scales, using hierarchical Bayesian analysis and the informed model was used for subsequent analyses

Task 7.2.2: Optimum design of materials – next generation RCs, Participants: NTUA, ETHZ/CSELab, UCY, TUM Duration: M24-M42

In this Task, optimum designs of RCs reinforced with 3D structured networks of carbon inclusions was computed using topology the results (material) obtained in Task 7.2.1 and topology optimization leading to next generation RC compositions with optimal mechanical properties.

Task 7.3: DCoMEX-BIO and DCoMEX-MAT commercialisation plans, Participants: NTUA, ETHZ/CSELab, UCY, TUM Duration: M20-M42

DCoMEX project employs novel HPC-enhanced Linear Algebra and Machine Learning (ML) methods in order to predict and monitor tumours growth and response to immunotherapy (DCoMEX-BIO), and design innovative materials and structures (DCoMEX-MAT). The main objective is to develop simulation software integrated with HPC methods to serve as a commercial tool for i) radiologists/medical doctors to differentiate responders from non-responders to immunotherapy protocols and make personalized/customised therapy decisions (DCoMEX-BIO) and ii) Engineers in construction and materials to design and virtual test new material compositions (DCoMEX-MAT).

Both of this software requires further development after the project's end before commercialization for: 1. Further improvement and optimization and 2. Development of user-friendly GUIs. To this purpose additional funding will be seeked via applications for research grands, both national and international, a number of which has already been send by members of the consortium. At the present state, and after an extensive market research, the consortium realised that the competition in software products related to materials and structures is very high, with new products launched and supported by established parties and compamies in the field such as ANSYS and ABAQUS. Even though DCoMEX-MAT includes significant innovations, wspecially in the HPC and ML related technologies, it is foreseen that it will be extremely hard to effectively position DCOMEX-MAT in the market. On the contrary, as will be analysed below in detail, DCoMEX-BIO has a large potential with respect to current market competition. Therefore, the consortium has decided to focus on DCoMEX-BIO and put all efforts in taking the steps further to evolve it.

Focusing on the DCoMEX-BIO commercialization plan, this may involve patent development and licensing and establishing a spin-off company and or partnering with industrial players. Additional strategies include attracting venture capitalists and considering licensing or co-development with industrial partners. The Minimum Viable Product (MVP) targets end-users like radiologists and oncologists in the EU for a small-scale trial, evaluating technical aspects and generating interest from potential investors or partners in oncology, biotech and industry. The general plan is at the end to construct a joint venture formed by DCoMEX members and the relevant SMEs that will own the product. To this purpose, we are already in the process of signing a MoU with 2 European SMEs (NCOMP, AnaBiosi-Data Ltd).

In D7.7, we first analyze the external macroenvironment so that to reveal threats (risks) and opportunities. Then, bearing in mind the characteristics of the project we present a SWOT analysis, which is followed by a global market overview in the related industries. This is followed by a strategy section where options for monetisation and go-to-market are presented. Thereafter, the report analyses the business opportunity in the EU and sets-up a strategic commercialization plan to achieve it.

1.2.8 Work package 8

Task 8.1 Evaluation and improvement of efficiency and Scalability (M8-M40)

For this task WG4 has initiated its activities. Following the MSolve/Korali integration in Piz Daint and using similar procedures, WG4 launched the deployment of MSolve/Korali integrated software (DCoMEX platform) in ARIS and MELUXINA supercomputers. In parallel to this deployment, a continuous monitoring-evaluation of the software in terms of scalability, parallel efficiency, energy efficiency, and data locality has been performed As a final outcome of this Task, energy efficiency were also tested and reported D8.1.

Task 8.2: Evaluation of fault tolerance and error resilience (M8-M40)

Following the completion of Task 6.4 with the deployment of DCoMEX/BIO and DCoMEX/MAT in Piz Daint, ARIS and MELUXINA. This Task monitors the deployed DCoMEX software with respect to fault tolerance and error resilience. This evaluation has been completed successfully and reported in D. 8.2

1.2.9 Work package 9

Tasks 9.1, 9.2, 9.3 and 9.4

Tasks 9.1, 9.2, 9.3 and 9.4 correspond to communication, dissemination and exploitation activities, respectively. A detailed plan and actions for all these activities was prepared (M6) and reported in Deliverable 9.2, including the DCoMEX website (D9.1). These documents outline the planning of the communication, dissemination and exploitation activities undertaken by the consortium members to maximize the project's outreach and visibility, raise awareness over the project's actions and share its results with all interested third parties. These documents also illustrate the strategy and implementation steps followed by each partner to achieve these goals along with a general timeline. A list of action for the first 12M of the project is described in detail in D9.2, for the next period (until 24M) in D9.3, while a concluding report that contains the final period (until M42 - end of the project) in D9.4. In brief this is presented in the following:

Communication activities

Project's website (D9.1): 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.

Use of WEB 2.0: A social media channel was established using the Facebook platform (https://www.facebook.com/dcomex.eu). New content was regularly posted to notify the audience about the recent developments of the project, hosted events and our conference participations.

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/), which is regularly updated.

Dissemination activities

Type of Dissemination	Status	Title	Authors	Journal
Journal article	published	Machine learning accelerated transient analysis of stochastic nonlinear structures	S. Nikolopoulos, I. Kalogeris, V. Papadopoulos	Engineering Structures, 2022 https://www.sciencedirect.com/science/article/pii/S0141029622001663
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, 2022, https://www.sciencedirect.com/science/article/pii/S0045782522004510
Conference Paper	published	A for-loop is all you need. For solving the inverse problem in the case of personalized tumor growth modeling	I. Ezhov, M. Rosier, L. Zimmer, F. Kofler, S. Shit, J.C. Paetzold, K. Scibilia, F. Steinbauer, L. Maechler, K. Franitza, T. Amiranashvili, M.J. Menten, M. Metz, S. Conjeti, B. Wiestler, B. Menze	Proceedings of Machine learning Research, 2022, https://proceedings.mlr.press/v193/ezhov22a/ezhov22a.pdf
Journal article	published	An adaptive semi-implicit finite element solver for brain cancer progression modeling	K. Tzirakis, C.P. Papanikas, V. Sakkalis, E. Tzamali, Y. Papaharilaou, A. Caiazzo, T.	International Journal for Numerical Methods in Biomedical Engineering, 2023

			Stylianopoulos, V. Vavourakis	https://onlinelibrary.wiley.com/doi/abs/10.1002/cnm.3734
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, 2023 https://www.sciencedirect.com/science/article/pii/S0017931022008894
Journal article	published	Multiscale analysis of nonlinear systems using a hierarchy of deep neural networks	S. Pyrialakos, I. Kalogeris, V. Papadopoulos	International Journal of Solids and Structures, 2023 https://www.sciencedirect.com/science/article/pii/S0020768323001580
Journal article	published	The stress-free state of human erythrocytes: data driven inference of a transferable RBC model	L. Amoudruz, A. Economides, G. Arampatzis, P. Koumoutsakos	Biophysical Journal, 2023 https://www.sciencedirect.com/science/article/pii/S0006349523001728
Journal article	Published	Learn-Morph-Infer: A new way of solving the inverse problem for brain tumor modeling	I. Ezhov, K. Scibilia, K. Franitza, F. Steinbauer, S. Shit, L. Zimmer, J. Lipkova, F. Kofler, J.C. Paetzold, L. Canalini, D. Waldmannstetter, M.J. Menten, M. Metz, B. Wiestler, B. Menze	Medical Image Analysis, 2023 https://www.sciencedirect.com/science/article/pii/S1361841522003000
Journal article	Published	Toward image-based personalization of glioblastoma therapy: A clinical and biological validation study of a novel, deep learning-driven tumor growth model	M.C. Metz, I. Ezhov, J.C. Peeken, J.A. Buchner, J. Lipkova, F. Kofler, D. Waldmannstetter, C. Delbridge, C. Diehl, D. Bernhardt, F. Schmidt-Graf, J. Gempt, S.E. Comps, C. Zimmer, B. Menze, B. Wiestler	Neuro-Oncology Advances, 2023 https://academic.oup.com/noa/article/6/1/vdad171/7502543?login=true
Journal article	published	AI-enhanced iterative solvers for accelerating the solution of large-scale parameterized systems	S. Nikolopoulos, I. Kalogeris, G. Stavroulakis, V. Papadopoulos	International Journal for Numerical Methods in Engineering, 2024 https://onlinelibrary.wiley.com/doi/10.1002/nme.7372
Journal article	published	Fusing nonlinear solvers with transformers for accelerating the solution of parametric transient problems	L. Papadopoulos, K. Atzarakis, G. Sotiropoulos, I. Kalogeris, V. Papadopoulos	Computer Methods in Applied Mechanics and Engineering, 2024 https://www.sciencedirect.com/science/article/pii/S004578252400330X
Journal article	published	Personalized in silico model for radiation-induced pulmonary fibrosis	E. Ioannou, M. Hadjicharalambous, A. Malai, E. Papageorgiou, A. Peraticou, N. Katodritis, D. Vomvas, V. Vavourakis	Journal of the Royal Society Interface, 2024 https://zenodo.org/records/13766990
Journal article	published	Solving inverse problems in physics by optimizing a discrete loss: Fast and accurate learning without neural networks	P. Karnakov, S. Litvinov, P. Koumoutsakos	PNAS nexus, 2024 https://academic.oup.com/pnasnexus/article/3/1/pgae005/7516080
Workshop paper	published	Improving the accuracy of Coarse-grained Partial Differential Equations with Grid-based Reinforcement Learning	JP. von Bassewitz, S. Kaltenbach, P. Koumoutsakos	ICML AI4Science workshop https://openreview.net/pdf/415fef02819878bd898609f08910380a7521b08a.pdf

Journal article	published	An efficient hierarchical Bayesian framework for multiscale material modeling	S. Pyrialakos, I. Kalogeris, V. Papadopoulos	Composite Structures, 2025 https://www.sciencedirect.com/science/article/pii/S0263822324006986
Journal article	submitted (accepted)	Generative Learning for the Effective Dynamics of Complex High-dimensional Systems	H. Gao, S. Kaltenbach, P. Koumoutsakos	Accepted at Nature Communications Preprint available at https://arxiv.org/abs/2402.17157
Journal article	submitted (under review)	Individualizing Glioma Radiotherapy planning by Optimization of a Data and Physics-Informed Discrete Loss	M. Balcerak, J. Weidner, P. Karnakov, I. Ezhov, S. Litvinov, P. Koumoutsakos, R.Z. Zhang, J.S. Lowengrub, I. Yakushev, B. Wiestler, B. Menze	Preprint available at https://arxiv.org/pdf/2312.05063
Journal article	submitted (under review)	Interpretable learning of effective dynamics for multiscale systems	E. Menier, S. Kaltenback, m. Yagoubi, M. Schoenauer, P. Koumoutsakos	Preprint available at https://arxiv.org/abs/2309.05812
Journal article	submitted (under review)	Interpretable reduced-order modeling with time-scale separation	S. Kaltenbach, P.S. Koutsourelakis, P. Koumoutsakos	Preprint available at https://arxiv.org/abs/2303.02189
Journal article	submitted (under review)	Closure Discovery for Coarse-grained Partial Differential Equations with Grid-based Reinforcement Learning	JP. von Bassewitz, S. Kaltenbach, P. Koumoutsakos	Preprint available at https://arxiv.org/abs/2402.00972
Journal article	submitted (under review)	A learnable prior improves inverse tumor growth modeling	J. Weidner, I. Ezhov, M. Metz, S. Litvinov, S. Kaltenbach, M. Balcerak, L. Feiner, L. Lux, F. Kofler, J. Lipkova, J. latz, D. Rueckert, B. Menze	Preprint available at https://arxiv.org/abs/2403.04500
Journal article	submitted (under review)	Predictive surrogates for Aerodynamic Performance of Wind Propulsion System Configurations	M. Reche-Vilanova, S. Kaltenbach, P. Koumoutsakos, H.B. Bingham, M. Fluck, D. Morris, H.N. Psaraftis	-
Journal article	submitted (under review)	Quantitative 3D histochemistry reveals region-specific amyloid-β reduction by the antidiabetic drug netoglitazone	F. Catto, E. Dadgar-Kiani, D. Kirschenbaum, A. Economides, A.M. Reuss, C. Trevisan, D. Caredio, D. Mirzet, L. Frick, U. Weber-Stadblauer, S. Litvinov, P. Koumoutsakos, J.H. Lee, A. Aguzzi	Preprint available at https://www.biorxiv.org/content/10.1101/2024.08.15.608042v1.full
Journal article	submitted (under review)	Generative Learning of the Solution of Parametric Partial Differential Equations using Guided Diffusion Models and Virtual Observations	H. Gao, S. Kaltenbach, P. Koumoutsakos	Preprint available at https://arxiv.org/abs/2408.00157

Table 1: Overview of scientific publications in peer reviewed Journal papers

Type of Dissemination	Date	Presenter	Title	Title of Conference/Workshop
Conference	9.06.2022	G. Sotiropoulos	Large deformation multi-scale analysis of thin nanocomposite shell structures	ECCOMAS 2022, Oslo

Workshop	14-15.06.2022	G. Stavroulakis	(responsible for DCoMEX booth)	Teratec Forum, The European meeting for Experts in Digital technologies Simulation, Paris
Workshop	19-20.09.2022	G. Stavroulakis	(responsible for DCoMEX booth)	First EuroHPC19 Projects collaboration workshop. Madrid
Conference	29.09.2022	V. Papadopoulos	Data Driven Material Design at Exascale	International Symposium on Polymer Nanocomposites (ISPN 2022), France
Conference	20-23.03.2023	V. Papadopoulos	DCoMEX: Data Driven Computational Mechanics at Exascale (poster session)	EuroHPC Summit 2023, Gothenburg, Sweden
Conference	12-14.06.2023	G. Stavroulakis	MSOLVE – A Loosely coupled multiparadigm HPC computational simulation suite	5th International Conference on Uncertainty Quantification in Computational Science and Engineering, Athens, Greece
Conference	12-14.06.2023	I. Kalogeris	AI-SOLVE: FUSING LINEAR ALGEBRA WITH MACHINE LEARNING TO ACCELERATE THE SOLUTION OF LARGE-SCALE PARAMETRIZED SYSTEMS	5th International Conference on Uncertainty Quantification in Computational Science and Engineering, Athens, Greece
Conference	23-27.07.2023	M. Balcerak	Inference of Brain Tumor Dynamics From a Time Series of Tumor Segmentations for Personalized Therapy Design by a Discrete Loss Optimization	17^{th} U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico, US.
Conference	23-27.07.2023	I. Kalogeris	Multiscale Analysis of Structures Composed of Composite Materials Using a Hierarchy of Deep Neural Networks	17^{th} U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico, US.
Conference	23-27.07.2023	V. Papadopoulos	AI-Solve: Fusing Machine Learning and Linear Algebra to Accelerate the Solution of Large-Scale Parametrized Systems	17^{th} U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico, US.
Conference	28-30.08.2023	S. Kaltenbach	Efficient Uncertainty Quantification and Bayesian Analysis for Computational Mechanics at Scale	3^{rd} International Conference on Computational Science and AI in Industry, Trondheim, Norway
Workshop	11-13.12.2023	S. Kaltenbach	Korali: Stochastic Optimization and Bayesian Inference	Mathematical Opportunities in Digital Twins, Washington
Conference	12-16.05.2024	E. Chroni	DCoMEX: Data-driven computational mechancis at exascale	ISC High Performance, Hamburg, Germany
Workshop	12.06.2024	S. Kaltenbach	Physics-aware reduced order modelling for forecasting the dynamics of high-dimensional systems	Scientific machine learning for simulation and inverse modelling, KTH Royal Institute of Technology, Sweden

Conference	24-26.06.2024	M. Balcerak	Modeling Brain Tumor Mass Effect via Optimization of a Physics-Informed Discrete Loss	8th International Conference on Computational & Mathematical Biomedical Engineering, George Mason University, Virginia, US.
Conference	3-7.07.2024	S. Kaltenbach	Learned Effective Dynamics (LED) and Bayesian methods for patient-specific cancer immunotherapy	ECCOMAS 2024, Lisbon
Conference	3-7.07.2024	M. Balcerak	Integrating Mass Effects in Glioma Radiotherapy planning by Optimization of a Data and Physics informed discrete loss	ECCOMAS 2024, Lisbon
Conference	3-7.07.2024	G. Sotiropoulos	AI-based Surrogate Modelling Techniques for Time Dependent Parametrized Mathematical Models of Cancer Immunotherapy	ECCOMAS 2024, Lisbon
Workshop	26.07.2024	S. Kaltenbach	Improving the accuracy of Coarse-grained Partial Differential Equations with Grid-based Reinforcement Learning	ICML AI4Science Workshop, Vienna
Workshop	2-3.09.2024	V. Papadopoulos	Data Driven Computational Mechanics at Exascale: DCoMEX project results	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
Workshop	2-3.09.2024	I. Kalogeris	A transformers -based AI approach for generating physics informed dynamics	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
Workshop	2-3.09.2024	S. Litvinov	Scaling Up: DCoMEX-Framework for Surrogates and Uncertainty Quantification at Exascale	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
Workshop	2-3.09.2024	G. Sotiropoulos	Surrogate models for large and coupled bioengineering problems	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
Workshop	2-3.09.2024	B. Menze	Modeling tumor growth for radiation treatment planning in DCoMEX and Beyond	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
Workshop	2-3.09.2024	T. Stylianopoulos	Mathematical modeling to guide cancer immunotherapy	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
Workshop	2-3.09.2024	G. Goumas	Computations on sparse data perform embarrassingly bad. Can we do something about it	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens

Table 2: Overview of participations in conferences/workshops

Exploitation activities

This exploitation activities for the project’s results 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.

The key exploitable results of the project, as stated in the proposal, are given in table 3.

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 were tasked with promoting it to relevant stakeholders, SMEs, academic institutions, and other research groups in the HPC ecosystem. The following concrete steps were undertaken towards this direction:

1. The UCY partner responsible for **R6** DCOMEX-BIO demonstrated the progress of the project and its potentials with AI and data analysis company AnaBioSi-Data Ltd (https://www.anabiosi-data.com/).
2. The TUM partner responsible for the pre- and post-processing of **R6** DCOMEX-Bio developed specialized software tools to facilitate the analysis and visualization of complex biological simulations. These tools were designed to improve the accuracy and efficiency of bio-mechanical modeling, such as simulations of tumor growth and fluid flow in biological systems. Demonstrations of the pre- and post-processing open-source software were conducted for academic partners within the consortium and at the host institutions.
3. The NTUA partner responsible for **R7** DCOMEX-MAT developed a demonstrator showcasing the software's capabilities in designing new high-performance materials with target mechanical properties**.** Adopting an in-person sales model, the capabilities of the software were presented to two SMEs, namely TWT (https://twt-innovation.de/en/) from Germany and Trygons (https://trygons.com/el/) from Greece. A pilot project was initiated with TWT for the design of lightweight vehicle parts with increased crashworthiness, made up carbon nanomaterial reinforced polymers. Similarly, a second pilot project was discussed with Trygons for the development of ship hulls made up of reinforced polymers.
4. The assets **R2**, **R3** and **R4** are expected to have a strong academic impact and therefore these results were communicated to researchers through journal publications and conference presentations, aiming to establish long-term collaborations.
5. The ETH partner responsible for Results **R3** and **R5** published the code related to DCoMEX on GitHub (https://github.com/DComEX) such that the framework is easily accessible for further use. Moreover, a minisymposium titled 'Advancing Predictive Simulations under Uncertainty: AI and UQ for Computational Mechanics' was organized at ECCOMAS 2024 to provide a platform to present results and increase awareness for the project within the scientific community.
6. During the project's operation, we achieved the deployment of the DCOMEX HPC framework in the Piz Daint, Aris and Meluxina HPC centers (**R5**). Efforts will be further pursued towards promoting the installation of this framework and its related constituents (**R1** and **R4)** to other supercomputing centers.
7. 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 were pursued by NTUA to companies developing simulation software, to advertise its capabilities and seek product sales and/or co-development.

In general, all members took actions towards the establishment of tactical alliances with other industrial or research organizations that hold the potential of promoting the DCOMEX results.

Collaboration plan

The Collaboration plan organizes all efforts to establish synergies and collaboration with the complementary grants listed under Article 2 of the DCoMEX Grant Agreement. The First Deliverable (6month) is the work plan of this project (New Deliverable 9.6) has been successfully delivered. The Project Agreement has been prepared and signed by DCoMEX partners.

The following actions were coordinated in this period:

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.

We have initiated such collaboration with SparCity project, and we have identified 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, we have arranged two preparatory meetings to exchange project description and app description, identify common objectives and proceed with the preparation of the collaboration plan (Milestone 1). We have also established a common working group to further develop our synergy, identify Tasks and explore the potential of achieving the Objectives (Milestone 2). For the forthcoming period we are planning to arrange quarterly meetings with the working group to update each other on project progress (Milestone
3).

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

2. Financial monitoring

The 75% pre-financing arrived at NTUA was distributed to all partners according to the approved project's budget as follows:

	Total EU requsted (€)	Prefinincing	%
Project	1.359.375	1.019.531,25	75
NTUA	465.625	349.218,75	75
ETHZ	506.250	379.687,5	75
UCY	125.000	93.750	75
TUM	153.125	114.843,75	75
GRNET	109.375	82.031,25	75

An additional 10% arrived at NTUA after the midterm review was distributed to all partners according to the approved project's budget as follows:

	Total EU requested (€)	After review	%
Project	1.359.375	135.937.5	10
NTUA	465.625	46.562.5	10
ETH	506.250	50.625.0	10
TUM	125.000	12.500	10
UCY	153.125	15.312.5	10
GRNET	109.375	10.937.5	10

3. Data management

As described in detail in the Data management plan (D9.6), the DCoMEX data outputs are collected and managed by the following web-based tools and repositories:

DCoMEX project's portal: This portal can be found in http://mgroup.ntua.gr/dcomex/ which acts as the first layer of the data management system for research in the field of computational mechanics and HPC computing. It has a link with all publications, data sets, software and other types of research products available online.

ZENODO: an open online research data repository. This repository is provided by OpenAIRE and it allows researchers to deposit both publications and data, providing tools to link them through persistent identifiers and data citations. Its purpose is to facilitate the finding, accessing, re-using and interoperating of data sets, in compliance with FAIR data principles. In this regard, it enables researchers, scientists, EU projects and institutions to:

-Share research results in a wide variety of formats including text, spreadsheets, audio, video and images across all fields of science

-Display their research results and get credited by making the research results citable and integrating them into existing reporting lines to funding agencies like the European Commision.

-Easily access and reuse shared research results.

-Integrate their research outputs with the OpenAIRE portal.

In addition, Zenodo allows performing simple and advanced search queries using keywords.

- GitHub: Git-based repository, where all code implementations and documentation will be stored, and data versioning and backups will be performed. For the moment the following codes have been stored:

  - https://github.com/mgroupntua/MSolve.core
  - https://github.com/cselab/korali
  - https://github.com/dcomex
  - https://github.com/dcomex-BIO
  - https://github.com/dcomex-MAT

All files and folders at data repositories will be versioned and structured by using a name convention of the following format: DCOMEX_Dx.y_YYYYMMDD_Vzz.doc, referring to the specific deliverable of the project, the date it was created and its version.

4. 18M Review meeting and ERS

The evaluation result summary (ERS) of the Review meeting that took place on 9th November 2022 in Luxemburg was very satisfactory with an overall positive evaluation of the project. The reviewers raised the following comments for which we have initiated corresponding reactions:

[Comment 01] The baseline at the start of the project in terms of software development as well as contributions per partner needs to be clearly defined and documented. In order to justify and claim the declared resources, this should be provided in sufficient detail in the next review, at the latest. The information should be documented in detail in the next progress report.

Reaction: As stated in the technical part of the DCoMEX submission, MSolve is a robust, high-performance multi-physics and multi-scale distributed solver. It is designed with parallelism in mind, supporting distributed execution of both multiprocessor CPU and GPU kernels using MPI and CUDA, respectively. Its core components have been tested in HPC platforms, however its state before the start of the project was at TRL 5. The solvers supported were the standard CG with Jacobi preconditioners along with Cholesky factorizations. A previous fork of MSolve had a TRL 2 level module for hierarchical parallelism with DDM but it has not been ported to the current version of MSolve. Moreover, no modules pertaining to AMG, artificial intelligence and their combination whatsoever were developed and there were no plans for block variants of CG, relaxed precision arithmetic and communication optimization for the algorithms.

On the other hand, Korali is a high-performance framework for uncertainty quantification, optimization, and deep reinforcement learning. Its engine provides support for large-scale HPC systems and a multi-language interface compatible with distributed computational models. Korali has been developed by the CSElab at ETHZ.

[Comment 02] The work performed during the project has to be clearly reported with respect to this baseline.

Reaction The work done to MSolve until now and the work to be done until the end of the project is connected to the work described in the WPs of the project. Specifically, all work of WP3 which comprises AISolve is manifested as a series of MSolve modules (e.g.: block-CG, extra DDM preconditioners, relaxed precision arithmetic, etc.) along with some basic AI modules (e.g.: diffusion maps, convolutional auto encoders, neural networks, etc.). AISolve uses these modules in order to construct the appropriate pipeline for it to solve computational mechanics problems using the fusion of all these methodologies. This pipeline is customized for the DCoMEX framework, for the solution of the specific problems of WP7. Moreover, tasks 6.5, 6.6 and WP8 also affect the aforementioned MSolve modules with respect to their performance and robustness. Progress of all this work is described in detail in the present report.

Regarding Korali, we have significantly extended its engine during the project, with respect to the aforementioned baseline. We have added algorithms based on TMCMC to specifically sample from hierarchical Bayesian posteriors in a massive parallel way. Moreover, we have provided the possibility to pass the Bayesian posteriors as probabilistic graphical models to Korali and have implemented a check that ensures that these graphical models are acyclic. In WP 4.3 we have additionally added a gradient-based version of the novel TMCMC algorithm that can speed-up the computations in case gradients should be available. For latent variables model, we have added modules based on CMAES and the Expectation-Maximization algorithm. Another improvement to Korali pertains to define an easily accessible interface to combine Korali with frameworks such as MSolve, which was implemented during the DCoMEX project.

Additionally, we have made Korali available directly in a (docker) container such that the software framework can be easily used on a cluster or other high-performance computing system. Extensive benchmarks have been run to ensure that the container-based versions scale well for parallel computing.

[Comment 03] The consortium shall homogenize their deliverables, using the same template and avoid submitting unedited scientific publications. Each deliverable should be self-contained and provide sufficient technical detail and analysis.

Reaction: Rejected deliverables D4.1, D.4.3, D5.1, D5.3, D9.1 and 9.3 have been enriched, homogenized and resubmitted.

[Comment 04] A risk mitigation strategy should be developed factoring in the possible of key personnel departure. This is of particular importance with respect to the contribution of partners subject to departure of the Principal Investigator (ETHZ and TUM).

Reaction: These risks have been addressed. Indeed, we faced the leave of some key personnel in 2 partners. Specifically, the persons in charge in ETH and TUM, Prof. P. Koumoutsakos and Prof. Bjoern Menze have left these institutions and consequently the project as well. However, both of their working research teams remain in ETH and TUM, respectively and remain fully active in DCoMEX. In TUM, Prof. Daniel Rukkert is now officially in charge of the DCoMEX research team. Therefore, we do not foresee any problem with the continuation of TUMs participation and contribution to the project in the future. Regarding ETH and Prof. Koumoutsakos leave, he has been officially replaced by Prof. Eleni Hantzi, as the new person in charge of the DCoMEX project on behalf of ETH. The 2 PostDoc students that are already involved in the DCoMEX project, Dr. Sebastian Caltenbach and Dr. Sergey Litvinov will remain in ETH and continue working in the development of the KORALI integration into the DCoMEX framework and applications under the supervision of Prof. Hatzi. In addition, both Prof. Koumoutsakos and Prof. Menze have expressed their willingness/commitment to support the newly appointed WP leaders and provide them with their expertise and guidance.

[Comment 05] It is not fully transparent that all resources spent on travel activities were necessary to achieve the objectives of the DoA. A detailed list, including all attended meetings, scopes and participants from the consortium, shall be provided. Otherwise, the JU might reserve the right to withhold travel funding.

Reaction: The list has been provided and approved by the JU.

[Comment 06] The collaboration between DCoMEx and SparCity needs to be continued further even expanded to training and dissemination activities. Further connections need to be established with NCCs to approach a wider audience.

Reaction: DComEx and SparCity continue their collaboration. They established two EuroHPC-19 CPCB workstreams on Sparse computations and HPC applications and first results will be presented in the CPCB meeting in Turin, 7 June 2023. DCoMEX is also in close collaboration with EUROCC via GRNET and has programmed the following joint actions:

-Repository

- Training

- Webinar on “**Fast and Powerful Machine Learning Tools in Engineering: Hands-On Applications**”, Online Workshop, organised by EuroCC@Greece in partnership with the National Infrastructures for Research and Technology (GRNET), the National Technical University of Athens (NTUA) and the University of Pretoria (UP), on May 11th.

- Identification and contact of regional SMEs

In addition, a few SMEs have been proposed by the EUROCC. These SMEs were reached by the DCmMEX EM and meetings have been arranged to presented DCmMEX results and exploit potential synergies.
A number of SMEs were invited in the final DCmMEX workshop in Athens (2-3 Sept 2024) and shared their results. A round table was organized and a fruitfull discussion took place, which concluded in a roadmap witn next steps towards adoption of DCmMEX results as well as HPC practices form regional SMEs.

[Comment 07] The consortium shall improve the project's internet presence.

Reaction: The Dissemination and Exploitation Manager has initiated the process of communicating the project’s internet presence. All DCmMEX events and results will be posted in the project´s web page and communicated to social media.

[Comment 8] The consortium shall also link the software repositories from the project web site.

Reaction: This has been done for the software that already developed and will be done for the final products as well.

[Comment 09] The consortium is advised to improve dissemination actions in social networks.

Reaction: See reaction to R01

[Comment 10] Monitor potential end-users that can validate the performance and feasibility of the proposed methods in industrial relevant applications.

Reaction: Apart from the SMEs that were contacted, the DCmMEX Exploitation team develops a pilot material desing application with TWT Gmbh, while discussions are in progress with ANSYS UK in order to test the AI-SOLVE library in relevant industrial applications.

[Comment 11] The needs of the stakeholders and communities should be examined and monitored, and an exploitation plan should be prepared.

Reaction: As above (see reaction in R05 and R06)

[Comment 12] Dissemination and training activities need to be directed towards real user and industry needs. Success stories and use cases need to be documented, highlighted, and communicated.

Reaction: As above (see reaction in R06)

[Comment 13] A sustainability plan for the time after the project's ending should be developed.

Reaction: This was developed in D7.7.

[Comment 14] The combined Korali and MSolve/AI-Solve machinery should be ported to EuroHPC JU systems. This should be taken into account in a revised risk mitigation strategy, as requested in the preceding recommendations, and in an updated dissemination and exploitation plan.

Reaction: The combined Korali and MSolve/AI-Solve machinery was ported to MELUXINA.

[Comment 15] The collaboration with SparCity on sparse matrices should be continued and developed further and also extended training and dissemination activities. Connections with National Competence Centres for HPC should be established to approach a wider audience.

Reaction: As above (see reaction in R05)

5. CONCLUSIONS

Despite the financial and administrative obstacles that some of the project members are facing from national funding bodies, all targets of the project have been met successfully. Deliverables and milestones have been reached and delivered with small delays. Success story of the project was demonstrated by the project's applications and disseminated by all members of the consortium via the dissemination channels of the project. The results of the project are open and reachable via the project's website as well by open access to ZENODO and GITHUB repositories of the project. A commercialization plan has been prepared leading to the next day of the project which will be oriented to both research and business. Towards this, a number of follow-up proposals have already been submitted, while others are going to be submitted in the forthcoming period. A first version of a business plan is being prepared targeting a joint venture between SMEs and partners of the project.