Data driven Computational Mechanics at EXascale

DCoMEX

Data driven Computational Mechanics at EXascale

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MANAGEMENT : Second Year Progress Periodic Report

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1.0	14/05/2023	Vissarion Papadopoulos	NTUA	Initial version

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 second year 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

SO1: Construction of AI-Solve an AI-enhanced linear algebra library

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 and ref [1-3].
- We are continuously developing and improving AI-Solve library 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 (ref [4]).

SO2: Exascale deployment of MSolve and Korali software engines.

Results of the project with respect to this objective:

- We are continuously optimising MSolve to fully utilise the combined CPU and GPU potential of modern supercomputers. Demonstrate software capabilities by providing performance and correctness test on physics-based computational models.

- We are extending and upgrading the Korali engine to include state of the art sampling algorithms that harness extreme computation architectures (See D4.1).

SO3: Pre-processing of experimental image data

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).

SO4: Integration of the DCoMEX framework, application and performance evaluation.

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 are in the process of producing the baseline frameworks DCOMEX-BIO and DCOMEX-MAT for the applications of WP7
- Continuous monitoringand evaluation of the software in terms of scalability, parallel efficiency, energy efficiency, and data locality is in progress. Energy efficiency considerations are foreseen at a later stage of the project’s progress.
- We are developing 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 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.

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).

The DCoMEX Advisory Board (AB) has not yet been assembled. We plan to assemble it and have feedback in the forthcoming period of the project.

Monitoring of Software codes under development

The following software codes are being 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 will be 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 is related to deliverables D3.1-D3.3 and will be integrated in MSolve (NTUA).
● Software module for UQ aware image segmentation that will be 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 customised version of MSOLVE/KORALI integration for cancer immunotherapy optimization related to D7.2. (NTUA/ETHZ/TUM/UCY).
● DCoMEX-MAT, a customised 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 is 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 MSOLVE code development and testing
- ● CSCS Piz Daint Supercomputer: 50.000 node hours per semester to conduct preliminary scaling experiments.
- ● ARIS SC at GRNET

As suggested by the ESR, we will also deploy DCOMEX in MELUXINA in the forthcoming period.

Global Consortium assemblies

Three global Consortium assembly meetings were conducted during this period. In the second year of the project the third global meeting was conducted on 1st July 2022 as an in-person meeting that took place in Spetses island in Greece. The Consortium was reassmbeled before the Midterm review on 19/10/2022 for wrapping up preparation for the review meeting that took place on 9/11 in Luxemburg. Next meeting is planed for July 2023 in Athens.

3rd in person meeting (2 July 2022 in Spetses island - Greece) summary Participants: NTUA: V. Papadopoulos, George Stavroulakis, S. Pyrialakos, Theofilos Christodoulou, George Goumas, Panos Metsis, I. Kalogeris, ETH: Sergey Litvinov, Sebastian Kaltenbach, Lucas Amodruz, UCY: Triandafyllos Stylianopoulos (remotely), Vasileios Vavourakis (remotely), TUM: Ivan Ezhov, Bjorn Menze (UZurich), Giles Tetteh (TUM), GRNET: Ilias Hatzakis (remotely), Dimitris Dellis (remotely), EuroHPC Project Officer: C. Scalese (remotely).

4th preparatory meeting (19 October 2022 remotely) summary Participants: NTUA: V. Papadopoulos, George Stavroulakis, George Goumas, I. Kalogeris, ETH:, Sergey Litvinov, Sebastian Kaltenbach, UCY: Triandafyllos Stylianopoulos, Vasileios Vavourakis, TUM: Ivan Ezhov, Bjorn Menze (UZurich), Giles Tetteh (TUM), GRNET: Ilias Hatzakis , Dimitris Dellis.

Working groups

The following working groups have been established and are active also in the second year of the project.

1. (WG1) TUM/NTUA group, integrates the TUM image processing tools to MSolve platform
2. (WG2) NTUA/UCY for the development DCOmEX-BIO software. This group develops the mathematical framework of the tumor growth model, implements it in MSolve and validates the results with results from existing models in COMSOL software. In a later stage starting from 1/07/2022, the group was augmented as TUM/NTUA/UCY/ETHZ for the preparation of the clinical data processing in the MSolve/Korali framework.
3. (WG3) NTUA/ETH(CSELab and CSCS). A working group has been established for the integration of MSolve and Korali at Piz Daint.
4. (WG4) NTUA/ETH/GRNET NTUA/ETH (CSELab and CSCS). A working group has been established for the integration of MSolve and Korali to ARIS network for testing and then possibly to LUMI for benchmarking.

All groups have regular meetings and report directly to the PC.

Deliverables and Milestones monitoring

An internal peer review is 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.

In this first period, all deliverables were delivered on time with small deviations. Specifically

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	31.3.2022	2.6.2023
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	Amended to M26	-
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	Cancelled
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
D6.1	System requirements, design and architecture	ETHZ	R	PU	31.9.2021	5.10.2021
D6.2	DCoMEX codes baseline prototype (Software)	ETHZ	O	PU	31.9.2021	5.11.2022
D6.3	DCoMEX codes baseline prototype (Report)	ETHZ	R	PU	31.9.2021	5.11.2022
D6.4	DCoMEX DCoMEX modules integrated in MSolve/Korali (Software)	ETHZ	O	PU	31.9.2021	5.11.2022
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 (report on activities – redesign and plan)	ETHZ	R	PU	3.11.2022	3.11.2022
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 for this period have been met and verified according to the following table

Milestone 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

Next Milestones that are on track, include the Milestones for critical software releases are presented in the following table

Milestone No.	Milestone name	WP	Due date	Means of verification
5	DMAP and CAE implementation and validation Report	2	M26	Software released and validated, Documentation
6	Second year Progress Periodic Report	1	M24	Documentation
7	AI-Solve performance evaluation (report)	3	M28	Documentation
8	Incremental versions of Korali	4	M28	Software released and validated
9	DCoMEX-MAT and DCoMEX-BIO developed	7	M30	Software prototypes released and validated
10	Protocols for optimum cancer immunotherapy treatment	7	M36	Documentation
11	Optimal material composition for reinforced concrete applications	7	M36	Documentation
12	Post-processing methodology Report	5	M36	Documentation
13	Data processing software final evaluation and documentation (report)	5	M36	Documentation
14	Performance evaluation of DCoMEX-MAT and DCoMEX-BIO prototypes	8	M36	Software released, validated, evaluated and documented
15	Third year Progress Final Report	1	M36	Documentation
16	Project end	1	M36	Documentation

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

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/ and it will act as the first layer of the data management system for research in the field of computational mechanics and HPC computing. It will link 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

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.

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 an amendment request.

Task 2.3 Implementation of surrogate model (M9-M24)
This Task has been completed. Due to the delay in Task 2.2 this task has also to be delayed until 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 has also to be delayed until 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 has also to be delayed until M26.

1.2.3 <u>Work package 3</u>

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 following Tasks 3.5 “Communication Optimization” (M5-M30), 3.6 “Fault Tolerant- Energy aware operation” (M5-M30) and 3.7 “Algorithmic Implementation of AI-Solve exascale considerations” (M7-M36), have been initiated and are progressing according to the schedule. We have prioritized these Tasks in the next period.

1.2.4 <u>Work package 4</u>

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 in order 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. The corresponding deliverable is cancelled and an alternative strategy will be pursued in the project in replacement of this Task. A report has been initiated justifying this conclusion. The PC has been informed that this issue is minor and does not affect the progress of the proposal. We need to extend the deadline for this Task form M10 to M26

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

This Task has been initiated and is progressing according to the schedule. Due to the delay in the Tasks of WP2 this task has also to be delayed until 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.

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 will be delayed until M36 since the first prototype of DCoMEX-BIO was available on M24.

Work on the optimization will be performed by the partners in WG3 responsible for each software module, NTUA for MSolve/AISolve and ETHZ-CSELab for Korali, when the first prototype DCOMEX-BIO model is available. We need to extend the deadline of this Task from M24 to M36.

Task 6.6 Testing and benchmarking (M13-M36)

The framework for testing and deploying the DCoMEX Framework has been prioritised - given the complexity requirements of the software modules. CSCS took the lead on this work to: i) provide a containerised 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 prototype to perform benchmarks on representative workloads. Implementation of representative benchmarks will be performed by NTUA, with the assistance of CSELab in M20. The partners TUM and UCY also plan to provide use cases and models for testing and validation of the framework. We need to extend the deadline of this Task from M24 to M36.

1.2.7 Work package 7

Task 7.1 BioEngineering Application: Verification and model validation with preclinical and clinical data (M5-M36)

For this Task, WG2 (NTUA/UCY) has been created for the development, testing and validation of the DCOmEX-BIO software. The group meets on a weekly basis. UCY developed the mathematical framework of the tumour growth model and worked together with MGroup for the implementation of the equations in the MSolve Platform. A first prototype is already available and tested against simple advection-diffusion-reaction equations. At the moment WG2 extends DComEX-BIO to include the total parameters and equations of the tumor growth model and validate the results with results from existing models in COMSOL software as well as with pre-clinical data obtained from the UCY team and related to cancer immunotherapy. In a later stage, starting from 1/07/2022, the group was augmented with the addition of ETHZ (TUM/NTUA/UCY/ETHZ) for the preparation of the clinical data processing in the MSolve/Korali framework. A validated and tested prototype version of the DComEX-BIO software has been launched on M24.

Task 7.2 Material Design Application: Verification and model validation (M5-M36)

In This Task, the DCoMEX integrated platform project, has been customized for material design applications. Towards this, the DComEX-MAT version of the DComEX platform is being developed in parallel to Task 6.5 (DComEX integration). The focus until now by the NTUA team has been the investigation of heat transfer phenomena on polymers reinforced with carbon nano-materials such as carbon nanotubes and graphene sheets. It has been theorised that the synergy between polymers and carbon nanomaterials would lead to highly thermally conductive materials. However, recent experimental works showed that this is not the case due to the significant negative impact of thermal resistance at the interface of polymers and nanomaterials [5]. This phenomenon has been numerically studied by the NTUA team members, and optimal microstructural configurations for certain scenarios have been identified [6]. The outcome of this investigation demonstrated that nano-reinforced polymers can attain higher conductivity values under certain conditions, but not as high as initially expected. Some further investigation on this will be conducted. Due to the aforementioned deviation from the initial target of obtaining a highly conductive material and in order to pursue the aim of a successful material design story in the frame of the DComEX project, NTUA team decided to extend the research to structural problems, as well. Carbon nanomaterials can greatly enhance the mechanical properties of conventional building materials such as concrete and the overall structural performance since they have an extraordinarily high modulus of elasticity (0.1-1.7 TPa), they are lightweight, fatigue and corrosion resistant, and they act as crack arrestors. This change has been decided to be included in an amendment request later this year together with some extra PMs to account for the additional effort but without requesting additional budget. The DCOMEX/MAT validated version will be launched in M26.

1.2.8 Work package 8

Task 8.1 Evaluation and improvement of efficiency and Scalability (M8-M36)

For this task WG4 has initiated its activities. Following the MSolve/Korali integration in Piz Daint and using similar procedures, WG4 has launched the deployment of MSolve/Korali integrated software (DComEX platform) in ARIS and LUMI supercomputers. In parallel to this deployment, a continuous monitoring-evaluation of the software in terms of scalability, parallel efficiency, energy efficiency, and data locality is in progress. Energy efficiency considerations are foreseen at a later stage of the project progress.

Task 8.2: Evaluation of fault tolerance and error resilience

This task follows the completion of Task 6.4 with the deployment of DCOMEX/BIO and DCOMEX/MAT in Piz Daint and ARIS. This Task has been initiated and proceeds according to the scheduled plan.

1.2.9 Work package 9

Tasks 9.1, 9.2 and 9.3

Tasks 9.1, 9.2 and 9.3 correspond to communication, dissemination and exploitation activities, respectively. A detailed plan for all these activities has been prepared (M6) and reported in Deliverable 9.2, including the DCoMEX website (D9.1). This document outlines the planning of the communication, dissemination and exploitation 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. A list of action for the first 12M of the project is described in detail in D9.2. The updated list for the 18M period is as follows:

Journal Articles:

1. **Machine learning accelerated transient analysis of stochastic nonlinear structures**, S. Nikolopoulos, I. Kalogeris, V. Papadopoulos, *Engineering Structures*, Volume 257, 2022
2. **Domain Decomposition Methods for 3D crack propagation using XFEM**, S. Bakalakos, M. Georgioudakis, M. Papadrakakis, Computer Methods in Applied Mechanics and Engineering, in press (https://doi.org/10.1016/j.cma.2022.115390), 2022.
3. **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*, to appear in Volume 200, January 2023
4. **AI-enhanced iterative solvers for accelerating the solution of large-scale parametrized systems,** S. Nikolopoulos, I. Kalogeris, G. Stavroulakis, V. Papadopoulos, submitted to the *International Journal of Numerical Methods in Engineering*, *under review* *(preprint available at* arXiv:2207.02543v3*)*
5. **Multiscale analysis of nonlinear systems using a hierarchy of deep neural networks**, S. Pyrialakos, I. Kalogeris, V. Papadopoulos, submitted to *International Journal of Solids & Structures*, V. 271–272, 1 June 2023, 112261, International Journal of Solids and Structures.
6. **The stress-free state of human erythrocytes: data driven inference of a transferable RBC model**, Amoudruz, L., Economides, A., Arampatzis, G., & Koumoutsakos, P., 122(8):1517-1525, doi: 10.1016/j.bpj.2023.03.019, Biophysical Journal 2023.

Conference presentations:

1. **Data Driven Material Design at Exascale** (plenary talk), International Symposium on Polymer Nanocomposites (ISPN 2022), September 2022, France
2. **Data Driven Material Design at Exascale,** invited talk at Laboratoire Modelisation et Simulation Multi Echelle (MSME), University Gustave Eiffel, Paris, France
3. **Large deformation multi-scale analysis of thin nanocomposite shell structures,** G. Sotiropoulos, V. Papadopoulos, ECCOMAS 2022, Oslo
4. **Quantum Computing for uncertainty quantification in engineering,** K. Atzarakis, V. Papadopoulos , ECCOMAS 2022, Oslo
5. (Upcoming) **EuroHPC** minisymposium in **UNCECOMP 2023, June 2023, Athens**

Exhibitions:

1. **Teratec Forum 2022** – DCOMEX presence in EuroHPC booth at the Europa Village, Paris, France, 2022
2. **EuroHPC Summit 2023** - DCOMEX presentation, Goteborg, 2023
3. **ISC 2023** (upcoming): DCOMEX participation in common EuroHPC booth exhibition area.

Workshops:

1. Workshop **"Quantum Computing and its synergy with High Performance Computing in Engineering Sciences and Applications"**, Spetses Island, Greece, July 2022. The workshop was carried out in parallel to the regular 3rd DCOMEX program meeting and explored the synergies of HPC with quantum computing tools.
2. First EuroHPC19 Projects Collaboration Workshop, Madrid 2022
3. HiPEAC workshop Monday Jan. 16, 2023

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 in order 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. Use of resources

The following deviations regarding the use of resources are foreseen:

1. Reduce PM allocation for ETHZ by 7 PM, from 95 PM to 88 PM (to adjust for higher per PM costs in CH, with commitment to meet obligations with slightly fewer resources):

-12 FTE reduction to ETHZ/CSCS (from 23 to 11)
· CSCS allocation is now 11 FTE
· CSCS focusses on WP6 and WP1
- 5 FTE increase for ETHZ/CSElab (from 72 to 77)
· ETHZ/CSELab takes responsibility for CSCS' previous small contributions in WP3, WP8 and WP9.

3. 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, the following SMEs have been proposed by the EUROCC. These SMEs were reached by the DCOMEX EM and meetings have been arranged to presented DCOMEX results and exploit potential synergies.

BIOEMTECH	https://bioemtech.com/	Παναγιώτης Παπαδημητρούλας	panpap@bioemtech.com	HEALTH	biochemistry - Provision of high performance and low cost imaging systems
DELTA MPS	www.delta-ms.gr	Μάριος γκουλεμάνης	mgoulem@delta-ms.gr	MATERIALS	digital tools/ materials, nanomechanics
FEAC engineering	www.feacomp.com	Σωτήρης Κόκκινος	sotiris.kokkinos@feacomp.com	ENGINEERING	digital twins/ engineering simulations
GIVE ENGINEERING	https://www.give-engineering.com/Capability.html	Ηλίας Νασιόπουλος	i.nassiopoulos@gmail.com	ENGINEERING	aerodymanics and computational fluid dynamics
SOFISTIK	http://www.sofistik.gr/	Σωτήρης Μπιτζαράκης, Νίκος Κόκλας,	info@sofistik.gr, linkedin.com/in/sotiris-bitzarakis-9840517	CFD, CAD	engineering software
ENIOS	https://e-nios.com/	Ελευθέριος Πιλάλης	info@e-nios.com	HEALTH	biomarkers, drug design
Scienomics	https://www.scienomics.com/	Ξενοφών Κροκίδης	info@scienomics.com	MATERIALS	Materials
METPIKON	www.metricon.gr	Κωνσταντίνος Νικολάου	nikolaou@metricon.gr	Manufacturing	automation
ABcurD	https://abcured.com	Κατερίνα Χατζάκη	achatzak@med.duth.gr	HEALTH	biomarkers, drug design
ADVANTIS	https://advantis.io/	Dimitris Rozakis, Zoi Giavri	info@advantis.io	HEALTH	Medical Imaging

[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 DCOMEX 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 DCOMEX 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 R0..)

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

Reaction: This will be developed and incorporated in D9.4

[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 will be ported to MELUXINA. This deployment has been initiated.

[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)