EuroHPC
Joint Undertaking

Data driven Computational Mechanics at EXascale

DCoMEX

Data driven Computational Mechanics at EXascale

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MANAGEMENT

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1. DESCRIPTION

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

The purpose of the present document (D1.1) is to outline the first year management and progress report issues of the project. These include coordination of the project, reporting supervision and intra-consortium communication support. More specifically, the report provides with 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.

2. MANAGEMENT ACTIONS SUMMARY

The Consortium Agreement Management actions of the project coordinator (PC) conducted in the first period of the project are summarized here. These include first research coordination actions, i.e. Work Package and Task coordination, including software development and integration actions, data management actions coordination, the administrative coordination of documents and reports delivered in the EU (i.e. deliverables) in relation to the project objectives and milestones and finally, contractual and administrative issues and possible project amendments and finally the actions for the horizontal collaboration plan and the Consortium agreement signed by all relevant project participants.

2.1. Project management and coordination

The consortium management ensures that each task leader is being supported adequately in his responsibility for administrative coordination and performance control of the Task-related operations, (e.g., meetings, cost-statements, summary reports, deliverables etc.) ensuring that adequate resources are at the disposal of the project. In this direction, the following Committees and corresponding persons in charge were agreed and initiated in the KoM of the project:

The Exploitation Manager (EM): Exploitation, dissemination and Intellectual Property Rights issues will be coordinated at the consortium level by the Exploitation Manager. The Exploitation Manager will be the Leader of WP9 dealing with demonstration, evaluation, exploitation and dissemination of the project results. The Exploitation Manager will be responsible for the Deliverables of WP9 (Innovation management and Technological Implementation). The DComEX EM role was assigned to **George Arampatzis** (ETHZ).

Communication Manager: The communication manager makes an intensive use of available communication tools such as teleconferences and videoconferences as well as electronic mail communications in order to promote speed and efficiency of interactions. The CM will be responsible for DCoMEX website. A secure site hosted by the coordinator (NTUA) will allow all partners access the collection of all data and information. The DCoMEX CM role was assigned to **George Stavroulakis** (NTUA).

The DComEX Steering Committee (SC).

The SC represents the interests of all partners in the project. Each partner will have one representative on the SC. An agreement will be typically sought through building consensus amongst the partners. Consensus will follow the rule of simple majority; all decisions should be supported by half plus one of the partners. A conflict resolution mechanism will be implemented as defined later in General Agreement (GA) and Consortium Agreement (CA). The SC will be responsible for interacting with the project's Advisory Board. The SC will be chaired by the Coordinator and will meet once every six months or more often if this is required. The Project SC has been assembled in the frame of the first and

second global DComEX meetings and agreed to proceed to the requested project amendments as these are described in Section 7

The DComEX Advisory Board (AB).

The AB of the project consists of Prof. Bernhard Schrefler, University of Padova (research field: mechanics of biological materials and bioengineering applications), Prof. Yousef Saad, University of Minnesota (research field: numerical methods for sparse linear systems), Prof. Karen E. Willcox, University of Austin, TEXAS (research field: Reduced-order and multi-fidelity modeling). The AB has not yet been assembled.

2.2 Monitoring of Software codes under development

The following software codes are being developed and integrated in the frame of 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 exascale 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 customized version of MSOLVE/KORALI integration for cancer immunotherapy optimisation related to D7.2. (NTUA/ETHZ/TUM/UCY).
- DCoMEX-MAT, a customized 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

- 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.

2.3 Project meetings

2.3.1 Global Consortium assemblies

Two global Consortium assembly meetings were conducted during this period. The first one was the kick-off meeting conducted on 11th of May 2021 and the second one conducted on the 6th of December 2022. Due to COVID pandemic, both meetings were virtual (by teleconference). The third meeting is programmed for the 1st July 2022 and is going to be an in person meeting in Spetses island in Greece.

Kick-off meeting (11th of May 2021) summary

Participants. NTUA: V. Papadopoulos, George Stavroulakis, I. Kalogeris, S. Nikolopoulos, G. Sotiropoulos, S. Pyrialakos, Theofilos, George Goumas, ETH: Petros Koumoutsakos, George Arampatzis, Martin Sergio, Benjamin Cumming, UCY: Vasileios Vavourakis, Odysseas Kokkinos, Miranda Panagi, Fotos Mpekris, TUM: Ivan Ezhov, Bjorn Menze (UZurich), GRNET: Ilias Hatzakis, Dimitris Dellis

The meeting followed exactly the following meeting Agenda, as scheduled.

Agenda

Time (CET)	Topic	Lead
10:00	Welcome - Review of the Agenda - Goals	NTUA
10:15	DCoMEX in the EuroHPC framework – Goals	D.Opalka (Officer)
10:30	Project overview	NTUA
11:00	Introduction of partners (5 minutes per Partner)	All
11.30	WP1 Management Issues	NTUA
11:45	WP2 Surrogate Modeling	NTUA
12:00	WP3 AI-Solve Library	NTUA
12:30	Break	
13:30	WP4 UQ and Bayesian analysis	ETHZ/CSELab
14:00	WP5 - Preprocessing (Data manegement)	TUM
14:30	WP6 – Software Integration, Optimization and Testing	ETH/CSCS
15:00	Break	
15:30	WP7 - Applications	UCY/NTUA
16:00	WP8 – Performance Evaluation	GRNET
16:30	WP9 – Communication – Dissemination Exploitation plan	ETHZ/CSELab NTUA
17:00	Wrap-up discussions, next meetings	NTUA
17:30	End of Day	

The Project Coordinator V. Papadopoulos initiated the meeting, reviewed the Agenda and presented the Goals and Objectives of the project. Then, the project Officer Daniel Opalka, presented the framework of EuroHPC JU and positioned DCoMEX within this context. The Project Coordinator followed with a more detailed description if the DCoMEX project, reviewed its results, its expected impact, its specific Work Packages and tasks as well as deliverables and milestones with emphasis in those starting early (M1-M6).
At this point and when V. Papadopoulos (NTUA) referred to the HPC facilities that need to be committed, and particularly Piz Daint at CSCS and LUMI, Ben Cumming from CSCS commented that the requested resources might be excessive and in all cases a sub proposal should be prepared and submitted in due time in order for the project to access these facilities. Particularly LUMI, can be accessed via PRACE.

At that point, Petros Koumoutsakos (ETH) commented that a EuroHPC JU should facilitate the access of the funded grants to the European HPC facilities so that no additional proposals should be necessary for such access. The Project Officer answered that this is a discussion that is being active in the EuroHPC board but for the moment no such procedure is available and access should be granted via PRACE. The panel suggested that all members should activate their representatives to the EuroHPC board and asked Daniel Opalka to transfer such request on behalf of the project partners.

The project partners and specifically Benjamin Cumming from CSCS agreed to prepare such proposals for accessing LUMI and Piz Daint, while D. Dellis and I. Hatzakis said that they would also prepare similar proposals for other HPC facilities via PRACE. They also proposed that ARIS HPC facility (GRNET) could be used for development.
Next, the partners introduced their research teams and described their expertise with respect to the project.
After this presentation, each WP leader with the help of corresponding Task Leaders summarized the Work Packages and Tasks of the Projects.

V. Papadopoulos started with WP1 and presented the management structure of the project. The synthesis of the steering committee was discussed, consisting of one representative from each partner. Therefore, the following persons were decided to participated in the SC.

1. V. Papadopoulos (NTUA)
2. P. Koumoutsakos (ETH)
3. T. Stylianopoulos (UCY)
4. I. Ezhov (TUM)
5. I. Hantzakis (GRNET)

In addition, V. Papadopoulos informed the Consortium that the Pre-Financial Payment of 75% has been arrived to NTUA and will be distributed to the partners by the end of May.

The PC informed the Consortium about the parallel EuroHPC collaborative project and the contribution of DCoMEX to this effort. The consortium authorized V. Papadopoulos to represent DCoMEX in this collaborative project and sign the corresponding agreement when time comes. Finally, before the meeting break, the logo of the project and the Website Domain were presented.
Then, I. Kalogeris and G. Stavroulakis presented WP2 and WP3, respectively. I. Kalogeris developed the strategy for surrogate modeling, developed the tasks, deliverables and their timetable. He referred specifically to the testing of additional ML methodologies such as ANN, Autoencoders and POD as alternatives to Diffusion Maps.

Goerge Stavroulakis did the same for WP3. He mentioned the central role of WP3 in the project. He stated that a lot of work has already been carried out and preliminary results of the ML enhanced iterative solver is available, he developed the strategy for upgrading the DD solvers with the ML tools and deploy them in HPC environments, while taking care for error resilience fault tolerance and energy awereness. He finally mentioned the focal point of integration AI-Solve to Msolve and Korali framework in WP6. G. Arampatzis and S. Martin, presented WP4, B. Menze and I. Ezhov, presented WP5, Ben Cumming and S. Martin presented WP6 and I. Kalogeris presented WP7. I. Hatzakis presented WP8 and deployed the role of GRNET in the performance evaluation and its optimization in terms of efficiency and scalability as well as error resilience and fault tolerance of the DCoMEX platform.

Finally, G. Arampatzis and V. Papadopoulos presented the dissemination plans for WP9. They agreed to collaborate in order to present a detailed exploitation plan of the Project Results by M6. Meanwhile the Project Website will be prepared and a press release document has been released to the partners for locally announce the project initiation. In addition, the data management strategy was discussed, we all agreed to the open source model adopted in the Project except for the market oriented products DCoMEX-BIO and DCoMEX-MAT which are going to be IPR protected. A data management plan will be prepared up to M6.

Finally, in the Wrap up discussions it was concluded that Monthly Group meetings (virtual) should take place in order to boost and initiate the DCoMEX integration process. Specifically the following meetings were scheduled:

1. NTUA-ETH: Msolve-Korali Integration (6.4). Ongoing process already initiated by the two Groups. Next meeting scheduled for last week of May.
2. NTUA/ETH/GRNET: System requirements (Tasks 6.1, 6.2, 6.3), connected to early deliverable D6.1 System requirements, design and architecture (report) M6. The meeting is scheduled for the last week of May.
3. NTUA/ETH-CSELab/TUM/UCY: Data preparation and management for UseCase 1. Scheduled for the 1st week of June. Related to early Deliverable D5.1 (M8) and D5.2 (M12).
4. NTUA/ETH-CSLab/TUM: Data preparation and management for UseCase 2. Scheduled for the 1st week of June. Related to early Deliverable D5.1 (M8) and D5.2 (M12).

2nd meeting (6th of December 2021) summary

Participants. NTUA: V. Papadopoulos, George Stavroulakis, S. Pyrialakos, Theofilos Christodoulou, George Goumas, Panos Metsis, ETH: I. Kalogeris, Martin Sergio, UCY: Triandafyllos Stylianopoulos, Vasileios Vavourakis, Fotos Mpekris
TUM: Ivan Ezhov, Bjorn Menze (UZurich), GRNET: Ilias Hatzakis, Dimitris Dellis, EuroHPC Project Officer: C. Scalese

Agenda

Time (CET)	Topic	Lead

10:00	Welcome - Review of the Agenda	NTUA
10:15	Welcome address and EuroHPC update from the Project Officer	D.Opalka C. Scalese
10:30	Project process - deliverables	NTUA
10.45	WP1 Management Issues	NTUA
11:00	WP2 Surrogate Modeling Potential amendments in Task 2.2 and 2.3	NTUA
11:30	WP3 AI-Solve Library	NTUA
12:00	Break	
13:00	WP4 UQ and Bayesian analysis	ETHZ/CSELab
13:30	WP5 - Preprocessing (Data management)	TUM
14:00	WP6 – Software Integration, Optimization	ETH/CSCS
14:30	Break	
15:00	WP7 - Applications	UCY/NTUA
15:30	Discussion on data for application 7.1 Discussion on amendments in 7.2	NTUA-UCY-TUM NTUA/ETHZ/CSELa
16:00	WP8 – Performance Evaluation	GRNET
16:30	WP9 – Communication – Dissemination	ETHZ/CSELab NTUA
17:00	Consortium Agreement for Collaboration plan, wrap-up discussions and next meeting	NTUA
17:30	End of Day	

The Project Coordinator V. Papadopoulos initiated the meeting, reviewed the Agenda presented the Goals and reviewed the status of the project. Then, the on behalf of the project Officer, C. Scalese informed the consortium about the news of the EuroHPC community regarding the HPC facilities and their access policy. The project partners D. Dellis and I. Hatzakis agreed to prepare proposals for accessing in the HPC facilities via PRACE at the beginning of the second year of the project. The Project Coordinator followed with a more detailed description of the status of the DCoMEX project completed and ongoing Tasks and reviewed the completed (M1-M6) and upcoming deliverables and Milestones (M6-M12). At this point, he informed the consortium about the data management plan of the project (Deliverable 9.5) and the new deliverable 9.6 regarding the horizontal collaboration plan between EuroHPC projects and specifically the collaboration planed with SPARCITY project. Finally, he informed the consortium of the established working sub-groups of DCoMEX.
After this presentation, each WP leader with the help of corresponding Task Leaders summarized the Work Packages and Tasks of the Projects.

Then, I. Kalogeris and G. Stavroulakis presented WP2 and WP3, respectively. I. Kalogeris developed the strategy for surrogate modeling, developed the tasks, deliverables and their timetable. He referred specifically to the testing of additional ML methodologies such as ANN, Autoencoders and POD as alternatives to Diffusion Maps and suggested to invest in Autoencoders since they exhibit certain advantages with respect to the other methods. At this point, the coordinator suggested that this would require an increase of the PMs for this Task and agreed with the Project Officer to discuss the possibility of an amendment in case this is necessary.

Next, George Stavroulakis presented WP3. He mentioned the central role of WP3 in the project. He presented the building blocks of the AI-Solve library and referred to the DDM methods and preconditioners that are being developed. He mentioned that that a lot of work has been carried out and preliminary results of the ML enhanced iterative solver is available, he developed the strategy for upgrading the DD solvers with the ML tools and deploy them in HPC environments, while taking care for error resilience fault tolerance and energy awareness.

Then, I Kalogeris, developed the sampling schemes that were developed in WP4 in conjunction with the TMCMC Bayesian frameworks. Following this, a detailed discussion took place with respect to the tools developed in WP5 for image segmentation and data processing. Bjorn Menze developed the methodologies and tools to be applied in MSolve and discuss a plan with both V. Papadopoulos and Triantafyllos Stylianopoulos, regarding the integration of his tools to the Computational Model of UCY that is being developed in MSolve-BIO module. Two working groups were established. One between TUM/NTUA for the integration of TUM image processing tools to MSolve platform and one between TUM/NTUA/UCY/ETH for the clinical data processing in the MSolve/Korali framework.

Further on, I Kalogeris developed the Task 7.2 application and suggested that the material design heat transfer application has proven a bit discouraging with respect to the expected advancement of the heat properties of the composite, since the high thermal resistivity of CNT/matrix interfaces blocks the composite from developing a conductance mechanism. He suggested to switch to an alternative application regarding concrete materials and structures, reinforced with CNTs. Early results of this combination demonstrate that this combination seems very promising for significantly enhancing both the strength as well as the durability of the material. As in the case of WP2, the coordinator suggested that this would again require an increase of the PMs for this Task and agreed with the Project Officer to discuss the possibility of an amendment in case this is necessary. The consortium also agreed to this amendment if needed.

At the end, I. Kalogeris developed the dissemination and exploitation plan of the project as this is presented on Deliverable D9.1.
Finally, the consortium planned the next meeting in June 2022 to be held in Athens, provided that the COVID situation will allow for such a plan.

2.4. Data management

As described in detail in the Data management plan (D9.6), the DCoMEX data outputs will be 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 also tools to linking 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

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.

2.5. Working groups

The following working groups have been established and are active in 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 modeling 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 will be 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 to LUMI for benchmarking.

All groups have weekly meetings and report regularly to the PC.

3. FINANCIAL MONITORING

NTUA follows the project expenses and track deviations in coordination with the accounting system. The project cost management includes the processes required to ensure that the project is completed within the approved budget. Concerning cost control for the project, NTUA abides by the Commission requirements, including monitoring of the cost performance to detect deviations from the original plan, accurate recording in the cost baseline, preventing incorrect, inappropriate, or unauthorized changes of the contract.

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

4. DCOMEX DELIVERABLES AND MILESTONES MONITORING

Deliverables

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 end.

In this first year 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
D2.1	DMAP algorithm prototype	NTUA	O	PU	30.11.2021	24.1.2022
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

D4.3	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
D9.1	DcomEX Website	ETHZ	DEC	PU	30.6.2021	30.9.2021
D9.3	Communication, dissemination and exploitation plan	ETHZ	R	PU	30.9.2021	2.11.2021
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

Milestones

All first year Milestones 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 validated
4	First year Progress Periodic Report	1	M12	Documentation

5. WPs and Tasks monitoring

In the first period all WP and Tasks were monitored by the WP leaders and the PC. All Tasks were progressed according to the plan and the Projects Gant with no significant problems or obstacles. Specifically:

Work Package 2

Task 2.2: DMAP surrogate implementation (M2-M8). This Task has been completed. However, as reported in the minutes of the 2nd project meeting, we decided το 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, will be included in an amendment request that has been decided by the DComEX SC.

Task 2.3, Implementation of surrogate model (M9-M16), has been initiated and is progressing according to the schedule.

Work Package 3

Task 3.1 DDM preconditioners for exascale systems (M1-M10)

A set of DDM preconditioners including PD-DDM and AMG were developed and implemented for accelerating the convergence of the solvers of Task 3.3. Direct solvers were incorporated for the solution of small local problems, further promoting data-locality and communication reduction.

Task 3.2 Surrogate models for preconditioning and coarse problem solution(M1-M20)

Tasks 3.3 Inexact Solvers for scalability end error resilience (M5-M24)

This Task has been initiated and is progressing according to the schedule. More specifically, the results of Task 3.2 on surrogate modeling have been integrated in an AMG based solution scheme, leading to an efficient first prototype of the AI-Solve concept.

Tasks 3.4 Sparse Computations (M5-M24)
This Task has been initiated and is progressing according to the schedule. For this Task a working sub-group within NTUA (MGroup/CSLab) has initiated common activities to enhance sparse matrix vector multiplications in the frame of SParseX library.

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-M30), have been initiated and are progressing according to the schedule.

Work Package 4

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

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)

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 Development of a load-balanced scalable sampling algorithm (M2-M10)

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.

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 a 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-M12)

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.

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 Tasks established a preliminary definition of the prerequisite software and hardware environments required by the DCoMEX

project. The testing and benchmarking technologies, frameworks, and methodologies that will be utilized throughout the project were specifically defined. In particular, we defined the design and architecture of the systems (supercomputers) to be used: i) Node architecture, GPU capability, and memory hierarchy and ii) Network architecture. In addition, the main software components were identified including: i) Their own software and hardware requirements ii) Analysis of their compute components, following the principles of the Berkeley Dwarfs, iii) Software libraries, modules, and frameworks we will require and iv) Energy considerations. These outcomes are described in detail in Deliverable D6.1

Task 6.4 Integration (M7-M24)

For the development of the MSolve/Korali platform integration, WG 3 was created. First the MGroup/ETH/CSELab, integrated MSolve and Korali and tested their combined functionality in a toy academic heat transfer problem. Following this, CSCS joint the team to deploy and test the MSolve/Korali platform in Piz Daint. The integration has been initiated and is progressing according to the plan. It is foreseen that the target of having the DComEX prototype deployed in Piz Daint by M15 will be meet successfully.

Task 6.5 Low level code optimization (M7-M24)

In parallel to the integration Step of Task 6.5 low-level code optimisations includes has been initiated by WG3 with the lead of CSCS. This Task has been initiated and is progressing according to the schedule. The same procedure will be followed by WG4, upon integration of DComEX in ARIS and LUMI supercomputers.

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 in a weekly basis. UCY developed the mathematical framework of the tumor growth modeling model and worked together with MGroup for the implementation of the equations in 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. In a later stage starting from 1/07/2022, the group will be augmented as with the addition of ETHZ (TUM/NTUA/UCY/ETHZ) for the preparation of the clinical data processing in the MSolve/Korali framework. It is foreseen that a validated and tested prototype version of the DComEX-BIO software will be launched before 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 carbon nanotubes and graphene sheets. It has been theorized 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 [1]. This phenomenon has been numerically studied by the NTUA team members, and optimal microstructural configurations for certain scenarios have been identified [2]. 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.

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 super computers. 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 later stage of the project progress.

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 is described in detail in D9.2.

Actions so far:

- Enrichment of the educational material for the courses 'Parallel Processing Systems" , "Advanced Distributed Systems", "Computational Mechanics", "Stochastic finite element methods" (NTUA)

    - G. Sotiropoulos, V. Papadopoulos, Large deformation multi-scale analysis of thin nanocomposite shell structures, Oslo, 2022

    - S. Nikolopoulos, I. Kalogeris, V. Papadopoulos, *Machine learning accelerated transient analysis of stochastic nonlinear structures*, Engineering Structures, 2022
    - S. Bakalakos, M. Georgioudakis, M. Papadrakakis, *Domain Decomposition Methods for 3D crack propagation using XFEM*, Computer Methods in Applied Mechanics and Engineering (under review)
    - Lucas Amoudruz, Athena Economides1, Georgios Arampatzis and Petros Koumoutsakos, *"The stress-free state of human erythrocytes: data driven inference of a transferable RBC model",* Biophysical Journal, (under review).

6. 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).

7. Deviations and amendments

The project is progressing satisfactory without any significant deviations, obstacles or changes with respect to the original plan. Some minor adjustments have been proposed and discussed in the 2nd global assembly meeting the Consortium where it has been decided to request an amendment that would include the following:

1. Task 2.2 Switch to auto-encoders in addition to DMAP algorithms
2. Change application in Task 7.2 to multiscale design of CNT reinforced Concrete

These changes along with the corresponding changes in the PM effort will be submitted to EU as an amendment request along with other minor changes such as PM and effort reallocations, extension of Tasks and Deliverable deadlines, etc.

8. REFERENCES

[1] G. Konstantopoulos, P. Maroulas, D. Dragatogiannis, S. Koutsoumpis, A. Kyritsis, C. Charitidis, “The effect of interfacial resistance and crystallinity on heat transfer mechanism in carbon nanotube reinforced polyethylene, Materials and Design (2021).

[2] S. Bakalakos, I. Kalogeris, V. Papadopoulos, “An extended finite element method formulation for modeling multi-phase boundary interactions in steady state heat conduction problems”, Composite Structures (2021).