



**Data driven Computational Mechanics at EXascale**



**DCoMEX**

**Data driven Computational Mechanics at EXascale**

**Work program topic: EuroHPC-01-2019  
Type of action: Research and Innovation Action (RIA)**

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**COMMUNICATION, DISSEMINATION AND EXPLOITATION REPORT**

**DELIVERABLE D9.4**

**Version No 1**



<http://www.dcomex.eu/>

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# **1. Executive Summary**

DCoMEX is a large-scale European project that aims to revolutionize computational mechanics by introducing novel numerical methods powered by artificial intelligence (AI). At the heart of this innovation is the creation of a scalable library of AI-enhanced algorithms for solving large-scale sparse linear systems of equations, which are fundamental to computational mechanics. The DCoMEX framework will be validated through two groundbreaking case studies: (i) the patient-specific optimization of cancer immunotherapy treatment, and (ii) the design of advanced composite materials and structures across multiple scales. Both case studies exemplify computational challenges requiring peta- and exascale computing resources, highlighting the project's transformative potential.

This document (D9.4) serves as the final report on the communication, dissemination, and exploitation activities carried out by the consortium members over the course of the project. The structure of the report is as follows: Chapter 2 presents an overview of the project's dissemination efforts, including conferences attended by DCoMEX researchers and the current status of scientific publications. Chapter 3 outlines the communication strategies employed, while Chapter 4 focuses on the exploitation of project results. Finally, Chapter 5 provides a summary of key takeaways and an evaluation of the overall impact of these activities.



## 2. Dissemination Activities

The dissemination activities of the DCoMEX project aim to share the scientific and technological knowledge developed within the project, targeting relevant research groups and user communities. These activities seek to raise awareness of the project's objectives and outcomes. In this direction, DCoMEX adopted a dual dissemination strategy, focusing on publishing results in prestigious international journals and conferences, while also providing open access (following the green open access model) to ensure broad availability of the project's outcomes.

The dissemination strategy was centered on maximizing the reach of DCoMEX within target audiences, sharing the scientific and technological advancements made, and building connections with other relevant projects and initiatives. To achieve these goals, DCoMEX researchers actively participated in 16 conferences and workshops, delivering 27 presentations on various topics related to computational science and high-performance computing (HPC). Table 1 summarizes these participations up to the project's end month, September 2024. Through these events, DCoMEX researchers have established valuable connections within the HPC community and fostered collaborations with other researchers and European projects in the field of computational mechanics.

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
Exhibition	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	17 <sup>th</sup> U.S. National Congress on Computational



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			Segmentations for Personalized Therapy Design by a Discrete Loss Optimization	Mechanics, Albuquerque, New Mexico, US.
<b>Conference</b>	23-27.07.2023	I. Kalogeris	Multiscale Analysis of Structures Composed of Composite Materials Using a Hierarchy of Deep Neural Networks	17 <sup>th</sup> U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico, US.
<b>Conference</b>	23-27.07.2023	V. Papadopoulos	AI-Solve: Fusing Machine Learning and Linear Algebra to Accelerate the Solution of Large-Scale Parametrized Systems	17 <sup>th</sup> U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico, US.
<b>Conference</b>	28-30.08.2023	S. Kaltenbach	Efficient Uncertainty Quantification and Bayesian Analysis for Computational Mechanics at Scale	3 <sup>rd</sup> International Conference on Computational Science and AI in Industry, Trondheim, Norway
<b>Workshop</b>	11-13.12.2023	S. Kaltenbach	Korali: Stochastic Optimization and Bayesian Inference	Mathematical Opportunities in Digital Twins, Washington
<b>Exhibition</b>	18-21.03.2024	V. Papadopoulos	DCoMEX: Data Driven Computational Mechanics at Exascale (poster session + presentation)	EuroHPC Summit 2024, Antwerp, Belgium
<b>Conference</b>	12-16.05.2024	E. Chroni	DCoMEX: Data-driven computational mechanics at exascale	ISC High Performance, Hamburg, Germany
<b>Workshop</b>	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
<b>Conference</b>	24-26.06.2024	M. Balcerak	Modeling Brain Tumor Mass Effect via Optimization of a Physics-Informed Discrete Loss	8 <sup>th</sup> International Conference on Computational & Mathematical Biomedical Engineering, George Mason University, Virginia, US.
<b>Conference</b>	3-7.07.2024	S. Kaltenbach	Learned Effective Dynamics (LED) and Bayesian methods for patient-specific cancer immunotherapy	ECCOMAS 2024, Lisbon
<b>Conference</b>	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
<b>Conference</b>	3-7.07.2024	G. Sotiropoulos	AI-based Surrogate Modelling Techniques for Time Dependent	ECCOMAS 2024, Lisbon



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			Parametrized Mathematical Models of Cancer Immunotherapy	
<b>Workshop</b>	26.07.2024	S. Kaltenbach	Improving the accuracy of Coarse-grained Partial Differential Equations with Grid-based Reinforcement Learning	ICML AI4Science Workshop, Vienna
<b>Workshop</b>	2-3.09.2024	V. Papadopoulos	Data Driven Computational Mechanics at Exascale: DCOMEX project results	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
<b>Workshop</b>	2-3.09.2024	I. Kalogeris	A transformers -based AI approach for generating physics informed dynamics	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
<b>Workshop</b>	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
<b>Workshop</b>	2-3.09.2024	G. Sotiropoulos	Surrogate models for large and coupled bioengineering problems	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
<b>Workshop</b>	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
<b>Workshop</b>	2-3.09.2024	T. Stylianopoulos	Mathematical modeling to guide cancer immunotherapy	“Data-driven Applications for Exascale Supercomputers” Workshop, Athens
<b>Workshop</b>	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 1:** Overview of participations in conferences/workshops

In addition to the aforementioned activities, the scientific contributions from all DCOMEX working groups have been published in prestigious peer-reviewed journals across a range of disciplines, including computational mechanics, biomodeling, medicine, medical imaging, material design and machine learning. To date, 13 journal articles acknowledging DCoMEX have been published in peer-reviewed scientific journals, with one additional journal article accepted for publication. Furthermore, the project has contributed to one conference paper, one workshop paper, and eight submitted journal articles that are currently under review, with preprints available in open-access repositories. Table 2 provides a detailed overview of all scientific publications up to September 2024.



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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 <a href="https://www.sciencedirect.com/science/article/pii/S0141029622001663">https://www.sciencedirect.com/science/article/pii/S0141029622001663</a>
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, <a href="https://www.sciencedirect.com/science/article/pii/S0045782522004510">https://www.sciencedirect.com/science/article/pii/S0045782522004510</a>
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, <a href="https://proceedings.mlr.press/v193/ezhov22a/ezhov22a.pdf">https://proceedings.mlr.press/v193/ezhov22a/ezhov22a.pdf</a>
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. Stylianopoulos, V. Vavourakis	International Journal for Numerical Methods in Biomedical Engineering, 2023 <a href="https://onlinelibrary.wiley.com/doi/abs/10.1002/cnm.3734">https://onlinelibrary.wiley.com/doi/abs/10.1002/cnm.3734</a>
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 <a href="https://www.sciencedirect.com/science/article/pii/S0017931022008894">https://www.sciencedirect.com/science/article/pii/S0017931022008894</a>
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 <a href="https://www.sciencedirect.com/science/article/pii/S0020768323001580">https://www.sciencedirect.com/science/article/pii/S0020768323001580</a>
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 <a href="https://www.sciencedirect.com/science/article/pii/S0006349523001728">https://www.sciencedirect.com/science/article/pii/S0006349523001728</a>
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 <a href="https://www.sciencedirect.com/science/article/pii/S1361841522003000">https://www.sciencedirect.com/science/article/pii/S1361841522003000</a>
Journal article	Published	Toward image-based personalization of	M.C. Metz, I. Ezhov, J.C. Peeken, J.A. Buchner, J.	Neuro-Oncology Advances, 2023





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		glioblastoma therapy: A clinical and biological validation study of a novel, deep learning-driven tumor growth model	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	<a href="https://academic.oup.com/noa/article/6/1/vdad171/7502543?login=true">https://academic.oup.com/noa/article/6/1/vdad171/7502543?login=true</a>
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 <a href="https://onlinelibrary.wiley.com/doi/10.1002/nme.7372">https://onlinelibrary.wiley.com/doi/10.1002/nme.7372</a>
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 <a href="https://www.sciencedirect.com/science/article/pii/S004578252400330X">https://www.sciencedirect.com/science/article/pii/S004578252400330X</a>
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 <a href="https://zenodo.org/records/13766990">https://zenodo.org/records/13766990</a>
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 <a href="https://academic.oup.com/pnasnexus/article/3/1/pgae005/7516080">https://academic.oup.com/pnasnexus/article/3/1/pgae005/7516080</a>
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 <a href="https://openreview.net/pdf/415fef02819878bd898609f08910380a7521b08a.pdf">https://openreview.net/pdf/415fef02819878bd898609f08910380a7521b08a.pdf</a>
Journal article	published	An efficient hierarchical Bayesian framework for multiscale material modeling	S. Pyrialakos, I. Kalogeris, V. Papadopoulos	Composite Structures, 2025 <a href="https://www.sciencedirect.com/science/article/pii/S0263822324006986">https://www.sciencedirect.com/science/article/pii/S0263822324006986</a>
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 <a href="https://arxiv.org/abs/2402.17157">https://arxiv.org/abs/2402.17157</a>
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 <a href="https://arxiv.org/pdf/2312.05063">https://arxiv.org/pdf/2312.05063</a>
Journal article	submitted (under review)	Interpretable learning of effective dynamics for multiscale systems	E. Menier, S. Kaltenback, m. Yagoubi, M.	Preprint available at <a href="https://arxiv.org/abs/2309.05812">https://arxiv.org/abs/2309.05812</a>



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			Schoenauer, P. Koumoutsakos	
<b>Journal article</b>	submitted (under review)	Interpretable reduced-order modeling with time-scale separation	S. Kaltenbach, P.S. Koutsourelakis, P. Koumoutsakos	Preprint available at <a href="https://arxiv.org/abs/2303.02189">https://arxiv.org/abs/2303.02189</a>
<b>Journal article</b>	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 <a href="https://arxiv.org/abs/2402.00972">https://arxiv.org/abs/2402.00972</a>
<b>Journal article</b>	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. Iatz, D. Rueckert, B. Menze	Preprint available at <a href="https://arxiv.org/abs/2403.04500">https://arxiv.org/abs/2403.04500</a>
<b>Journal article</b>	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	-
<b>Journal article</b>	submitted (under review)	Quantitative 3D histochemistry reveals region-specific amyloid- $\beta$ 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 <a href="https://www.biorxiv.org/content/10.1101/2024.08.15.608042v1.full">https://www.biorxiv.org/content/10.1101/2024.08.15.608042v1.full</a>
<b>Journal article</b>	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 <a href="https://arxiv.org/abs/2408.00157">https://arxiv.org/abs/2408.00157</a>

**Table 2:** Overview of scientific publications and papers

### 3. Communication activities

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

#### Project’s website

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

#### Project’s portfolio

The project’s portfolio was created, which contained the project’s logo, illustrative images, presentations, project flyers and brochures.

#### 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 (figure 1), hosted events (fig. 2) and our conference participations (fig.3)

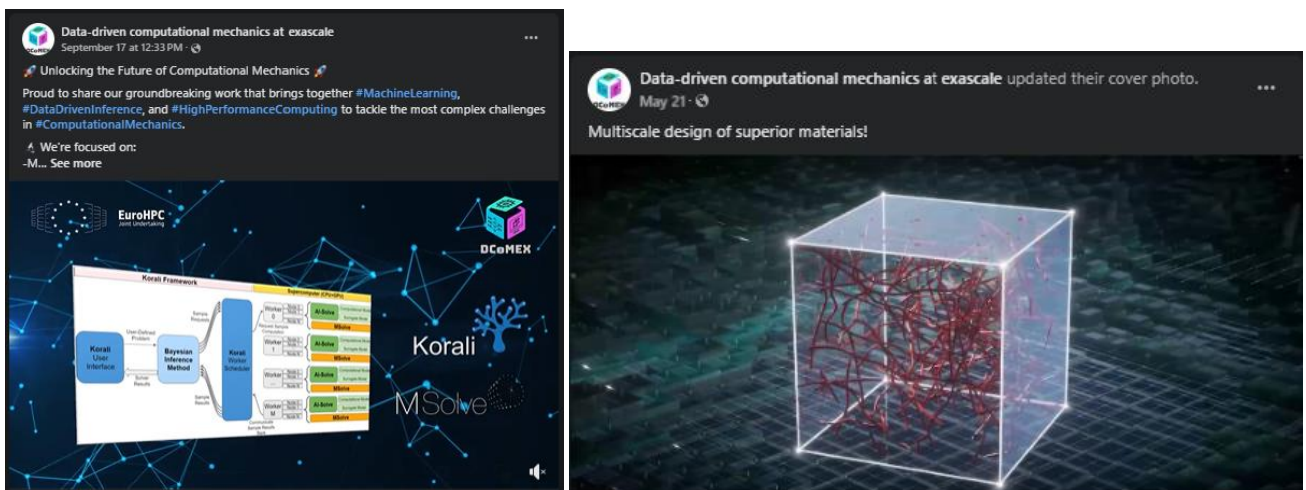


Figure 1: Facebook posts from September 17 and May 21, 2024



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Figure 2: Facebook post from September 2, 2024



Figure 3: Facebook posts from June 10 and May 14, 2024

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.

## Press releases

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





## Organization of meetings/workshops/conferences

In the effort to bring together experts from the HPC community and Computational Science community, members of the DCoMEX’s consortium organized a workshop titled “**Quantum Computing and its synergy with High Performance Computing in Engineering Sciences and Applications**” on July 2, 2022. This event was attended by thirty participants with physical presence and more than fifty people attended virtually.

**Quantum Computing and its synergy with High Performance Computing in Engineering Sciences and Applications**

**Saturday, 2<sup>nd</sup> of July 2022**

**PROGRAM**

**10.00 Welcome and Introduction**, Andreas Boudouvis (Rector of NTUA) - Vissarion Papadopoulos (NTUA/MGroup)

**10.20 Introduction to Quantum Computing**, George Stavroulakis (NTUA/MGroup)

**10.50 The landscape of HPC in Greece, Europe and worldwide**, George Goumas (CSELab/NTUA)

**11.10 Quantum and HPC technologies and infrastructures**, Vangelis Karkaletsis (IT/NCSR Demokritos)

Coffee Break

**12.00 Using quantum annealers to solve optimization problems and quantum games to securely transmit cryptographic keys**, Theofilos Andronikos (Ionian University)

**12.30 Quantum Computing for Uncertainty Quantification in engineering**, Konstantinos Atzarakis (NTUA/MGroup)

**13.00 Panel discussion - Quantum computing: Synergies and Actions in research and education**, Coordinated by Georgios Nounesis (President of NCSR Demokritos), Petros Koumoutsakos, (Harvard) and Nectarios Koziris (Dean of ECE/NTUA)

Lunch

ANARGYRION & KORGIALENION FOUNDATION  
SPETSES, GREECE

QR code: <https://constrain.kua.welke.com/en/meeting/23992?ID=760c97f6648c6d2034ee1646962be>

Figure 4: Invitation to “Quantum Computing and its synergy with High Performance Computing in Engineering Sciences and Applications” Workshop, in Spetses island, Greece

A second workshop, titled “*Data-Driven Applications for Exascale Supercomputers,*” was organized by the DCoMEX project members during the final month of the project (2–3 September 2024) in Athens, Greece. This two-day event focused on showcasing the project's outcomes and exploring the industrial applications of high-performance computing (HPC). The first day was dedicated to presenting the project’s results to a broad audience, including representatives from both the academic and industrial communities. The second day was aimed at industry professionals, who discussed the current challenges within the industrial sector that necessitate HPC solutions.

**"Data-driven Applications for Exascale Supercomputers" Workshop**

2 Sep 2024, 08:00 → 3 Sep 2024, 17:00 Europe/Athens

Description

Workshop  
**Data-driven Applications for Exascale Supercomputers**

SEPTEMBER 2-3, 2024 | 09:00 - 17:00 EET | ATHENS, GREECE

We are pleased to announce the "Data-driven Applications for Exascale Supercomputers" Workshop, organized by the National Technical University of Athens (NTUA) and the National Infrastructures of Research and Technology (GRNET), in the framework of the EuroHPC projects EuroCC 2 and DCoMEX. The workshop will take place on **September 2-3, 2024**, in the context of the EMCS conference.

**Dates:** September 2-3, 2024

**Location:** Deree - the American College of Greece (6 Gravias Street, Aghia Paraskevi, Athens, Greece)

**Audience:**

- Academic and Researchers** - Ideal for experts in machine learning, artificial intelligence, and computational mechanics, emphasizing recent research, innovative methods, and high-performance computing integration.
- Industry Professionals** - professionals across various sectors interested in enhancing operational efficiency and innovation through Supercomputing and Artificial Intelligence.
- Technical Experts in HPC and AI** - Essential for HPC and AI experts, focusing on the latest software frameworks and tools, providing insights into advanced technologies and frameworks.

**Cost:** free of charge

**Reservations:** Secure your spot by registering. Please note that space is limited.

Figure 5: Invitation to “Data-driven Applications for Exascale Supercomputers” Workshop, in Athens, Greece



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### Clustering activities

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

- a. With respect to Task 3.1: Domain Decomposition Method (DDM), we explored 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 explored additional mixed precision schemes with application to DCoMEX iterative solvers.

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

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

In addition to the aforementioned activities, we participated in the First EuroHPC19 Projects Collaboration Workshop, held in Madrid in 2022, where we initiated discussions for potential collaborations with other projects. We also showcased DCoMEX at the Teratec Forum in Paris, France, in 2022, with a dedicated booth in the *Europa Village*, an area focused on the European HPC ecosystem. Furthermore, members of the consortium attended the EuroHPC Summit in 2023 (Sweden) and in 2024 (Belgium), further strengthening our engagement with the HPC community.

### Educational activities

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

A seminar in HPC and programming was held in NTUA under the auspices of the DCoMEX project during the spring semesters of 2022 and 2023. The seminar was titled "Introduction to object-oriented programming in the C# framework" and more than 20 undergraduate students attended it.

## 4. 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
<b>R1:</b> UQ-aware image pre-processing engine	TUM	Open source	Industrial users, supercomputing centers
<b>R2:</b> CPU and GPU-enabled Msolve multiscale/Multiphysics solver	NTUA	Open source	Researchers on algorithms relevant to stochastic multiscale optimisation
<b>R3:</b> Adaptive UQ and Bayesian analysis Korali engines	ETHZ/CSElab	Open source	Researchers on algorithms relevant to stochastic multiscale optimisation
<b>R4:</b> AI-Solve library	NTUA	Open source	Industrial users, supercomputing centers, academic researchers
<b>R5:</b> The DCoMEX HPC framework	CSCS	Open source	Industrial users, supercomputing centers, researchers
<b>R6:</b> The DCoMEX-BIO software for cancer immunotherapy optimisation	UCY	Patent protected	Software development and medical systems companies, hospitals, cancer research centers, clinical oncologists
<b>R7:</b> 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.



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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.
8. 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.





## 5. Summary

This document outlines the dissemination, communication, and exploitation activities conducted during the DCoMEX project. These three areas were critical to the project's success, and each has been addressed individually, with the activities undertaken by the consortium members detailed thoroughly. Closing this final section, we would like to outline the overall achievement in these three fields:

**Dissemination:** DCoMEX researchers have maintained a strong presence at numerous conferences and workshops in the fields of high-performance computing (HPC) and computational mechanics. The project has generated significant new knowledge, leading to 13 publications in prestigious journals, one additional journal article accepted for publication, one conference paper, and one workshop publication. Furthermore, eight more submissions are currently under review. Consortium members will continue disseminating the research outcomes through future journal publications and conference presentations.

**Communication:** Consortium members contributed by creating new content based on project results, while also making concerted efforts to expand the project's community. The successful organization of two workshops fostered engagement, generating meaningful discussions for future collaborations and potential projects.

**Exploitation:** The consortium targeted each partner's exploitable assets to relevant stakeholders, creating new funding opportunities. Exploitation efforts will continue beyond the project's official end, ensuring the long-term impact and sustainability of its results.