EuroHPC
Joint Undertaking

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)

DCoMEX website: The fully functional DCoMEX website

DELIVERABLE D9.1

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http://www.dcomex.eu/
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DOCUMENT SUMMARY INFORMATION

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	Who	Affiliation	Date
Checked by internal reviewer	George Stavroulakis	NTUA	06/09/2021
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1.0	01.09.2021	Leonidas Papadopoulos	NTUA	
2.0	05.09.2021	Leonidas Papadopoulos	NTUA	

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CHAPTER1 Introduction

The project website, accompanied by a rich set of diverse activities such as blogcasts, videos, brochures & fliers, focused reports and announcements, aims to achieve the goals of **Task 9.1: Communication activities**:

(i) raise awareness within different target communities and the general public,

(ii) demonstrate progressively the project concept and system functionalities to key stakeholders at European level,

(iii) manage the attendance to relevant conferences and the production of publications in order to attain maximum effectiveness,

(iv) involve new end-user communities and IT providers and

(v) pave the way for exploitation of project results.

The project website was edited by **George Arabatzis**, **George Stavroulakis** and **Leonidas Papadopoulos** and checked by **Vissarion Papadopoulos** and **George Stavroulakis.**

CHAPTER 2 Webite Contents

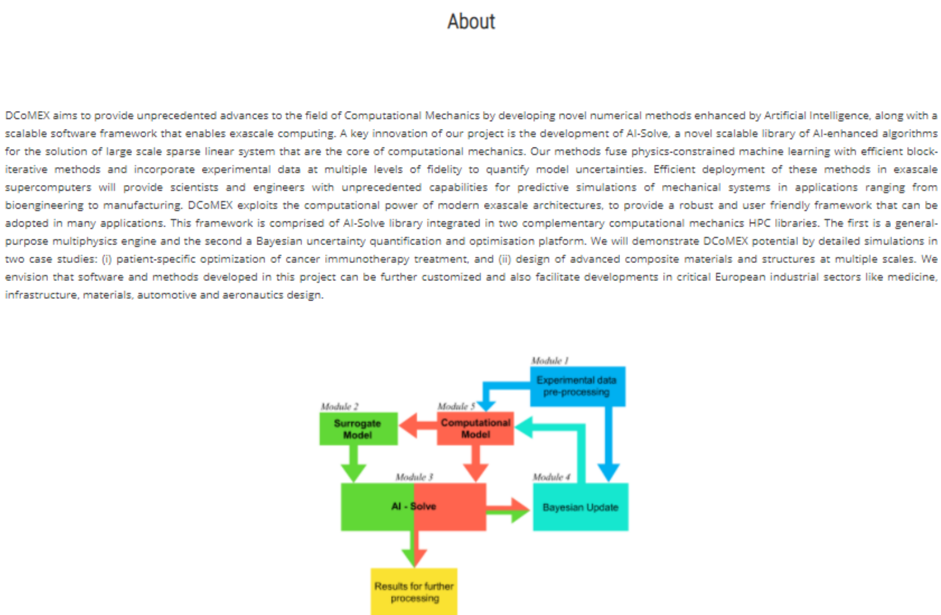
The project website consists of five sections, with some of them been further divided into a number of subsections.

2.1 Home

The Home page of the website features the logo of the project as well as a menu with drop-down buttons, allowing the user to navigate easily through the website. The menu is accessible through all the website sections.

2.2 About

This section describes the motivation, the methods and the goals behind the project, as well as its main innovations.



2.3 Project

This section is divided into three subsections:

(i) Facts, which contains the main information of the project,

Facts

1	**Project Title:**	Data Driven Computational Mechanics at Exascale
2	**Project Number:**	956201
3	**Project Acronym:**	DCoMEX
4	**Starting date:**	01/04/2021
5	**Duration in months:**	36
6	**Call Identifier:**	H2020-JTI-EuroHPC-2019-1
7	**Type of Action:**	EuroHPC-RIA
8	**Topic:**	EuroHPC-01-2019
9	**Fixed keywords:**	High performance computing; Scientific computing and data processing
10	**Free keywords:**	Data Driven Computational mechanics, Exascale Computing, Manifold Learning, Fault Tolerance, Scalability, Heterogeneous CPU+GPU computing, Bayesian analysis, Uncertainty Quantification

(ii) Objectives, which discuss the main strategical objectives of the project, and

Objectives

The DCoMEX is comprised of the following Strategic Objectives (SO):

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

(i) SO1.1: Development of a set of innovative machine learning (ML) methods for dimensionality reduction and surrogate modelling, including the diffusion maps (DMAP) manifold learning and deep neural networks (DNN).

(ii) SO1.2 Development of AI-Solve library fusing data-driven methods and surrogate models with efficient block-iterative sparse linear system solvers.

SO2: Exascale deployment of MSolve and Korali software engines.

(i) SO2.1: Optimisation of 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.

(ii) SO2.2: Extension of the Korali UQ and Bayesian analysis framework to include state of the art load-balanced sampling algorithms that harness efficiently extreme computation architectures.

SO3: Pre-processing of experimental image data

(i) SO3.1: Development of 3D image and data processing routines that extract geometries together with estimates of their uncertainties that can be propagated to predictive simulators.

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

(iii) Coordinator, which introduces the project coordinator, National and Technical University of Athens (NTUA).

Coordinator

The National Technical University of Athens is the oldest and largest educational institution of Greece in the field of technology. NTUA has a firm commitment to research thanks to its personnel and its extensive infrastructure, state-of-the-art laboratories and computing facilities. The personnel of NTUA have provided a broad list of publications in the international literature with high scientific impact and a large number of doctorate students are currently undertaking their PhD programs in research fields related to the project. Past EU funding includes numerous H2020, FP6 and FP7 projects, five ERC IDEAS Grants and many Marie-Curie networking projects.

The NTUA team consists of two research groups: The Multidisiplinary Computation Mechanics Research group (MGroup) which belongs to the Institute of Structural Analysis and Antiseismic Research (ISAAR) of the School of Civil Engineering of NTUA and the Computing Systems Laboratory from the School of Electrical and Computer Engineering of NTUA.

2.4 Consortium

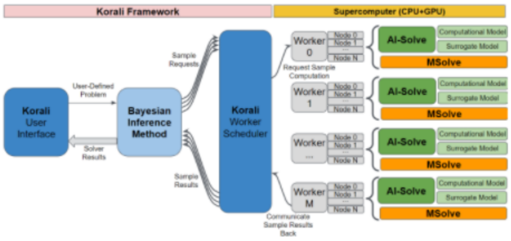
It consists of two subsections:

(i) About, which describes the expertise the different members of the Consortium bring into the project, and

About Consortium

The proposed project seeks, primarily to develop a novel data driven and AI-enhanced linear algebra library for solving linear systems of equations and integrate it into a software platform capable of handling very demanding computational mechanics problems, designed for exascale performance and bring to common practice these complicated and up to date restrictive analysis and design of complex and/or multiscale/multiphysics systems. The project is strongly interdisciplinary and as a consequence, the consortium is extensive in that it covers the basic mathematical, engineering and computer science backgrounds through to the medical and industrial applications. The consortium also reflects the breadth of the proposed project in that it consists of a strong and well-balanced blend of HPC centers and Universities. The consortium is defined by leading experts in academia and applied science. Expertise is being drawn from all of these resources in order to ensure that the project meets its intended objectives.

The participants in the project are drawn from Greece, Switzerland, Cyprus and Germany, so the consortium represents a cross-section of central and south European countries. The consortium covers such a number of countries, as to ensure that the required skills at the correct level are available to the project, rather than the skills being developed as a part of the project.



(ii) Members, which introduces the members of the Consortium.

Members

National and Technical University of Athens

The NTUA team consists of two research groups: The Multidisiplinary Computation Mechanics Research group (MGroup) which belongs to the Institute of Structural Analysis and Antiseismic Research (ISAAR) of the School of Civil Engineering of NTUA and the Computing Systems Laboratory from the School of Electrical and Computer Engineering of NTUA.

MGroup

The Multidisiplinary Computation Mechanics Research group (MGroup, http://mgroup.ntua.gr/) is a numerical simulation Lab specialized in large scale computational mechanics problems. MGroup is part of the Institute of Structural Analysis and Seismic Research of the Civil Engineer school of the NTUA (ISAAR). MGroup was founded by Asc Professor V. Papadopoulos and consists of 3 Faculty members 4 Post-doctoral students and 10 PhD students. Research activities of MGroup are related to material modeling, multiscale analysis and design, multiphysics, uncertainty quantification, optimum design, reduced order modeling, machine learning and artificial intelligence, accelerated computing and HPC. MGroup has developed MSolve software, an open source general purpose computational mechanics solver customized to solving large scale multiscale and/or multiphysics problems (https://github.com/isaar/MSolve).

National Technical University of Athens CSLab

2.5 Work Packages

It presents the nine work packages of the project, their main characteristics, their objectives and the deliverables associated to them.

Working Package 3

1	**Working Package number:**	WP3
2	**Working Package Title:**	AI-Solve
3	**Duration:**	M4 – M28
4	**Lead beneficiary:**	NTUA

This work package focuses on combining theoretical developments and state-of-the-art implementations of a set of solution methods for FEM-based physics informed computational models with innovative manifold learning methods in order to construct an innovative block-iterative solver that can drastically reduce the computational load, mitigate data transfers, recover from hardware errors and support energy-aware operation. To this direction, special focus will be given to: (i) DDM and AMG preconditioning, (ii) coarse problem formulations, (iii) usage of WP2 surrogate model for the coarse problem solution and preconditioning enhancements, (iv) data storage and partitioning, (v) communication avoiding strategies, (vi) inexact algorithms, (vii) hardware failure mitigation, (viii) energy-awareness and efficiency, (ix) validity, (x) scalability to a large number of nodes and cores, (xi) heterogeneity of the compute platform, (xii) robustness to input, (xiii) robustness to noise in data.

WP3 is led by NTUA which will be responsible for the design and implementation of AI-Solve and will drive the efforts for inexact solvers and communication optimisation. ETHZ/CSCS and GRNET will focus on hardware fault tolerance and energy awareness/minimisation. All three partners will have close collaboration in almost all the tasks of the work package. The work is divided into the following tasks:

Task 3.1: DDM preconditioners for exascale systems, **Participants:** NTUA, ETHZ/CSELab, **Duration:** M1- M10

A set of DDM preconditioners including PD-DDM and AMG will be investigated and implemented for accelerating the convergence of the solvers of Task 3.3. Some of these methods also incorporate direct solvers for the solution of small local problems, further promoting data-locality and communication reduction. All the aforementioned methods will be distributed and will be specifically designed to efficiently handle sparse data.