Data driven Computational Mechanics at EXascale

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1. Executive Summary

This report provides a performance report for the DCoMEX project and specifically for the DCoMEX-MAT framework. Here, we define the testing and benchmarking procedures that will be utilised for this report. In particular, we define:

- The design and architecture of the test cases considered
- The actual results in terms of computational time, speedup and network efficiency

2. Application benchmarks

Currently, the DCoMEX framework is a set of 2 application codes relying on MSolve. In the sections below, we describe the benchmark applications, the benchmark problems and the datasets.

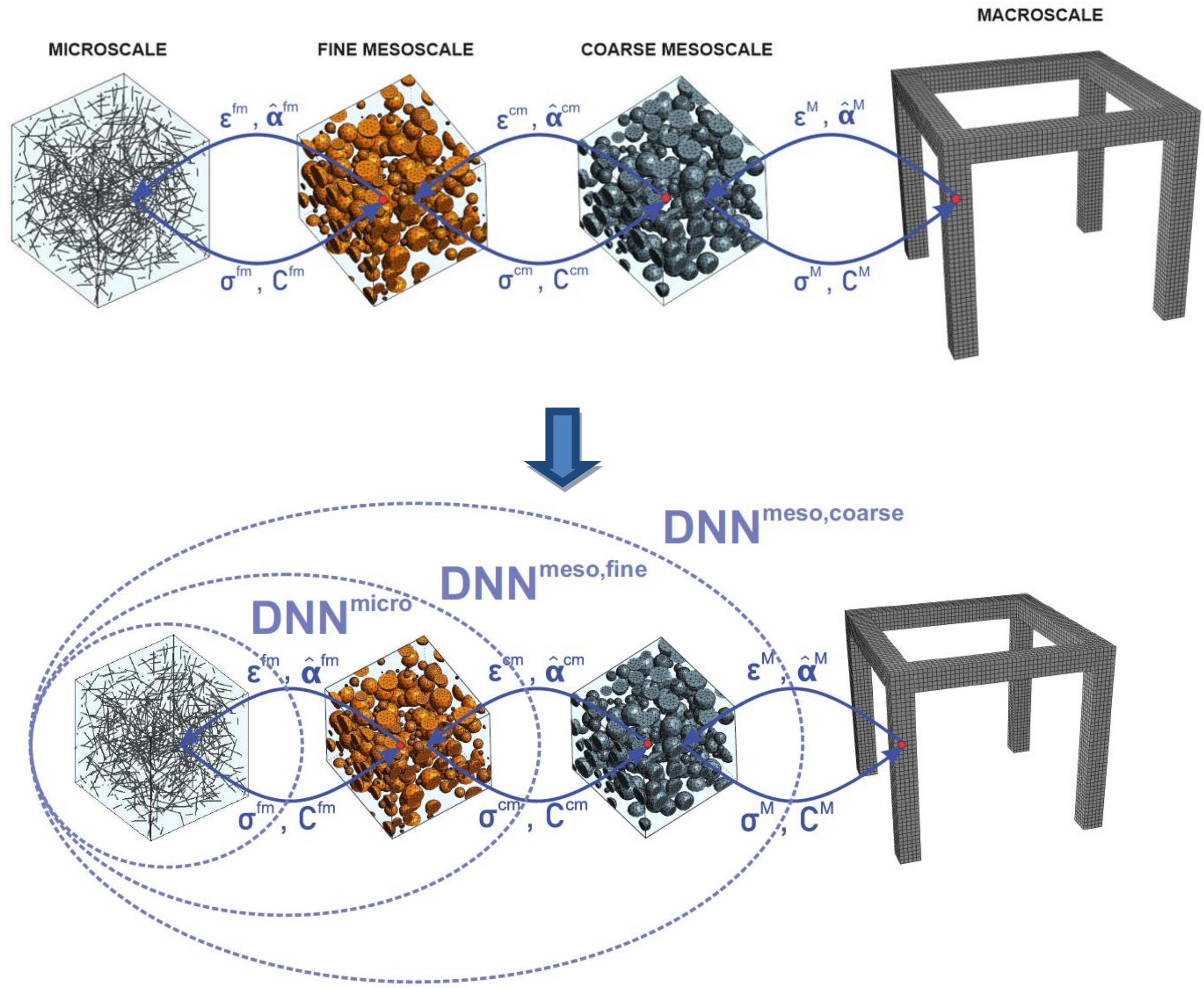
MSolve

MSolve, is a general-purpose computational mechanics solution platform with multiphysics and multiscale capabilities, developed at NTUA, that exploits combined multi-core central processing units (CPU) and graphics processing units (GPU).

1. Relevant Links
- Github: https://github.com/mgroupntua
- Documentation: https://mgroupntua.github.io/
2. Development Status
- TRL 6 - Under refactoring, most unit tests work.
3. Hardware Support
- CPU Intensive computation (Dense Linear Algebra mostly) using MKL
- Local Parallelism - It employs local parallel sampling through fork/join (multiprocessing).
4. Dependencies
- (Optional) SuiteSparse - For linear algebra module
- (Optional) Intel MKL - For linear algebra module
- Compiler: Roslyn, support for C# 7.0 and higher.
5. Platform Support
- Linux: Compiling
- MacOS: Compiling
- Windows: Compiling

2.1 DCoMEX-MAT

DCoMEX-MAT is a multiscale material modeling framework built on MSolve, designed to efficiently analyze complex composite materials. It offers an accurate and streamlined computational pipeline by leveraging the predictive power of nonlinear computational homogenization. By integrating neural networks as surrogate models, DCoMEX-MAT significantly reduces the computational time required for what is typically a resource-intensive process.



The approach involves using a series of deep feedforward neural networks (DNNs) to represent the

Figure 3: DCOMEX-MAT multiscale material model solution pipeline

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coarser ones, DNNs representing finer scales are embedded within those representing coarser scales. After training, a unified deep network is created, emulating the macroscopic behavior by integrating physical mechanisms from all finer scales. This process is illustrated in Figure [3], where the traditional 4-scale nonlinear computational homogenization process is replaced by the proposed surrogate modeling approach. As a result, this method enables efficient solutions to complex problems and facilitates multi-query analyses, such as Monte Carlo simulations for Bayesian inference, sensitivity analysis, and stochastic optimization. For a more detailed description regarding this framework the reader is referred to the report D7.4 (theory manual) of DCoMEX-MAT.

2.2.3 Test cases

To illustrate the presented framework, the interfacial mechanical properties of CNTs in cementitious material configuration have been explored. Specifically, a stochastic propagation analysis was performed by means of the Monte Carlo method on how these microstructural interfacial parameters affect the macrostructural response. The tests are taken from experimental reports from the literature and these include a 3-point bending test of a CNT-reinforced cement specimen, a tensile test performed on CNT-reinforced mortar rods and a 4-point bending experiment on a CNT-reinforced concrete beam. Next, the details for each experimental case will be briefly presented along with the multiscale model that reproduces the material's scales as well as the overall structural and material behavior. More details can be found in D7.4 (theory manual) of DCoMEX-MAT.

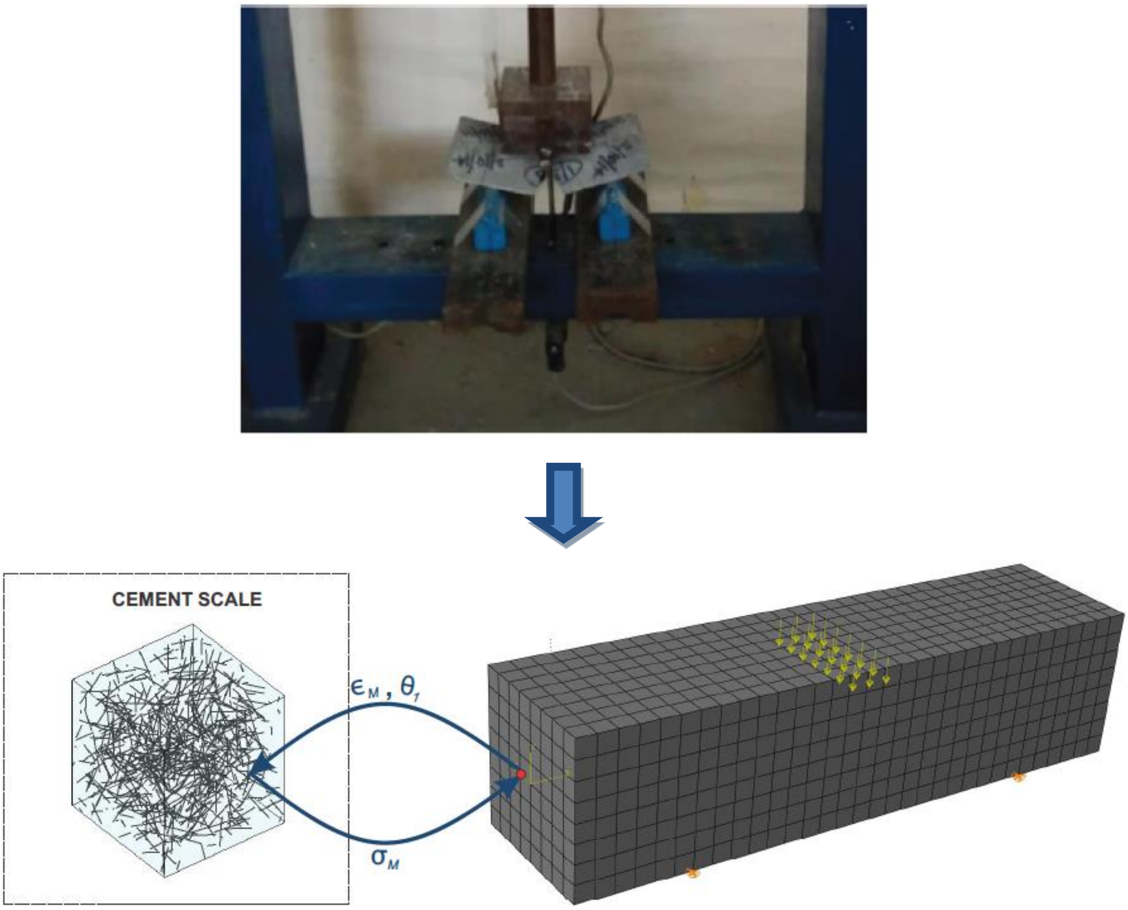

Figure 4: Experimental setup and multiscale model of the CNT-reinforced cement case

The first dataset was obtained from a 3-point bending test on a fully hydrated cement paste coupon (28 days old) reinforced with a 0.3% weight fraction of carbon nanotubes (CNTs). The testing beam specimen measured 160 mm x 40 mm x 40 mm, with two supporting rollers spaced 100 mm apart. A single, gradual point load was applied at the center of the beam's upper surface using a third roller. The CNTs had diameters ranging from 10 nm to 20 nm and lengths between 10 μm and 20 μm. To simulate the experiment numerically, a detailed multiscale model was developed, as illustrated in Figure [4]. The microstructural RVE was modeled by adding equivalent beam elements (EBEs) with random positions and orientations within the RVE until the specified weight fraction was achieved. For the macroscale model, 2048 hexahedral elements were used, resulting in a structural system with 8018 degrees of freedom (DOFs).
The second experimental data source is a tension test conducted on a cylindrical mortar rod, incorporating a 0.5% weight fraction of carbon nanotubes (CNTs) as fillers. The rod coupon had a length of 500 mm and a diameter of 30 mm. One end of the rod was fixed, while a gradually increasing tensile load was applied at the other. In this study, the CNTs had diameters ranging from 10 nm to 30 nm, with lengths between 1 μm and 2 μm. The CNT-cement scale is formulated similarly to the first

multiscale model. To model the mortar at the mesoscale, an RVE was developed, accounting for sand particles as inclusions within the mortar matrix. An additional length scale was introduced to capture these details. The macro-model was discretized using 3,666 tetrahedral elements, resulting in 18,966 structural DOFs. Both the experiment and the respective multiscale model are presented in Figure [5].

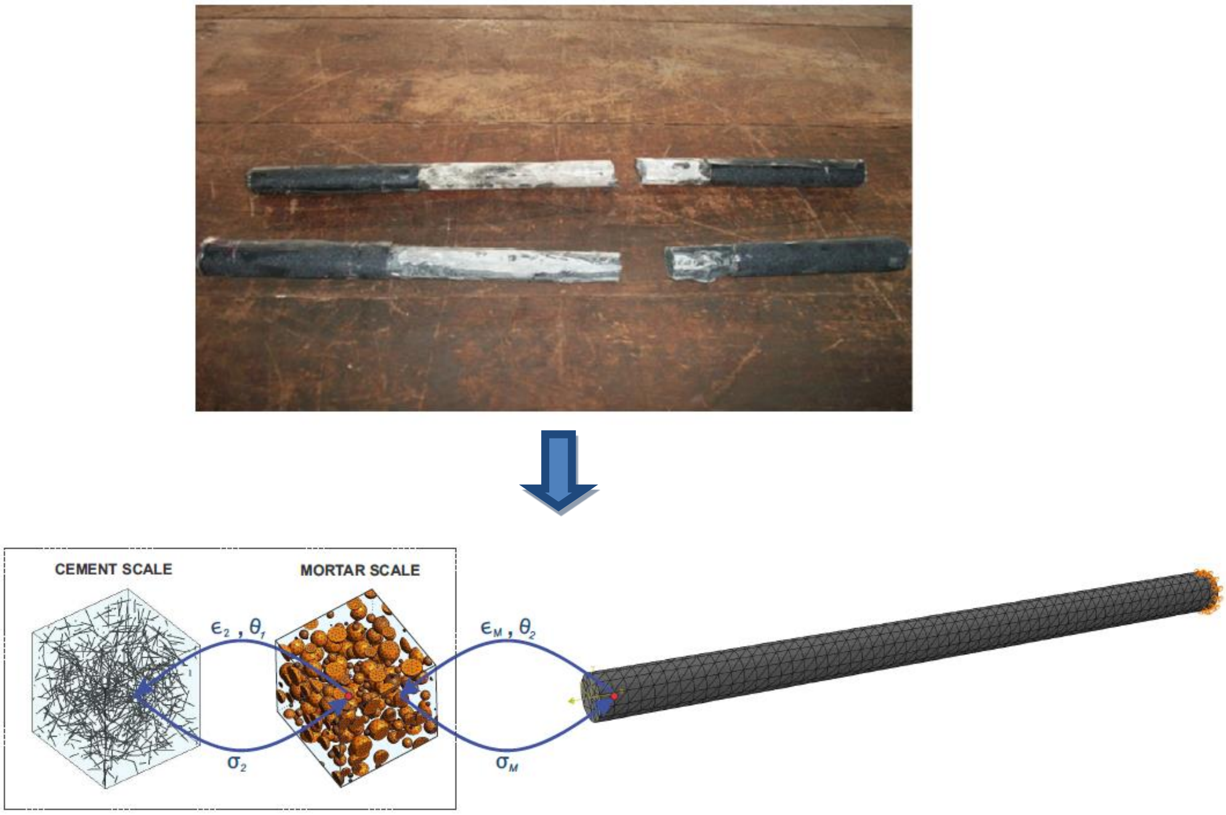

Figure 5: Experimental setup and multiscale model of the CNT-reinforced mortar case

The third dataset is derived from a four-point bending test conducted on a concrete beam reinforced with steel rebar and enhanced with 1% weight fraction of carbon nanotubes (CNTs). The beam measured 2100 mm in length, with a cross-section of 150 mm by 250 mm. Supports were placed 2000 mm apart along the lower side of the beam. The CNTs used had diameters ranging from 3 to 15 nm and lengths from 15 to 330 μm. During the flexural test, two incremental point loads were applied to the upper surface of the beam. In this analysis, the material behavior was represented by a three-scale model of cement, mortar, and concrete, as illustrated in Figure [4]. These scales were hierarchically connected to the macroscopic finite element (FE) model of the beam. The first two scales followed the formulations of the previous mentioned models, while the final scale captured the coarse aggregates at the mesoscale of the concrete specimen. The macrostructural system was discretized into 676 hexahedral elements and featured 1536 DOFs.

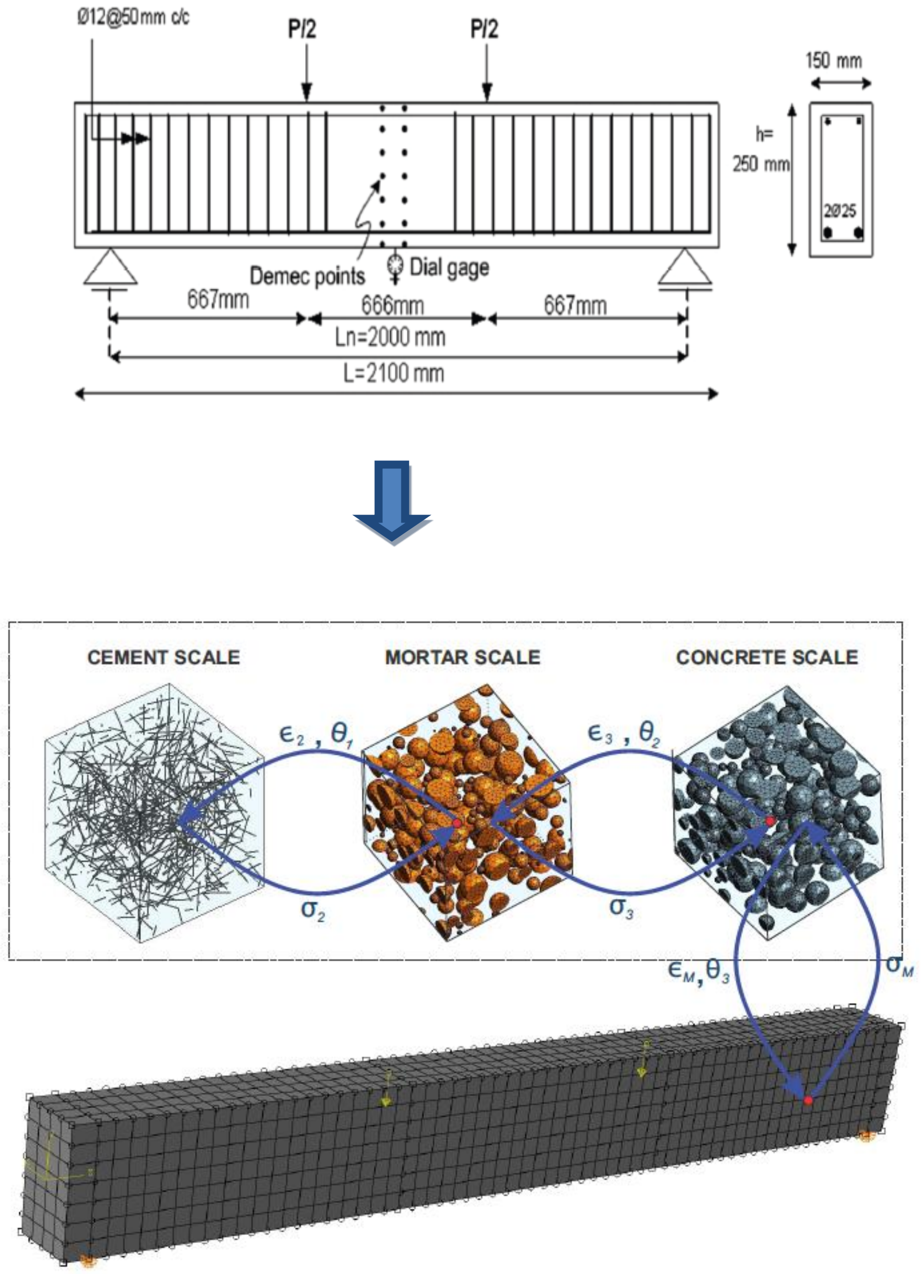

Figure 6: Experimental setup and multiscale model of the CNT-reinforced concrete case

3. Benchmark results

The following benchmarks have been run on MeluXina, on the cluster nodes, featuring AMD EPYC 7H12 64-Core Processors, 512GB of RAM and an InfiniBand (IB) HDR 200Gb/s high-speed fabric for node interconnection.

3.1 DCoMEX-MAT

Problem: 3-point bending test - cement

Nodes	Time (min)	Speedup (x)	Efficiency (%)

10	61.8	1.0	100
100	6.3	9.8	97
1000	0.7	96.5	94

Problem: 3-point bending test - mortar

Nodes	Time (min)	Speedup (x)	Efficiency (%)
10	74.1	1.0	100
100	7.8	9.5	99
1000	0.8	92.7	98

Problem: 3-point bending test - concrete

Nodes	Time (min)	Speedup (x)	Efficiency (%)
10	85.3	1.0	100
100	8.7	9.8	97
1000	0.9	94.6	97

4. Summary and Conclusions

In this report, the performance of DCoMEX-MAT was examined. In all test cases, scalability was near the optimum and all available computational resources were utilized in an optimum manner.