Data driven Computational Mechanics at EXascale

DCoMEX

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

Post-processing methodology

DELIVERABLE D5.3

Version No 1

http://www.dcomex.eu/
This project has received funding from the European High-Performance Computing Joint Undertaking Joint Undertaking ('the JU'), under Grant Agreement No 956201

DOCUMENT SUMMARY INFORMATION

Project Title	Data driven Computational Mechanics at EXascale
Project Acronym	DCoMEX
Project No:	956201
Call Identifier:	EuroHPC-01-2019
Project Start Date	01/04/2021
Related work package	WP 5
Related task(s)	Task 5.3
Lead Organisation	TUM
Submission date	11/7/2024
Re-submission date	
Dissemination Level	PU

Quality Control:

	Who	Affiliation	Date
Checked by internal Reviewer	I. Ezhov, B. Menze	TUM	1.7.2024
Checked by WP Leader	I. Ezhov	TUM	11.7.2024
Checked by Project Coordinator			

Document Change History:

Version	Date	Author (s)	Affiliation	Comment
1.0	1.7.2022	I. Ezhov, B. Menze	TUM	

Content

1. Description

Deliverable D5.3 describes the additions that enable the UQ-aware image processing module and software tool to visualize simulation outputs. The module enables the visualization of uncertainties resulting from boundary conditions as described in D5.2. As an extension to the modules described in D5.1, this report contains the specifications of Task 5.3, and describes means for visualizing uncertainties of model parameters in the DCoMEX image segmentation software tool.

1.1 Uncertainties Resulting from Local Uncertainties in the Modeling Domain

1.1.1 Local uncertainties in boundary conditions translate into local uncertainties in simulation results.

Taking real image data as input to extract boundary conditions of a modeling domain may lead to a well defined geometry in some cases, but images may also be associated with uncertainties in physical boundaries and, hence, to uncertainties in boundary conditions, in other cases.

The DCoMEX UQ image processing software is capable of extracting features that define boundaries in downstream simulations. Instead of discrete discontinuities between image segments, probabilities can be extracted. This can be done, or example, via general machine learning algorithms for general image processing tasks using the Ilastik software framework. In specialized applications in clinical neuroimaging this may be probabilistic boundaries extracted in the brain tumor image data pipeline that is part of the DCoMEX UQ image segmentation modules.

1.1.2 Implementation in the DCoMEX UQ aware image segmentation software

Uncertainties in the boundary conditions within the modeling domain are represented within the DCoMEX UQ-aware image segmentation software by sampling the domains in a structured way following [1,3,5], and presenting the downstream simulation with a set of likely simulation domains (D5.2). As such, even in a deterministic simulation, the output of simulating local state variable will be a set of parametric maps. To this end, the DCoMEX UQ-aware image segmentation software has implemented a visualization module for simulation outputs. It is capable of deriving – and presenting in the interactive 3D visualization mode – summary statistics of the simulation results, such as pixel- and voxel-wise averages, standard deviations, or other descriptors of the given pixel-specific distribution.

1.2 Uncertainties Resulting from Global Uncertainties of Parameters of the Simulation Model

1.2.1 Global parametric uncertainties translate into local uncertainties in simulation results.

Uncertainties in global parameters of the simulation model are another source of uncertainty in simulation output. Bayesian models typically lead to samples generated from instances of the distributions. As a consequence, output in model spatially distributed parameters results in distributions at voxel level, and sets of image volumes at the more general data processing level. An optimal postprocessing will allow to interpret them within the original modeling domain, and enable the user to study meaningful summary statistics at the voxel level. This may be, for example, parametric maps featuring the mean (or mode) or variance (or dispersion) of the local uncertainty introduced into the simulation via the uncertainty propagated when sampling from the distributions of relevant global parameters.

1.2.2 Implementation in the DCoMEX UQ aware image segmentation software

Same as with uncertainties associated to the unknowns in the boundary conditions, the resulting simulation maps need to be, first, summarized and, second, visualized. The latter should be done within the coordinates of the original domain to enable a direct verification and interpretation of the results. As such, the DCoMEX image post-processing module can ingest the resulting simulation outputs, and visualize them in the original domain of images and boundary conditions. Same as for uncertainties in BCs, summary statistics of the distributions can be visualized, including parameters of the mode or dispersion of any pixel- / voxel-wise distribution.

2. Specifications

2.1. Visualizing Simulation Results

Any functions in the DCOMEX image processing tool are organized as modules, and built on 2D or 3D volumes associated with input to and output from the simulation models. For visualizing output, this set of modules has been adapted to enable a volumetric visualization for the aforementioned summary statistics.

The reformatting tool allows translating them from volumetric MSolve formats into common 3D formats of the DCoMEX visualization module, or the alternative visualization modules that are available within the DCoMEX pipeline. Importantly, while all visualization modules are interactive and allow for inspecting local parameter values and summary statistics, some can be used to “clean” simulation results, e.g., in case of simulation artefacts that should not enter any downstream analysis. Importantly, by offering standard file formats compatible with 3D data analysis in the biomedical domain, final simulation results can also be made available to specialist processing software, such as the 3D Slicer[1] or Napari[2] .

2.2 Tools and Optimization for DCoMEX Reference Applications

2.2.1 Integration into the DCoMEX image segmentation software

The visualization software has become a module in the DCoMEX UQ-aware image segmentation software, and an additional module in the overall toolbox. Visualization capabilities for inspecting image data can be reused to keep the overall installation slim, also offering interactive functionalities, for example, in the ITK-snap software or the dedicated VTK visualization module of DCoMEX. Aligning with the overall software tool, the postprocessing functionalities are installed jointly with the pre-processing software, using the same data transformation and processing capabilities as the preprocessing modules.

Importantly, the postprocessing module can be pipelined and executed in command line tools, similar to the pipelines for the preprocessing, enabling a straightforward interaction and processing also of large or repeated tasks.

[1] slicer.org
[2] napari.org

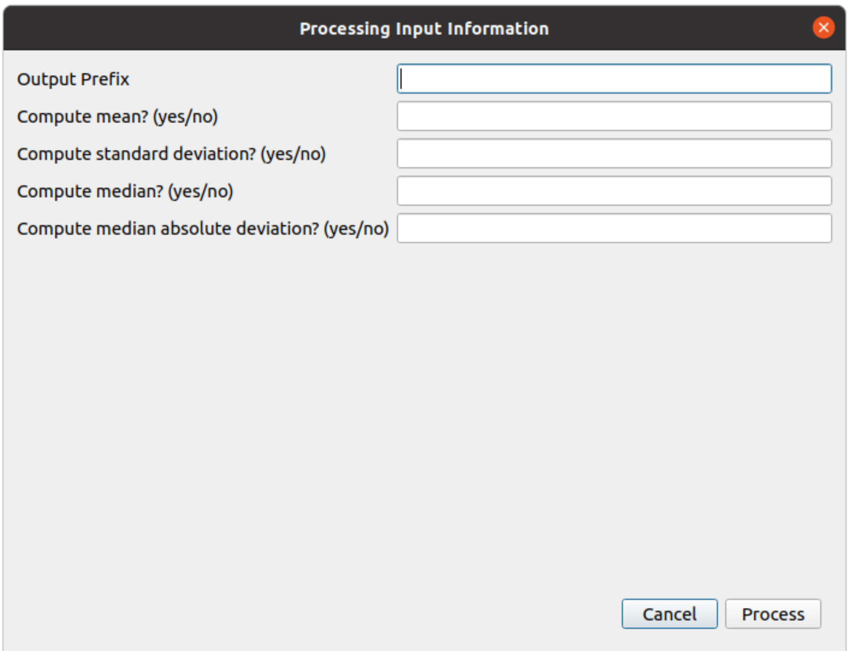
2.2.1 Structure, interfaces and functionality

The plugin is structured into the following primary components:

1. **Core Processing Module ("__init__.py")**: This handles the main computation tasks, including statistics calculations.
2. **Interface Layer ("settings.json")**: This defines the APIs for interaction with the plugin, including data input and result output interfaces.
3. **Data folder ("image_volumes")**: Serves as a placeholder for the images across which the statistics have to be computed.

These functions can interact with other components of the tool via interfaces that are:

1. **Input Interface**: Accepts a set of image volumes as input and requests for desired statistics to be computed. Same as other interfaces of the processing module, it appears as follows:



2. **Output Interface**: The output is returning data with calculated statistics

mean.nii.gz
std.nii.gz
mad.nii.gz
median.nii.gz

As indicated, different functionalities are implemented as default, including:

1. **Statistical Calculations**:

   Mean: Computes the element-wise mean value across image volumes.

   Standard Deviation: Computes the element-wise standard deviation value across image volumes.

   Median: Computes the element-wise median value across image volumes.

   Median Absolute Deviation: Computes the element-wise mean absolute deviation value across image volumes.

2. **Visualization**:

   DcoMEX visualization module utilizes the processed data to generate visual representations of the obtained statistics.

As all functions are implemented via python, they can straightforwardly be adapted to other summary functions.

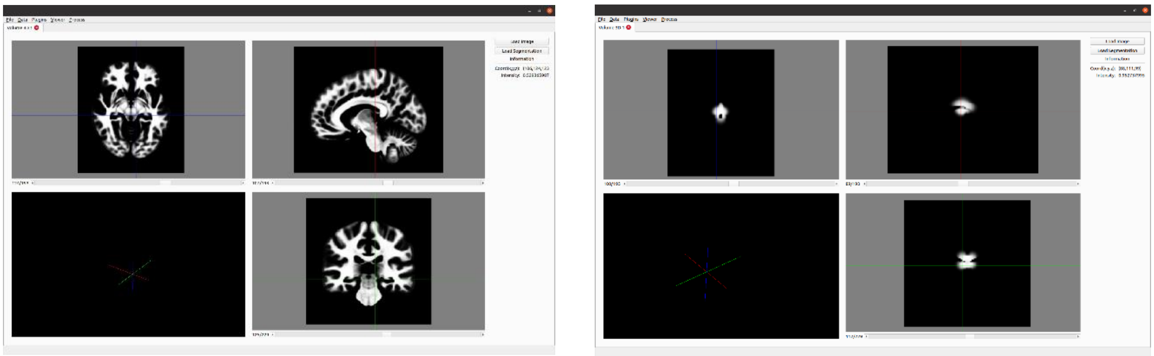


Figure 1. *Visualizing a patient anatomy in the DCoMEX Bio Usecase using the DCoMEX image data processing toolbox. For both input images and probabilistic tissue segmentations derived (left) and the resulting estimates of the tumor cell distributions (right) a visualization in a joint spatial domain is enabled by the DCoMEX image processing tool.*

2.2.3 An example for brain tumor simulation in the DCoMEX Bio Usecase

The Bio Usecase offers an example for the use of the uncertainty visualization module. To prepare the data, tissue compartments need to be estimated resulting in boundary conditions with associated uncertainties (D5.2). Fig 1 shows white matter tissue in the original patient domain. Using domain and image segmentations as input, an implementation of tumor growth model in MSolve, e.g., a simple Fisher Kolmogorov PDE mode, can be used to estimate model parameters, as well as their distribution conditioned on the given patient observations. As an alternative, a simple estimate can also be generated from the tumor image processing software module [6].

Sampling from the uncertain boundary conditions, as well as from the estimated parameter distributions, we obtain a set of tumor simulations that indicated a likely area of tumor cell infiltration. Summary statistics calculated across the resulting set of tumor simulations, 200 in the given example, can be generated directly from the output and visualized in the spatial domain of the patients anatomy for further inspection.

2.3 UQ Module Availability

The aforementioned processes for probabilistic image segmentation are part of the DCoMEX image segmentation tool and its interlinked third-party image segmentation tools (D5.2).

The software is developed as an executable or script based on Python. It has been developed and is available with open sources license from https://github.com/DComEX

3. References

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- [6] The Tumor Growth Toolkit Software, Michal Balcerak et al. https://github.com/m1balcerak/TumorGrowthToolkit