BIGMECA Data Platform

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COPIL – Chaire BIGMECA

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BIGMECA Chair PostDoc

Context

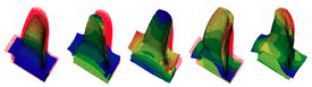
- Rise of automated 4D testing
- Maturity of HPC Material simulation
- 4D Characterization/Simulation of microstructure/damage/plasticity
- Mutltimodal Datasets :
  EBSD, SEM, DCT, XCT, FEM, FFT, CAD...

Challenges

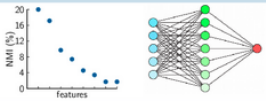
- Exploit data through complex numerical chains
- Develop a unified (open)data framework
- Applications : structure alloys
  $\rightarrow$lifetime assessment, damage, plastic localization

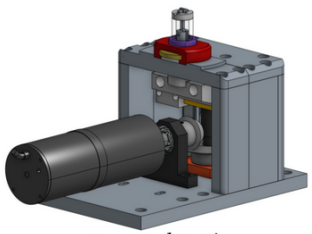
Données physiques
1D, 2D, 3D, 4D,
multimodales, in situ

Données de simulation
bilan, causalité,
de l'image au maillage,
réduction de modèles

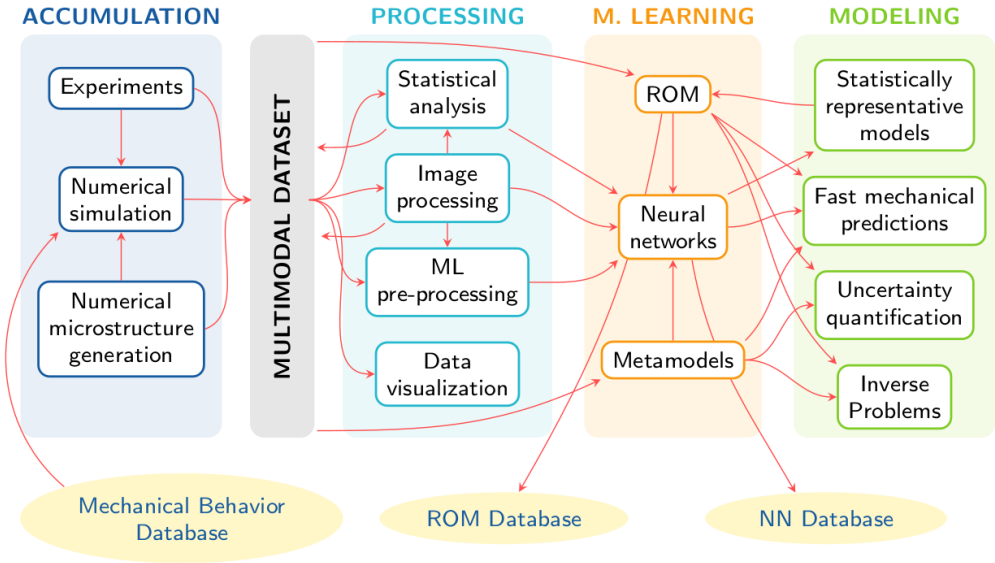


Algorithmes avancés
massivement parallèles,
machine learning,
neural networks





BIGMECA DATA FLOW



Overview

Technical Developments → **Applications**

Literature Review

Existing Platforms
File Formats, OpenData


BIGMECA Chair
Technical Report n° 1

Design and First Developments of the BIGMECA Data Platform

October 6, 2020

Aldo MARANO

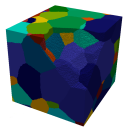
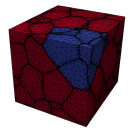
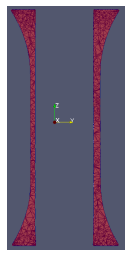
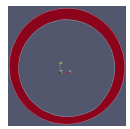
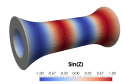
MINES ParisTech, PSL Research University
MAT - Centre des matériaux, CNRS UMR 7633
Evry BP 87 9103, France

Prototype

Data Format

HDF5 XDMF

Basic API & Data
Images/Meshes/Arrays
Metadata handling
Compression

Building Data Platform

PYMICRO integration

BasicTools integration
BT mesh I&O

Mesh Datamodel
Elset/Nsets
Nodal/Elt-cst fields
Vector/Tensor fields

Generic DataModel
Nodes naming system
Structured arrays

GrainDataTable

	bounding_box	center	idnumber	orientation	volume
0	[[72,74], [10,18], [3, 9]]	[0.24174044,...	12	[0.9882962 -0.09180787, 0.14053537]	39.
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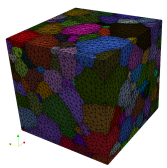
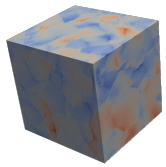
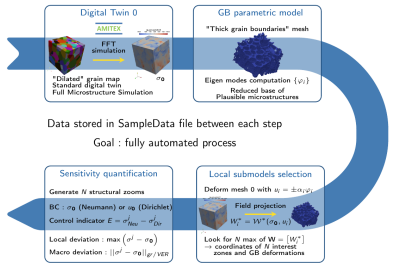
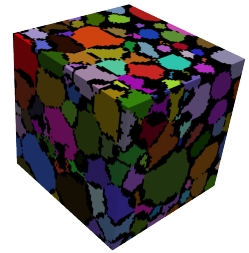
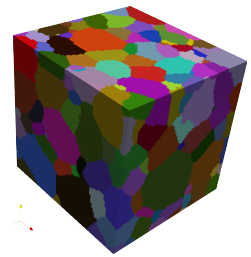



DCT uncertainty



Contents

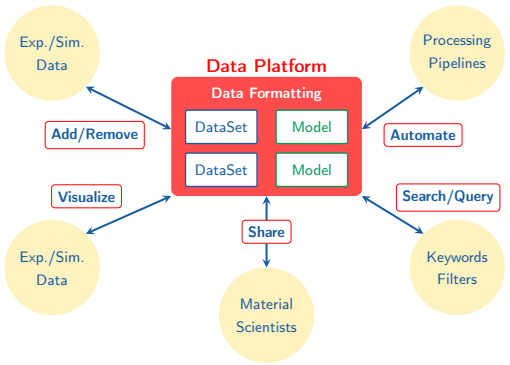
BIGMECA Data Platform

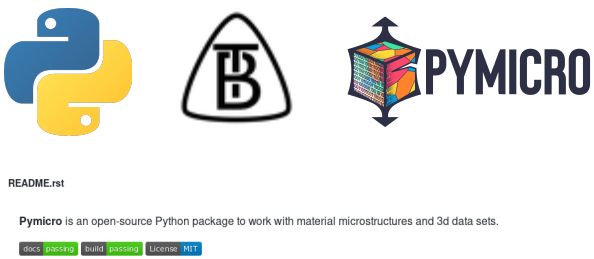
Features

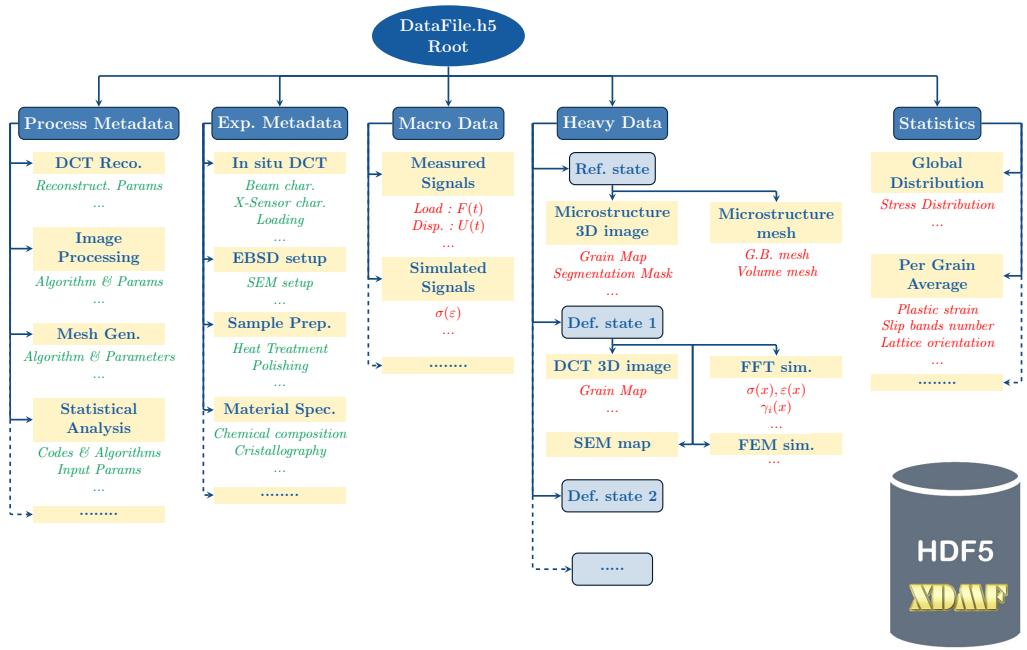
- XDMF/HDF5 – Compression
- "Multimodal" Paraview
- High-level user friendly API
- Interface with numerical tools
- GitHub / Documentation

Data Models

- Structured Arrays
- Grids : Images and Meshes – 2D & 3D
- Fields : array ↔ grid (Nodes, Elt, IP)
- Flexible & unlimited metadata







Data Platform Improvements Overview

- **Automatic meshing tools for multi-phase images :**
  - Integration of F. Nguyen Matlab tools
- **Integration with external numerical tools :**
  - Generic script generator and program caller
  - Basis for specific tools coupling classes generations
  - Coupled with : Paraview, ViTables, Zset
- **Integration of IP fields handling :**
  - IP field storage and visualization Data Model
  - Handling of mixed mesh topology

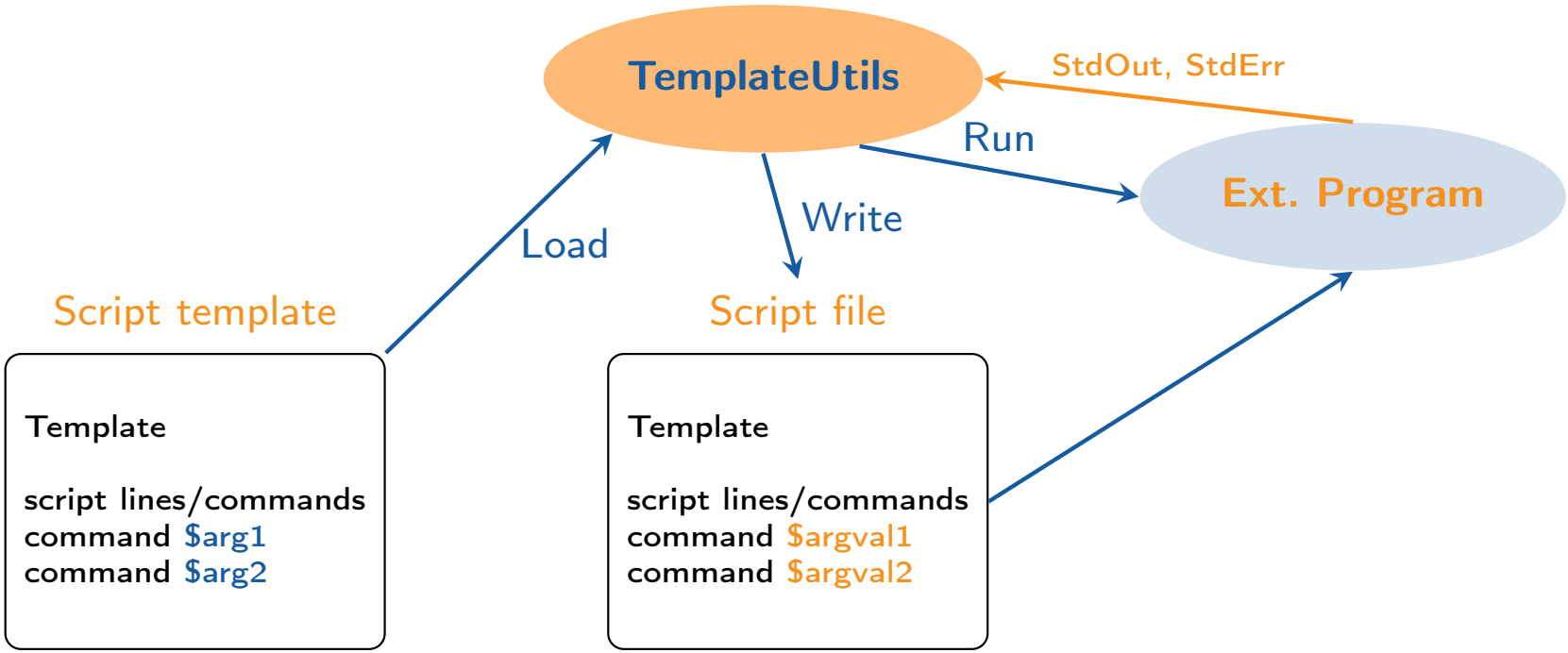
Coupling with external tools

TemplateUtils Class

- Gets a script template
- Set script argument values
- Run external program from Python
- Prints StdErr, StdOut

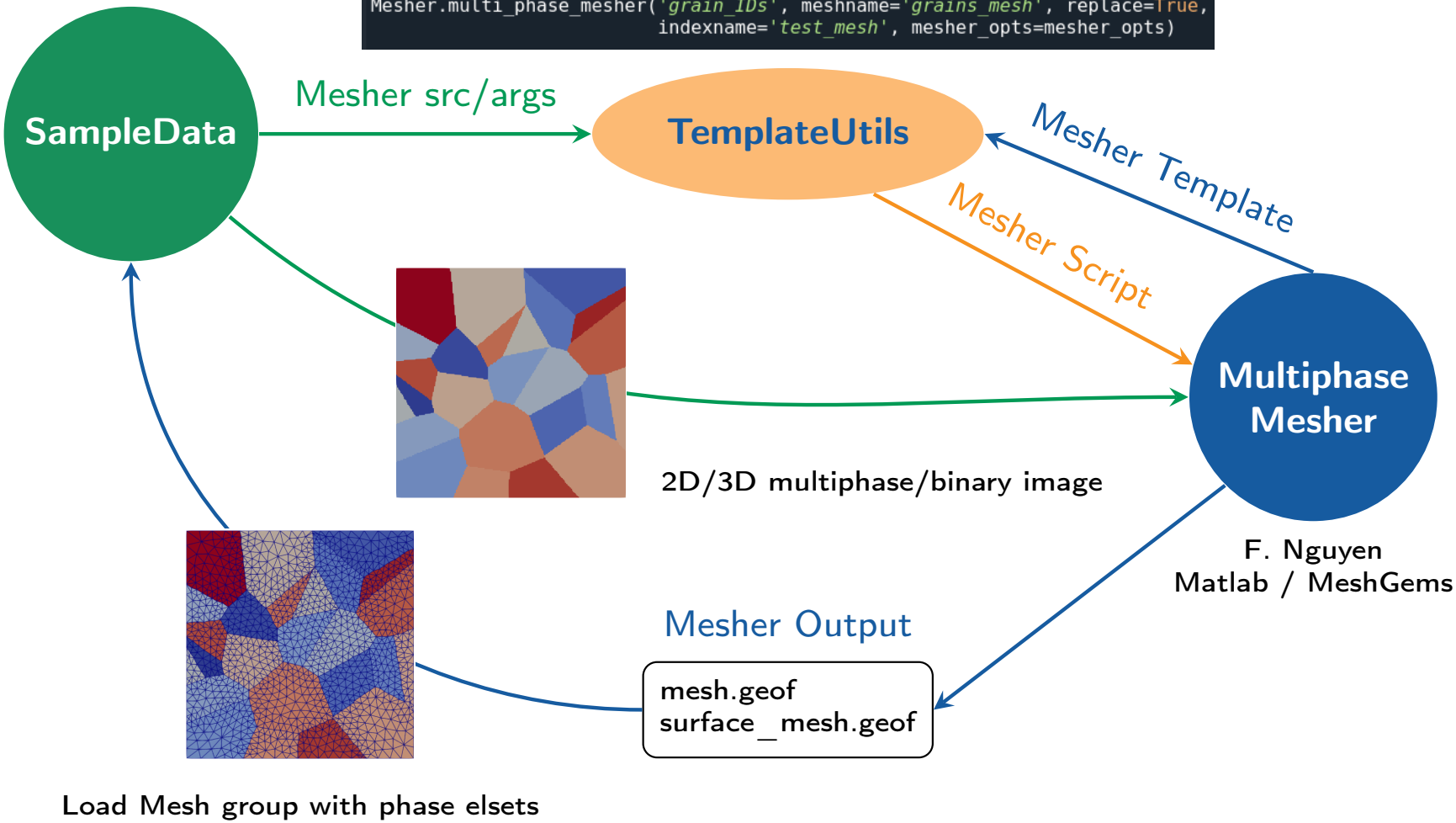
Perspectives

- Workflow manager
- Parallel cluster job manager
- Automatic parametric studies



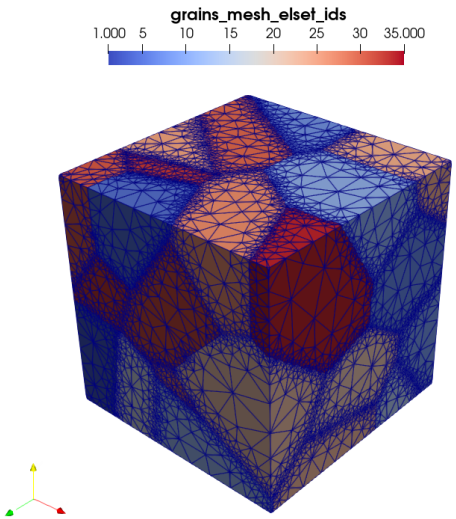
Automatic Mesher

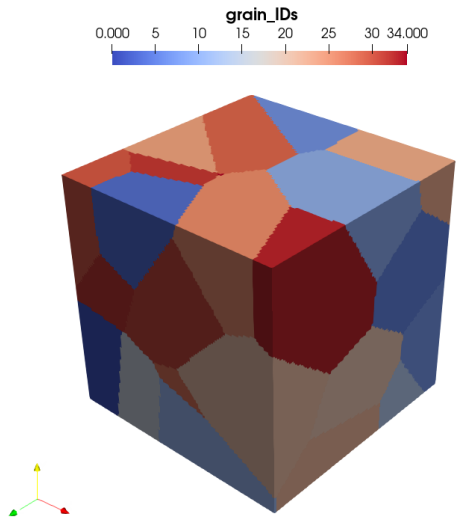
```
# Create Mesher instance
Mesher = SDImageMesher(data=data)

# Set up mesher options
# LS: line sampling rate (distance between points used to disretize curved
#      boundaries between image phases)
# HMIN/MAX : minimal and maximal size of mesh element edges
mesher_opts =  {'LS':5,'HMIN':5,'HMAX':100}

# Run mesher
Mesher.multi_phase_mesher('grain_IDs', meshname='grains_mesh', replace=True,
                          indexname='test_mesh', mesher_opts=mesher_opts)
```

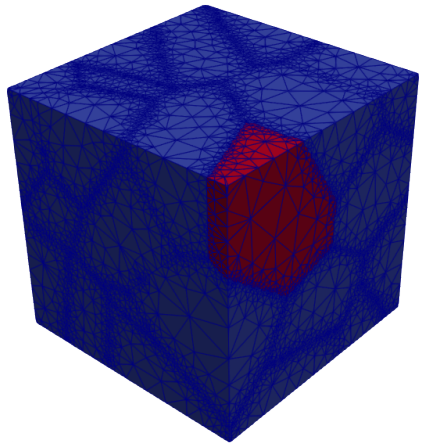


Automatic Mesher : Example

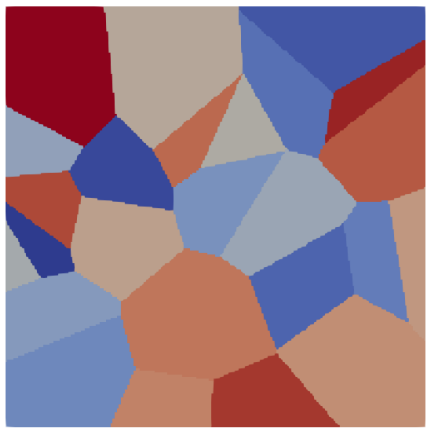
3D Voronoi tesselation

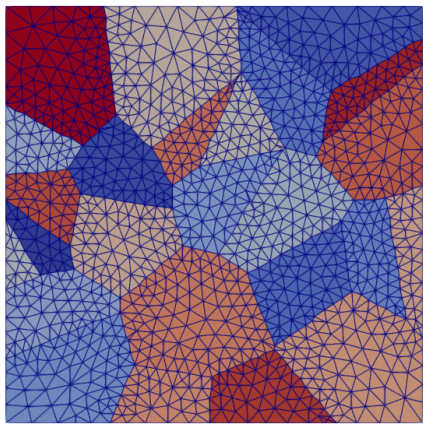




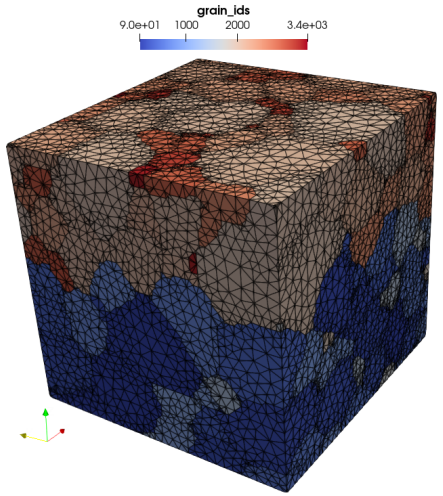


2D Voronoi tesselation





PSICHE DCT Ti subvolume



Zset coupling

SDZsetMesher, SDZsetFEA
SDZsetPostProcessing
SDZsetFieldTransfer

```
Nmodes = 10

FEA.set_inp_filename(filename='eigenmodes_calc')
FEA.set_material_file()
FEA.set_inputmesh(meshname='thick_boundaries_cut')
FEA.set_calculation_type('eigen')
FEA.set_eigenmode_lanczos_calculation(Nmodes, '1e10')
FEA.add_linear_elastic_material_block(volumic_mass=1.0, young_modulus=1.,
                                      poisson_ratio=0.)
```

```
set_bc = ['Xmax','Xmin','Ymax','Ymin','Zmax','Zmin']
dof_bc = ['U1', 'U1', 'U2', 'U2', 'U3', 'U3']
values_bc = ['0.','0.','0.','0.','0.','0.']
FEA.add_boundary_condition(bc_type='impose_nodal_dof', set_names=set_bc,
                           dof_names=dof_bc, values=values_bc)

FEA.set_fixed_set_bc(nset_list=['Thick_boundaries'])
```

SampleData

SDZset

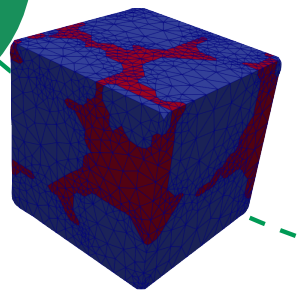
calc. set up

template.inp

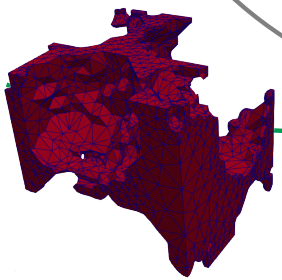
TemplateUtils

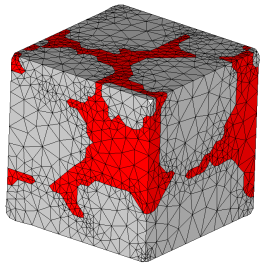
Problem.inp

mesh.geof

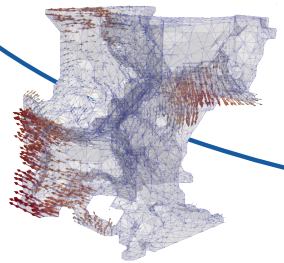


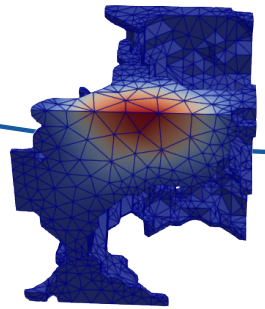
input mesh





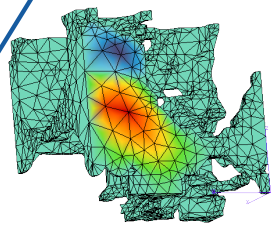
Zset





Problem.ut

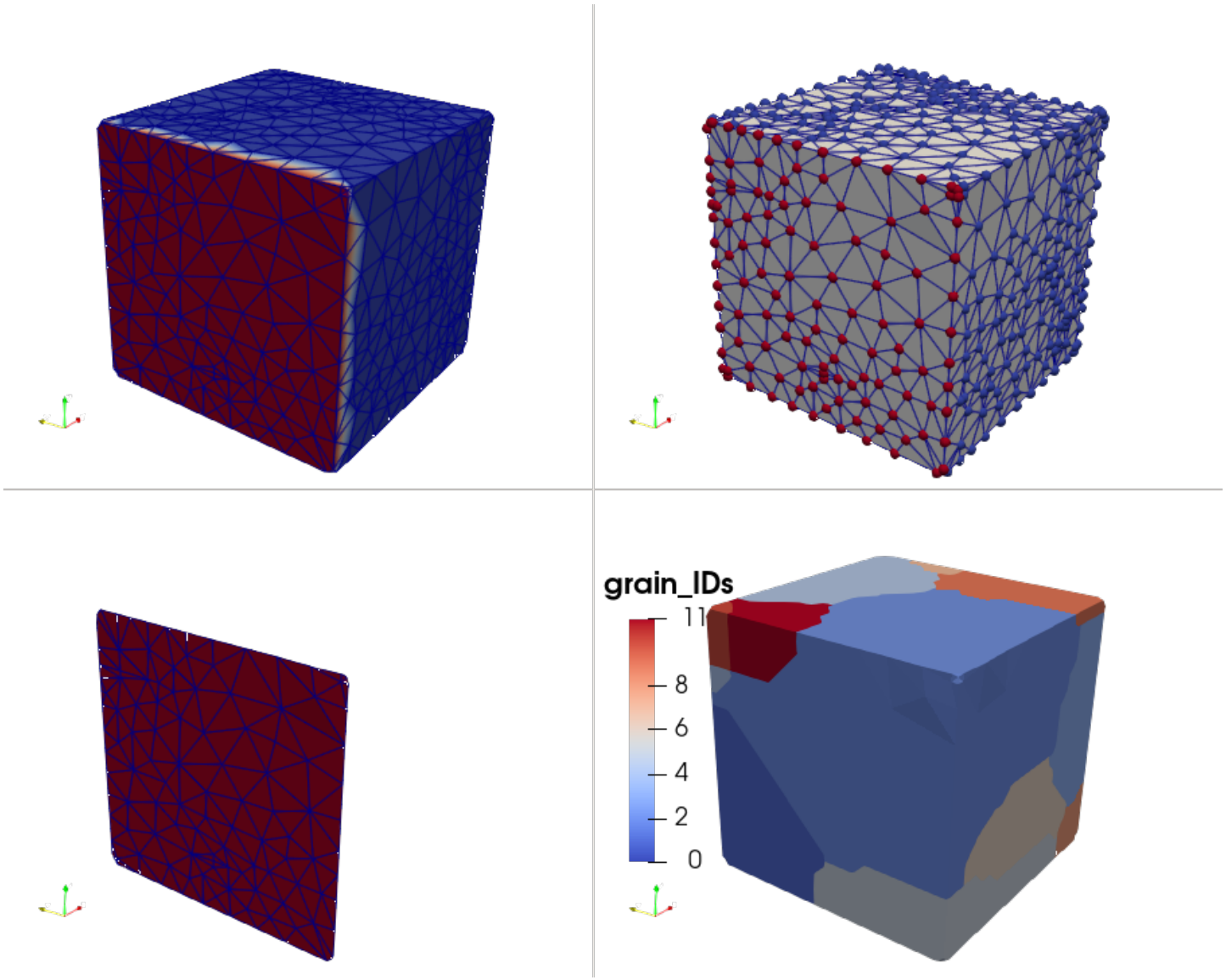
problem.node
problem.integ
...



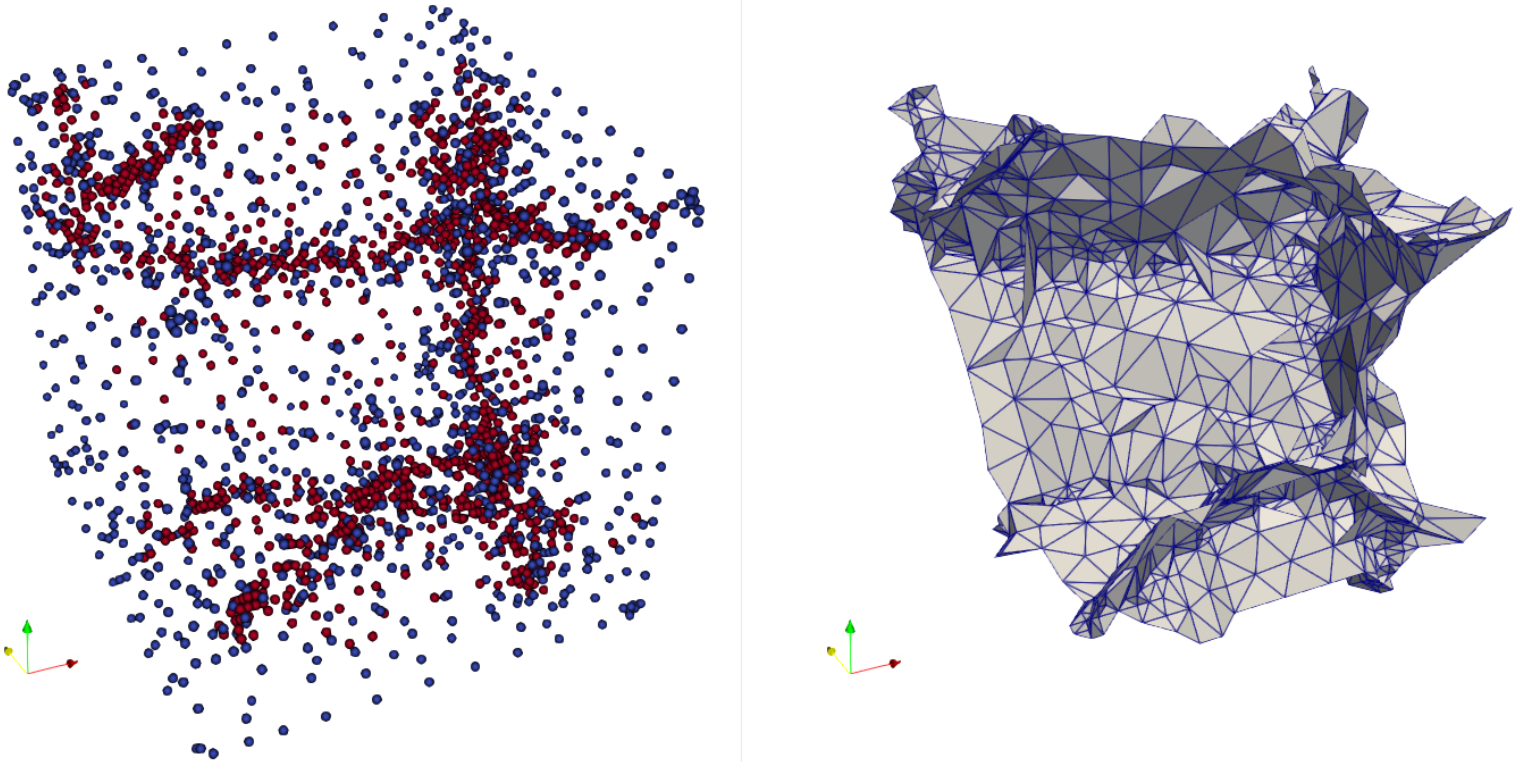
Zset output

```
FEA.run_inp(print_output=(False))
FEA.load_eigenmodes()
```

Zset Mesher example I



Zset Mesher example II



Gauss Point Fields

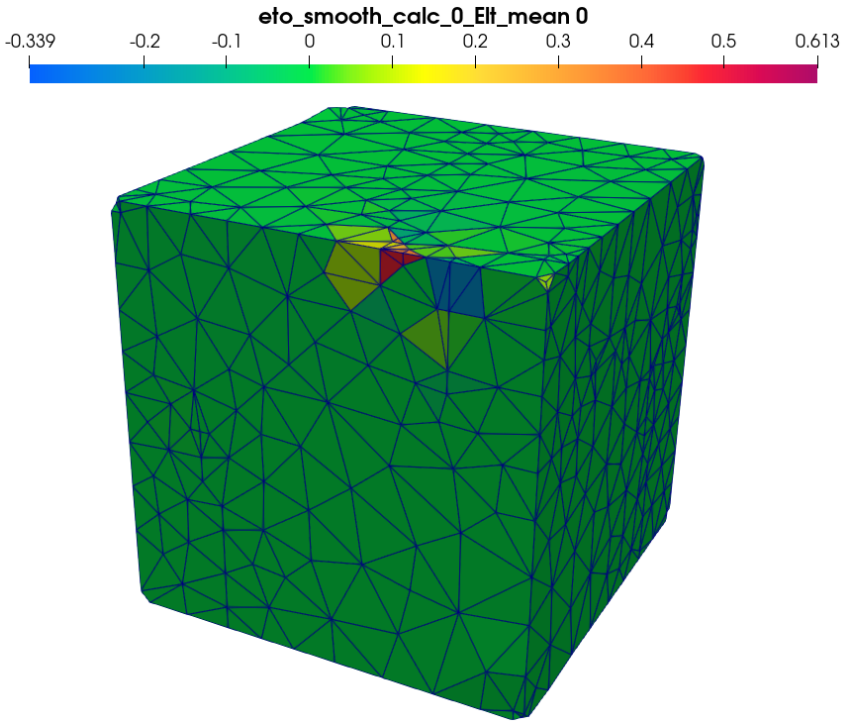
Storage

- Raw data Zset ordering convention
- Visualization array (mean, min, max/elt)
- Scalar, Vector, Tensor
- Shape verification

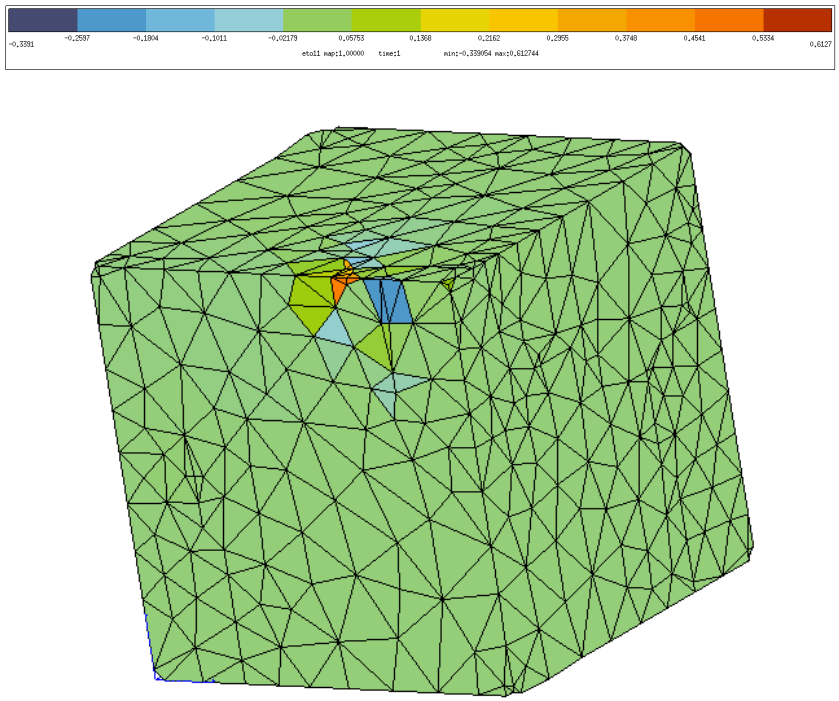
Complex mesh topology handling

- Can handle mesh with bulk & boundary elements
- Fields padding to match mixed connectivity shape
- Mixed XDMF topology format

SampleData ε_{11}



Zset ε_{11}



From images to Zset problems

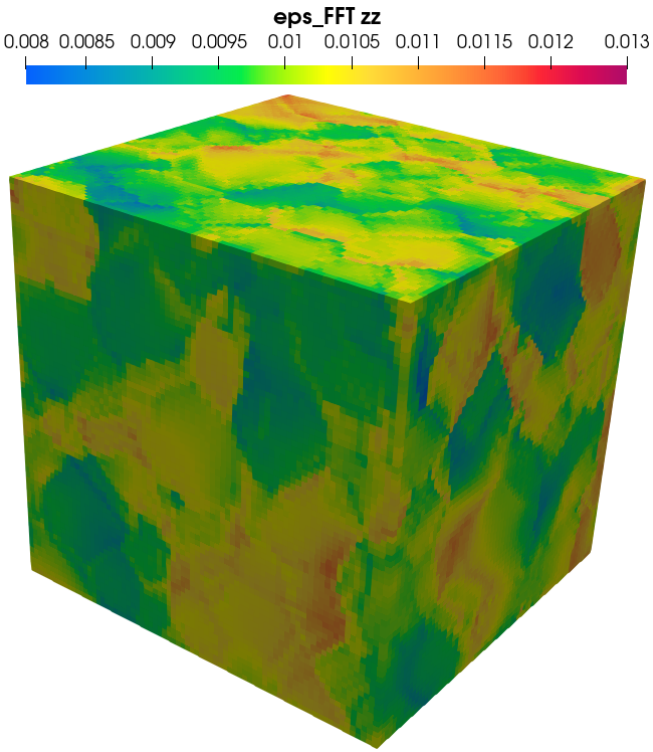
Implementation

- Write image as mesh of *c3D8r* elements
- Write image fields as IP fields
- SampleData $\rightarrow$ .ut problem output

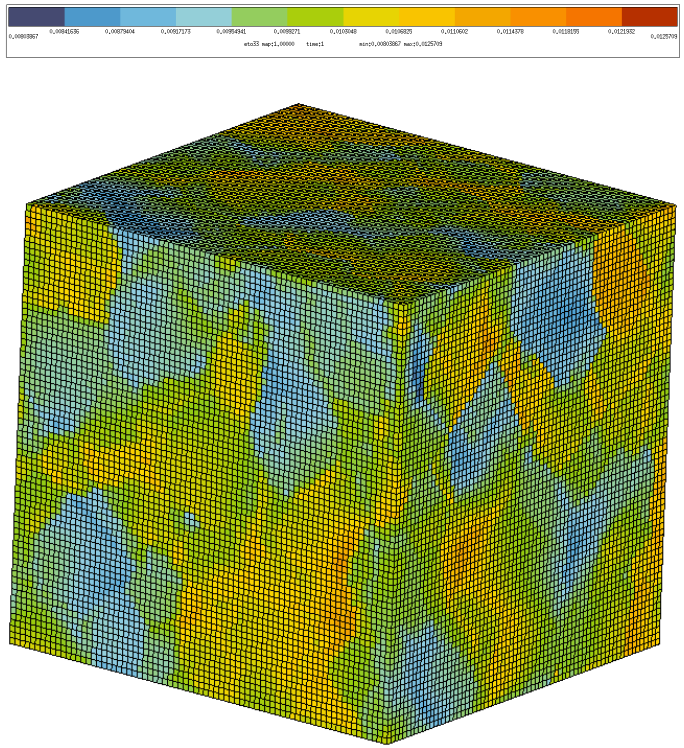
Usecases

- Use FFT Simualtion results as submodel BC
- Use FFT Simulation results with FEM output in post processings

SampleData FFT ε_{33}

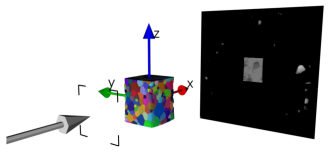


Zset ε_{11}



From DCT data to numerical simulation

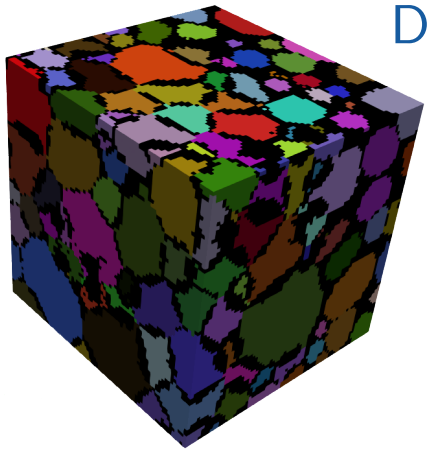
SOLEIL PSICHE



DCT

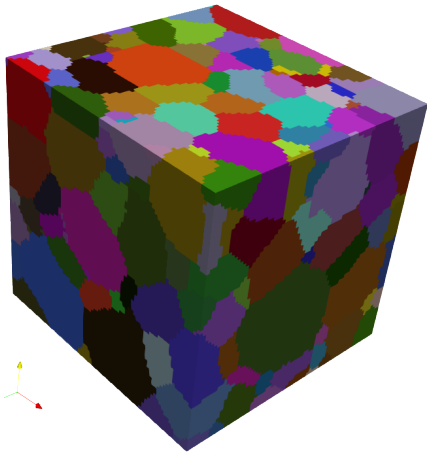
reconstruction

Digital Twin



morphological

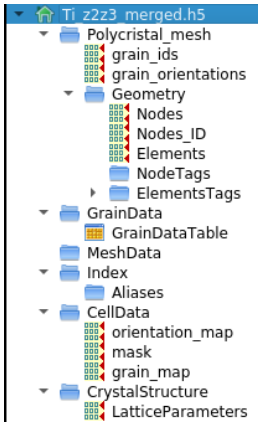
cleaning



storage

storage

Data Platform File



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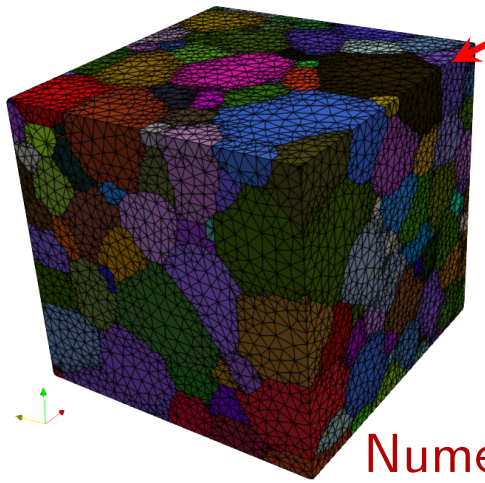
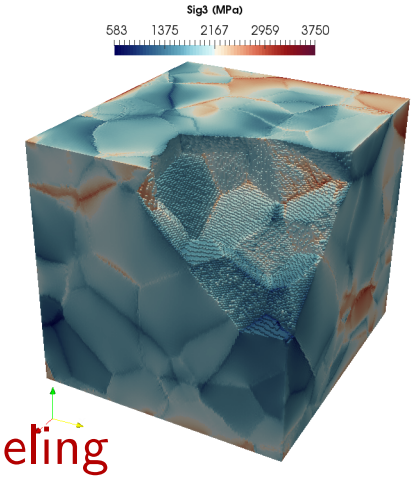
FFT Simulation

Automated meshing



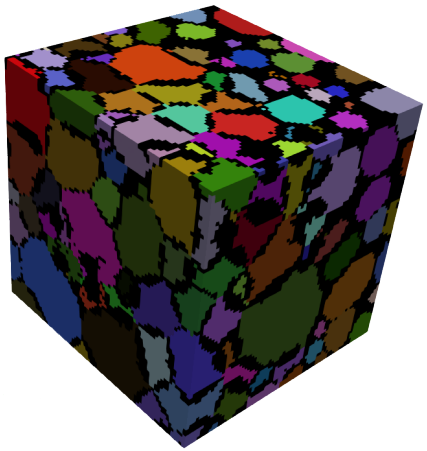


Numerical modeling

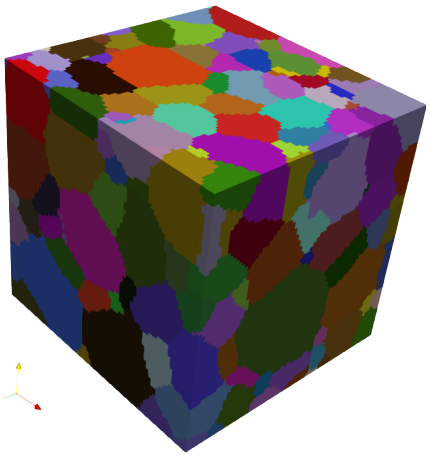
Contents

Problem Recall

DCT reconstruction output



Digital twin 0



Problem

- Exact position of GB ?
- Uncertainty associated to standard reconstruction ?
- Evaluate deviations from digital twin 0

Challenges

- Very large dimension
- How to chose simulations to perform ?
- Which uncertainty compute ?
- Automate process

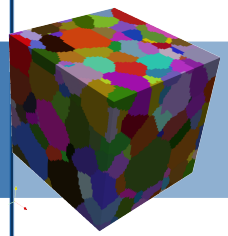
Method

- Parametric (& stochastic ?) generative model based on eigenmodes
- Simulation 0 : FFT. Evaluate local deviations from FEM structural zooms

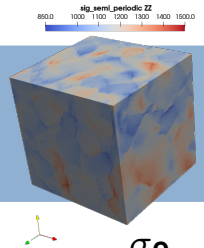
Numerical Chain Overview

Digital Twin 0

AMITEX



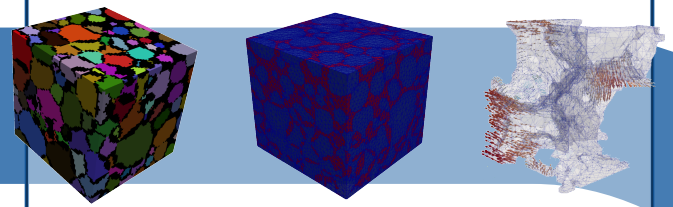
FFT simulation



σ_0

GB parametric model

"Thick grain boundaries" mesh



Eigen modes computation $\{\varphi_i\}$
Reduced base of
Plausible microstructures

Data stored in SampleData file between each step

Goal : fully automated process

Sensitivity quantification

Generate N structural zooms

BC : σ_0 (Neumann) or u_0 (Dirichlet)

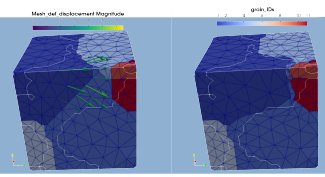
Control indicator $E = \sigma^j_{Neu} - \sigma^j_{Dir}$

Local deviation : $\max\left(\sigma^j - \sigma_0\right)$

Macro deviation : $||\sigma^j - \sigma_0||_{gr\,/\,VER}$

Local submodels selection

Deform mesh 0 with $u_i = \pm\alpha_i\varphi_i$



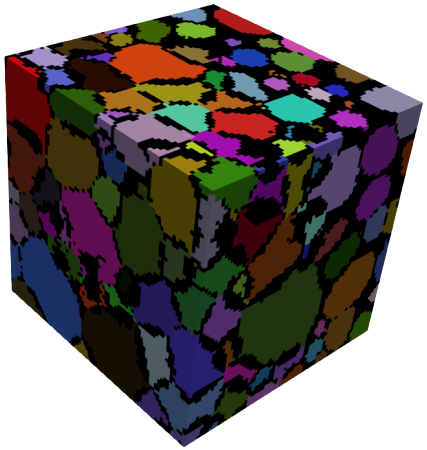
$W_i^* = \mathcal{W}^*(\sigma_0, u_i)$

Look for N max of $\mathbf{W} = [W_i^*]$

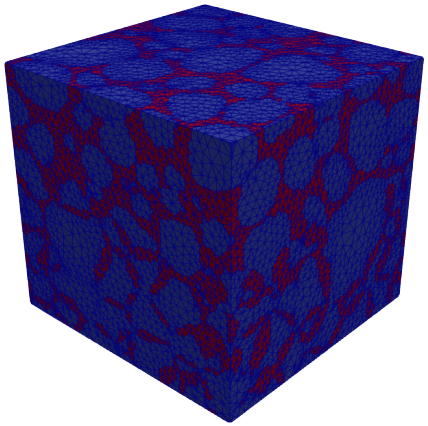
$\rightarrow$ coordinates of N interest zones

Eigenmodes computation 1

DCT reconstruction output



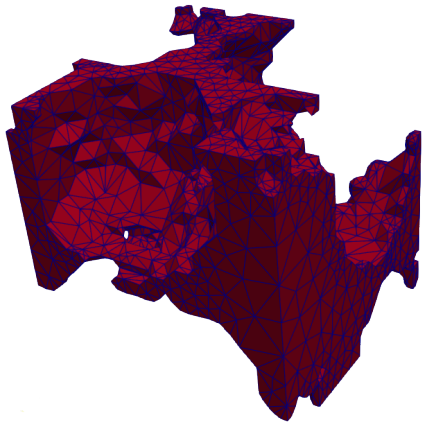
Uncertainty map mesh



Mesh uncertainty map

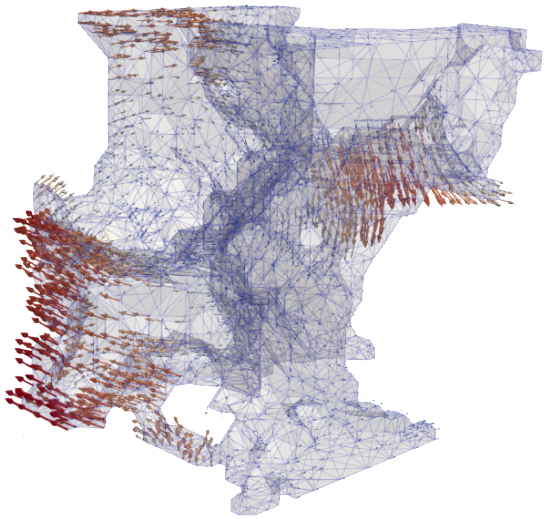
- Multiphase mesher on raw reconstruction output
- SDZset mesher to create mesh of uncertainty map
- SDZset mesher to create external surfaces elsets
- Automated
- Compute eigenmodes on uncertainty map "structure"

Uncertainty map structure



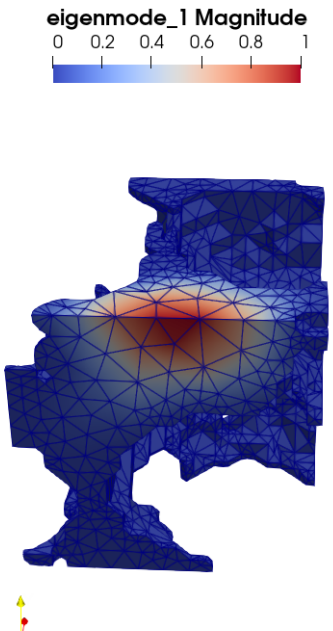
Eigenmodes computation 2

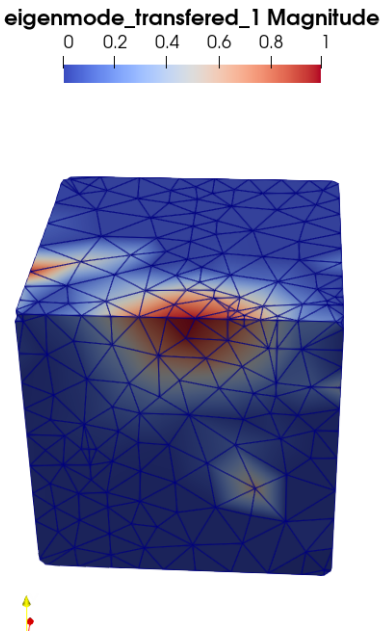
Uncertainty map modes

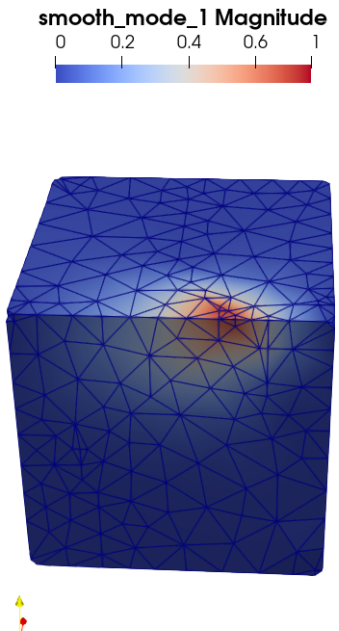


Modes for grain boundary deformation

- SDZsetFieldTransfer on grain mesh
- SDZsetFEA to smooth modes with elastic computation (ν=0)
- Get normalized $u^i = \phi_i$
- Projection on grain boundary normals
- Deform Mesh

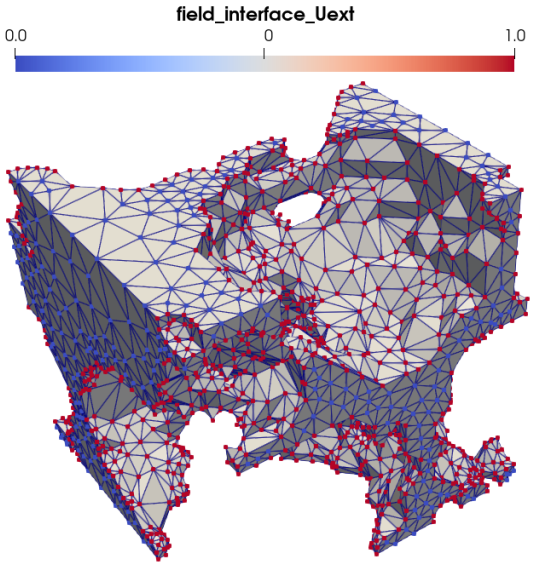






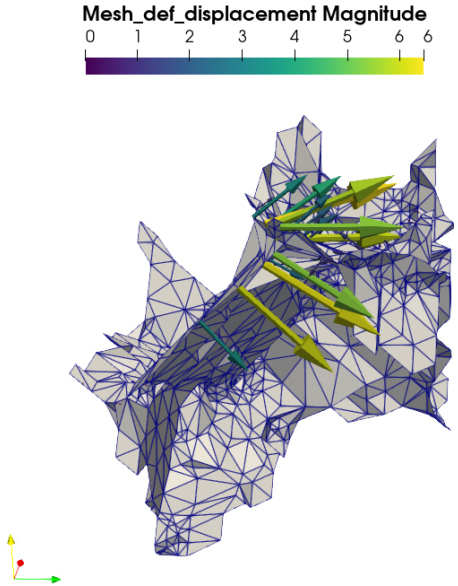
Eigenmodes computation 2

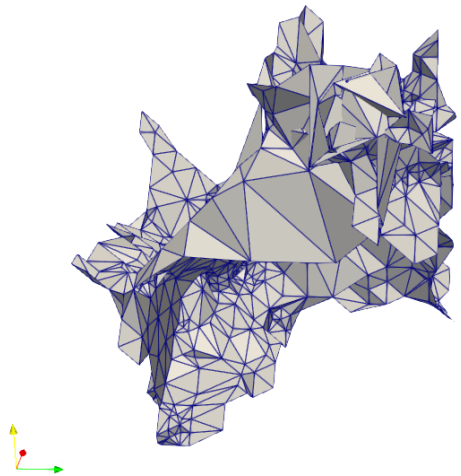
Boundary grains/uncertainty zone



Boundary conditions

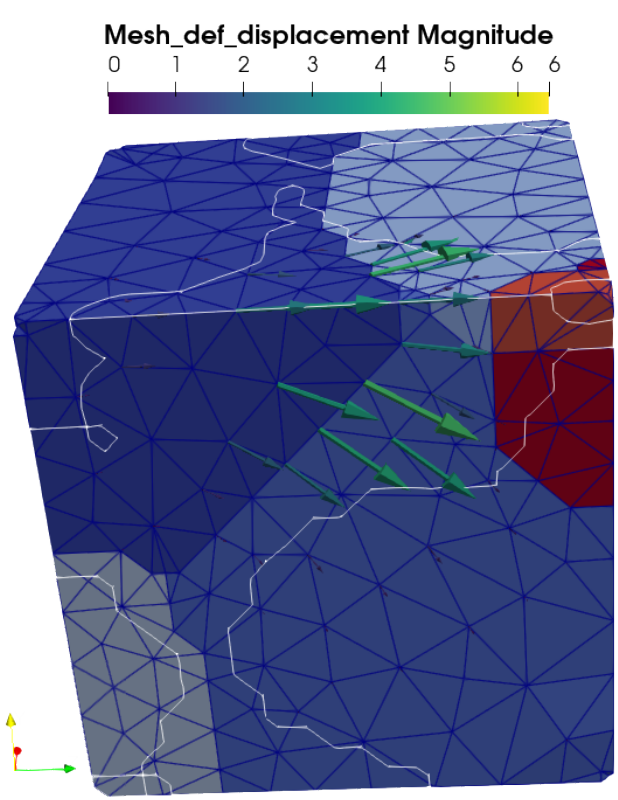
- Boundary uncertainty zone/grains : $\boldsymbol{u} = 0$
- External faces : $\boldsymbol{u} \cdot \boldsymbol{n} = 0$

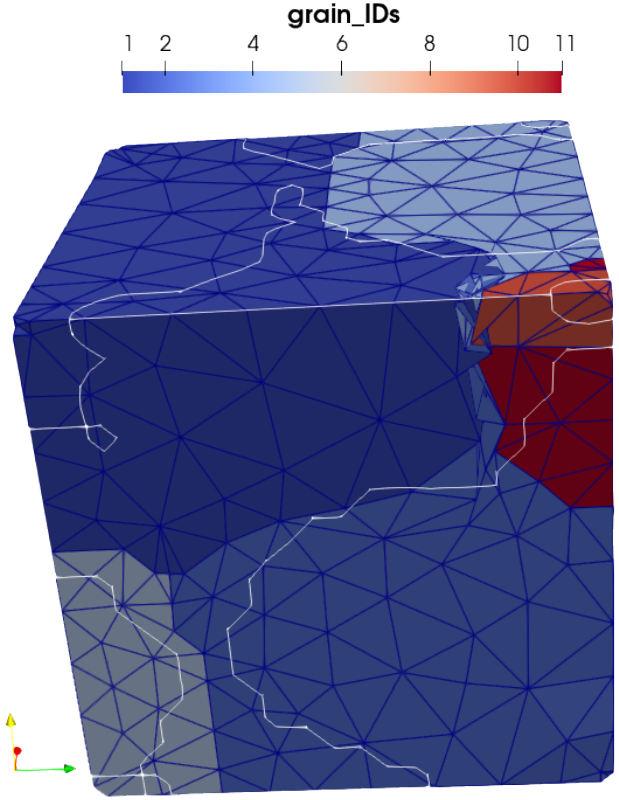




Deform mesh

Linear combination of 3 normal modes.

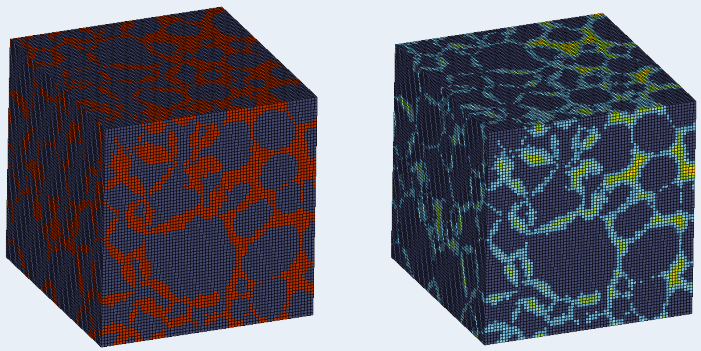




Next steps

Parametric Generative Model

- Explore different BC. Compute more modes on larger subvolume
- Apply projection and smoothing after linear combination ?
- Implement remeshing strategy
- Compute maximal modal amplitude from distance function



Submodels selection and simulation

- Generate maximal or random mesh deformations
- Compute joint virtual work of FFT σ_0 and modal deformation
- Polycristalline simulations of the N regions with maximal virtual work
- Evaluate uncertainties

Contents

Data Platform perspectives

Implementation

- Integration with FFT solveur AMITEX_FFTP
- Implement IP values visualization $\sim$ BasicTools Paraview plug-in ?
- Parallel I/O, datasets processing
- Most technical developments are done

Package

- Extend documentation
- Detailed Tutorial Notebooks
- Install and test on Jean Zay cluster

Support for Numerical chains

- H. Launay defect clustering chain
- From J. Bertoldo segmentation to simulation
- "Real-time" simulation of DCT digital twins

Applications

- Full digital twin of 4000 grains polycristal (from C. Ribart)
- Complete development of uncertainty evaluation chain
- Fully automate uncertainty evaluation chain
- Massive uncertainty propagation

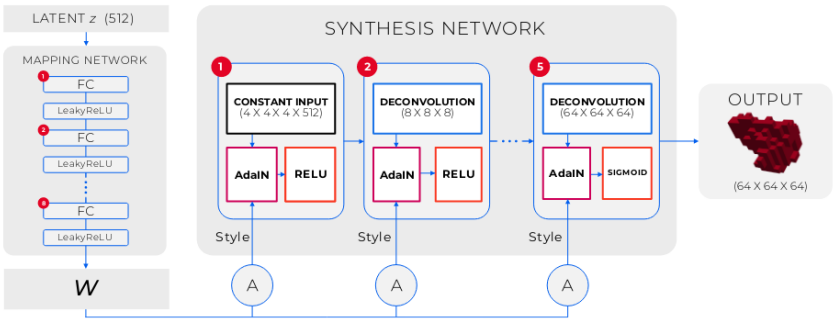
GANs for DCT reconstruction

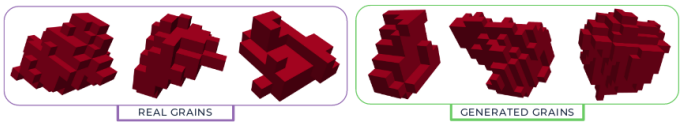
Goals

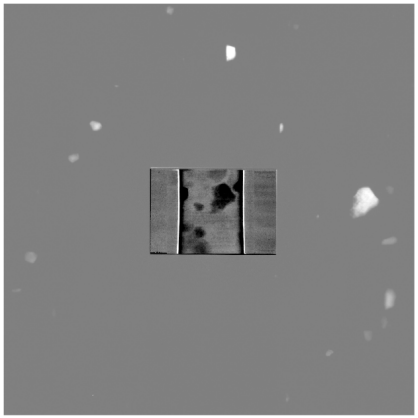
1. Generative model to fill uncertainty map with compatible microstructure
2. Generative model to fill uncertainty map with "true" DCT reconstruction
3. Extend model generality beyond eigenmodes

GANs (collaboration UCSB)

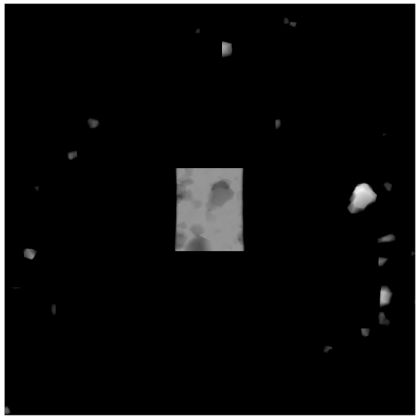
- 3DMaterialGAN
- Main challenge : gather meaningfull dataset
- Idea : Use simulation of DCT process from real and generated digital microstructures
- Preliminary phase : achievable goals ?







experimental $0 < \omega < 0{,}5°$



simulated $0 < \omega < 0{,}5°$