Accelerating scientific discoveries by mapping 3D imaging data to computational models for physics-based simulations

Bozo Vazic
Pania Newell

Department of Mechanical Engineering
The University of Utah

Introduction

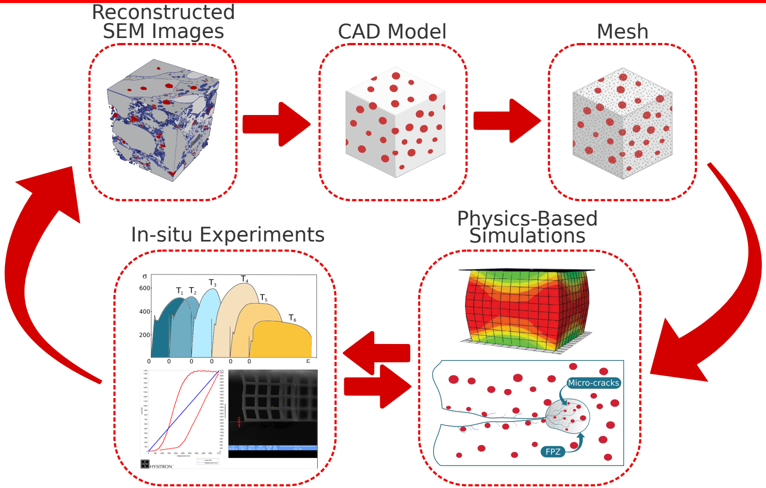
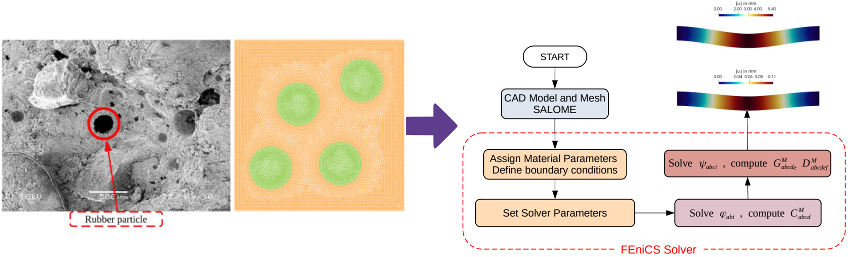


Image-based meshing creates new possibilities for the application of physics-based simulations to a wide range of previously intractable problems.

Motivation

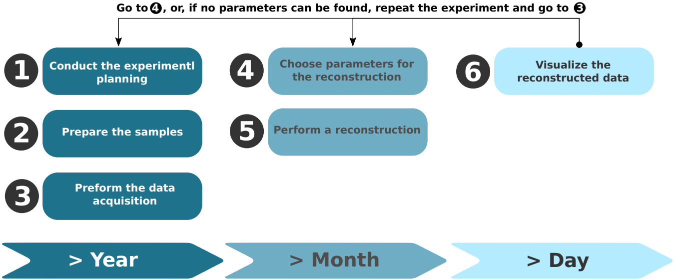
Homogenization translates behaviour of heterogeneous materials from the microscale level to the macroscale level. Most of the natural or man made materials are heterogeneous at some scale.



Upscaling material parameters and solving the macroscale problem

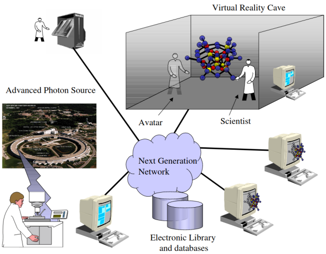
Objectives

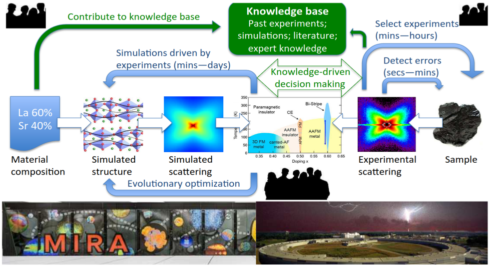
- **On-the-fly visualization of in-situ experiments**. On-the-fly visualization enables alteration and control of the experiment.
- **Physics-based simulation of the in-situ experiment in real time**. Rapid analysis can determine if data is useful.



Flow chart for microCT - from planning to visualisation of experimental data, Laszewski et al. (2000)

How it started ... How its going





How it started **How its going**

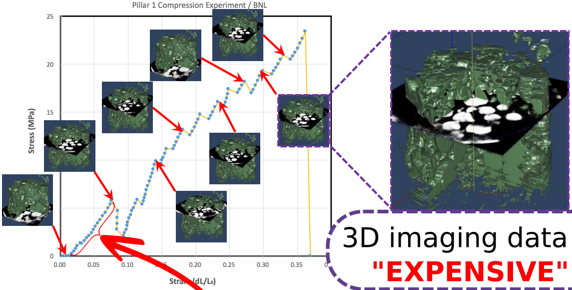
Accelerating discovery at an experimental facility, Laszewski et al. (1999) and Foster et al. (2015)

- Data movement: Existing shell tools lack required performance, ease of use, and reliability.
- Data management: Managing complex, high-volume scientific data across storage systems is a significant challenge.
- Data analysis: Managing runs across time scales, such as bridging short experiment-time computations versus month-long analysis studies is still challenging.

Computational Analysis

- Physics-based simulations can be performed in **real time** to determine whether data is useful and to provide other feedback to investigators during an experiment.
  - Fracture models to preemptively pause the experiments before catastrophic failure to study the fracture process zone
  - Homogenization models to quickly upscale material properties and compare them with macroscale results - sanity check
- Simulations can be performed **post experiment** to extract additional information and/or to compare with other data to provide new scientific insights and/or guide future experiments.

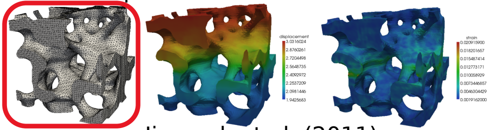
Computational Analysis



3D imaging data is **"EXPENSIVE"**

Just In Time Evaluation

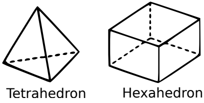
FEM Model From 3D Reconstructed Images
Displacement & Strain Data



Jirousek et al. (2011)

Mesh Generation

- Mapping 3D images into meshes necessitate user interaction and geometry simplification.
- Most of the approaches involve an intermediary step of surface reconstruction
- Unstructured 3D mesh generation techniques can be broadly divided into hexahedral (Hex) and tetrahedral (Tet) mesh generation - no technique can robustly mesh a arbitrary geometry and topology with good-quality hex elements.



Synopsys Simpleware - generates volume meshes with Hex & Tet combination or Tet only, showcasing the difficulty of generating Hex meshes.

Existing Software

- Synopsys Simpleware - licence needed - GUI - hexahedral & tetrahedral or tetrahedral elements
- Materialise Mimics - licence needed - GUI - tetrahedral elements
- Avizo - licence needed - GUI - tetrahedral elements
- iso2mesh - matlab/octave toolbox - tetrahedral elements
- OOF3D - open source - tetrahedral elements
- Gibbon - matlab toolbox - hexahedral & tetrahedral or tetrahedral elements
- CGAL - 3D Alpha Wrapping - open source - triangle surface mesh

All of them need a **watertight and orientable surface triangle mesh** as an input for creating a volumetric mesh - usually underlying data is not restricted to a specific format (triangle soups, polygon soups, point clouds, etc.)

Challenges

Computer Sciences

Distributed Computing
Computational Geometry
Data Science
Software Engineering
Data Structures
Image Processing
Computer Graphic & Visualisation
AI/ML

Engineering Sciences

Mechanical Engineering
Material Science
Geological Engineering
Bioengineering
Electrical Engineering
Civil Engineering

Mathematics & Physics

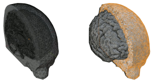
Applied Mathematics
Computational Physics
Applied Physics

Numerical Models

Meshing Algorithms

Data Management & Visualisation

Accelerating Scientific Discovery
via 3D Image Mapping



Concluding Remarks

1. Existing solutions do not have a clear pipeline from mapping 3D images to real time physics simulations - no unified framework.
2. Watertight and orientable triangle surface mesh is still a prerequisite for creating a volumetric mesh adding a layer of complexity.
3. Currently there is no automated mesh generation without significant human input increasing necessary processing time.
4. What is needed - a mesh generator (preferably with Hex elements only) that can create a high-quality volumetric mesh for physics-base simulations without intermediate surface generation (if possible) and with minimal human input.

Thank You for Your Attention!

- Von Laszewski, G., Westbrook, M. L., Barnes, C., Foster, I., Westbrook, E. M. (2000). Using computational grid capabilities to enhance the capability of an X-ray source for structural biology. *Cluster Computing*, 3(3), 187-199.
- Foster, I., Ananthakrishnan, R., Blaiszik, B., Chard, K., Osborn, R., Tuecke, S., ... Wozniak, J. (2015). Networking Materials Data: Accelerating Discovery at Experimental Facilities. In *Big Data and High Performance Computing* (pp. 117-132). IOS Press.
- Young, P. G., Beresford-West, T. B. H., Coward, S. R. L., Notarberardino, B., Walker, B., Abdul-Aziz, A. (2008). An efficient approach to converting three-dimensional image data into highly accurate computational models. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 366(1878), 3155-3173.
- Jirousek, O., Jandejsek, I., Vavrik, D. (2011). Evaluation of strain field in microstructures using micro-CT and digital volume correlation. Journal of Instrumentation, 6(01), C01039.

Contact:

Bozo Vazic, Ph.D.

email: bozo.vazic@utah.edu

webpage: www.newell.mech.utah.edu/