FINAL REPORT

FINAL PUBLISHABLE SUMMARY REPORT

TOMOMECH's main objective was to combine X-ray tomographic imaging for natural materials with computer simulations to determine mainly mechanical but also flow properties on the micro- and nanometre scale. Two natural porous materials were chosen to test the validity of this approach, the shell of the heart urchin (microstructured biological material) and chalk (nanostructured geological material).

Tomography, also known as CT, takes 2D projections of the internal structure of a sample using X-rays. These projections are essentially the same as radiographs in medicine. By rotating the sample and taking a large number of projections, it is possible to reconstruct the internal porosity of a sample in three dimensions. Tomography data are usually composed of a stack of grayscale images where the grayscale value corresponds to the local X-ray attenuation factor, i.e. the density of the material. In order to use these data for the computer simulations, it is necessary to segment the data into material and background. At the start of TOMOMECH, I developed an algorithm that uses different filtering steps to enhance the contrast in the images because at very high resolution, images can be blurred and thus segmentation becomes difficult. This algorithm proved itself superior to standard methods and was subsequently used for the rest of the project and was adopted into some of the work by my colleagues in our Research Section.

3D imaging of the heart urchin, which is a burrow dwelling cousin of the more commonly known sea urchins (Fig. 1 left), was performed using a laboratory X-ray tomography instrument with a resolution of about 1 µm. Macroscopically, the shell appears solid but tomography revealed an airy network of struts (Fig. 1 middle). Using image processing software, I was able to determine the thickness and spacing of the struts, which showed that there are two distinct regions in the shell, two finely structured regions (strut thickness of ~10 µm) on the outer and inner side of the shell and a coarser region (strut thickness ~25 µm) in the middle. Porosity in both regions varies between 30-70% and is achieved by varying the spacing of the struts not their thickness. This demonstrates an intricate biomineralisation process because the shell is entirely composed of magnesium enriched calcite ($CaCO_3$).

In order to study the relation between the microstructure and its mechanical function, I imported the 3D structure into a finite element (FE) simulation (Fig. 1 right). In FE simulations, an arbitrarily shaped object is approximate by a large number of small symmetric elements. The mechanical deformation of the object under external load can then be approximated numerically by evaluating the stresses and strains on the finite elements. Simulating loading along different axes for small subvolumes of the tomographic data, I determined the Young's modulus (stiffness) of the heart urchin shell at different locations. Around the mouth of the animal, the material is stiffer in the direction parallel to the mouth whereas on less differentiated positions of the shell, Young's modulus is isotropic. This clearly shows evolutionary adaptions to the expected loading direction but without changing the underlying building principle. On average, the shell performs mechanically close to an ideal foam, even at porosities of 70%. This part of TOMOMECH not only elucidated the evolutionary adaptions in this marine organism and demonstrated the validity of the approach, but also gives us a template for improving synthetic materials (biotemplating).

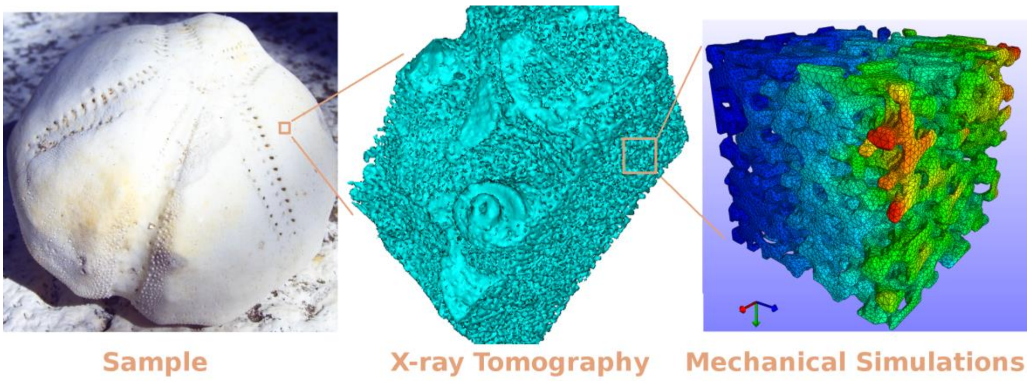

Figure 1: Work flow in TOMOMECH for deriving mechanical properties on the micro- and nanoscale: The sample (here: a heart urchin shell) was imaged using X-ray tomography. From the tomography data, a 3D model was derived and imported into finite element software for mechanical simulations.

Chalk (Fig. 2 left) is a biogenic limestone that serves as both aquifer and hydrocarbon reservoir. Thus, learning more about the mechanical properties at the pore scale can help provide information about the impact of drilling and chalk cliff stability. Chalk is formed from the remains of ancient algae, the coccolithosphorids, and depending on the degree of compaction, a great deal of the original biological structures survive. The pores and grains in chalk are thus often less than a micrometre in size which necessitates higher resolution. This can only be found at synchrotron radiation facilities. My host group had already recorded data for chalk (Fig. 2 middle) from both outcrops and drill cuttings provided by an oil company over a range of resolution. I used these data to derive simple petrophysical parameters, e.g. porosity and surface area, directly from the data and studied their dependence on porosity. I found that resolution of at least 25 nm voxel size is needed and accordingly, I chose this data set to perform mechanical simulations following the same approach as for the heart urchin shell. The results of these simulations clearly showed than chalk is much weaker than the heart urchin shell at the same porosity and that chalk's elastic properties drop rapidly with increasing porosity. However, subvolumes, in which more intact fossils could be found, performed better than regions consisting of only calcite crystals. Later on in the project, my host group acquired new data at even higher resolution. Using these data, I could also study the influence of nanometre sized fractures, which lead to a further decrease in mechanical strength. Comparing my results to macroscopic core plug measurements on chalk, I found very good agreement. Therefore, combining tomography and finite element simulations can deliver sensible results and is especially helpful when macroscopic testing is not possible.

In addition to the main objective of studying mechanical properties, I also applied a technique called dissipative particle dynamics (DPD) to simulate diffusion of particles in the nanoscale pore network of chalk. In this technique (Fig. 2 right), particles are simulated using classical equations of motion and force fields to described interactions between particles and the pore wall as well as particles with each other. Comparing the mean-square displacement for particles in the pores and in free diffusion, I was able to determine the tortuosity of the chalk samples. Tortuosity measures how twisted a pore system is and is itself needed to properly determine permeability. Permeability is an important material constant relating hydraulic pressure to fluid flow and thus describes the capability of a rock to promote fluid flow, i.e. in oil production or groundwater flow. The results of the DPD simulations showed that the size of the particles, i.e. molecules or larger aggregates, becomes important because of the very narrow pore throats in chalks. Thus, bigger oil components could be significantly slowed down. Furthermore, attraction of the particles to the surface causes a further decrease in mean square displacement up to the point where particles are basically trapped.

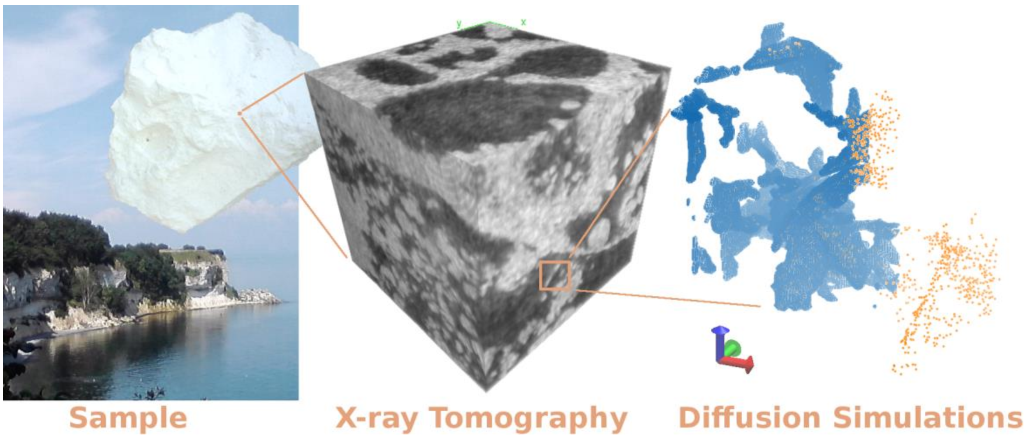

Figure 2: Work flow in TOMOMECH for simulating particle diffusion: The sample (chalk from an outcrop or drill cuttings) is imaged using synchrotron radiation X-ray tomography. The pore surface is computationally extracted from the tomography data and diffusing particles (red dots) are filled into the pores in a dissipative particle simulation.

Other work done in TOMOMECH includes 3D X-ray diffraction measurements on spines of the heart urchin, which show that the whole spine behaves much like a single crystal, as well as processing of tomography data for lattice Boltzmann simulations to derive permeability done by colleagues. In summary, TOMOMECH has achieved its goal of combining tomography and finite element simulations and its results have provided a method to derive material properties for industry applications but also insights into structure-function relationships in biomineralised materials.

A short description of TOMOMECH and all of its results and publications can be found on:

http://nanogeoscience.dk/projects/tomomech/

This site also contains links to other subpages explaining the techniques involved.