Heterogeneous materials power many modern technologies through unique properties that are determined by their microstructure. A heterogeneous material is one that is composed of domains of different materials/ phases (e.g., a composite) or the same material in different states. We are specifically interested in materials where the microscopic length scale, e.g. the average domain size within the material, is much larger than the atomic size, but much smaller than the characteristic length of the sample of interest. This consideration implies that domains possess can be viewed as a continuum and we can ascribe macroscopic/bulk/effective properties to the heterogeneous material. A number of Gore’s materials offerings fall under this specific description of a heterogeneous material (see 1 for an example). Characterizing the microstructure of such materials is necessary for development of structure-property relationships that are used to determine the suitability of the material in a specific application.

![A. ePTFE Membrane](image1.png) ![B. Catalyst Composite](image2.png)

Figure 1: SEM images of heterogeneous materials. Panel A shows an ePTFE membrane with two phases, polymer and void/air. This microstructure is typical of membranes used in several filtration applications. Panel B shows a catalyst composite material, used in Gore’s mercury control filter, made of 3 phases - catalyst, polymer, and void/air. Images taken from gore.com

Modern X-ray computer tomography (CT) has made it possible to extract three-dimensional images of the microstructure of materials. Developing structure-property relationships and models for the study of physico-chemical processes within these structures (see chapter 12 of [1]) from this 3D image data involves the following steps:

1. Image analysis to calculate microstructural metrics (e.g. two-point correlation functions)
2. Generating realizations of the heterogeneous material using the microstructural metrics. This step is referred to as reconstruction. Current methodology involves using lower order correlation functions and a stochastic optimization procedure [2] to generate realizations.
3. Simulating processes of interest for each realization and computing properties of interest as averages over all realizations

Our focus in this course will be on steps 1 and 2. Recently, generative neural network models trained on 3D images (or 2D slices from a 3D image) obtained through CT experiments (see Figure 2) have found applications in generation of ensembles of microstructures of heterogeneous materials [3, 4, 5]. Compared to stochastic methods
of image reconstruction, the implicit representation of the “learned” material distribution can be used to generate many realizations of the microstructure rapidly, at least theoretically. In practice, there are several challenges in developing and working with such models, limited availability of data being the primary problem. We would like to explore the use of generative models for 3D structure reconstruction from a limited dataset of computer tomography images. We would like to understand

1. What are the current state-of-the-art generative models for microstructure reconstruction?

2. Generative models are challenging to train and have some known issues (e.g. vanishing gradients, mode collapse). What techniques could we use while training to mitigate these problems?

3. How much data would we need to train such models such that the generated images faithfully reproduce the variations in the input data?

4. How can we ensure that new realizations are able to capture the effective properties of the material at various length scales?

5. If additional data (e.g. two-point correlation functions) on the structures or other physical insight are available, how could we use these in training the models? What additional data/physical metrics might be useful?

References


Learning outcomes

Beyond the larger learning outcomes listed in the course description, students working on this specific project will:

1. Understand, at a high level, techniques used in the characterization and modeling of heterogeneous materials.
3. Implement deep neural network models using python code built on top of the pytorch library. Train and validate the models on GPU/CPU compute clusters.
4. Develop skills in scientific software development, collaboration, and reproducible research.
5. Communicate their learning and finding through presentations to a broad audience possibly including industry practitioners working with heterogeneous materials.

Prerequisites

Students are expected to have:

- Working knowledge of linear algebra, probability theory, statistics, and differential equations at the senior level of a standard engineering curriculum.
- Experience in python programming at a level where you are comfortable working with object-oriented programming concepts and packaging code into reusable libraries.
- Basic working knowledge of a distributed version control system such as git.

Knowledge of statistical learning methods, quantitative image analysis, and materials characterization are not necessary, but desirable. If necessary, Gore can provide a tutorial on a) characterization of heterogeneous materials and b) convolutional neural networks and generative models as applied to image data.

Code and data considerations

1. Initial pytorch implementation of a generative model will be provided through a git repository with direct editing permissions. We expect at the end of the term all code generated will be available in this repository for future use.
2. We shall provide a selection 3D CT images in TIFF or HDF5 format. Additional training data can be obtained through online repositories or generated synthetically. For the latter, we shall point the students towards open-source codes that can be used.
3. All code and data are under a permissive license such as creative commons. All code and data generated in this course will fall under the same permissive license.