Developing a virtual materials laboratory

Tomographic imaging can now be routinely performed over three orders of magnitude in length scale with correspondingly high data fidelity. This capability, coupled with the development of advanced computational algorithms for image interpretation, three-dimensional visualization, and structural characterization and computation of physical properties on image data, allows for a new numerical laboratory approach to the study of real complex materials: the *Virtual Materials Laboratory*. Numerical measurements performed directly on images can, in many cases, be performed with similar accuracy to equivalent laboratory measurements, but also on traditionally intractable materials. These emerging capabilities and their impact on a range of scientific disciplines and industry are explored here.

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Once the thrill of acquiring tomographic data for the first time has worn off, it is not uncommon for users to ask: what do I do now? This question is difficult to answer in a broad sense, since analysis means many things; for biological or paleontological studies, comparative anatomical studies often suffice, but for materials researchers the reply is still largely being formulated. To address this need, we have developed tools for the specific materials problem of calculating the transport and mechanical properties of hydrocarbon-bearing rock. The result is the initiation of a Virtual Materials Laboratory that comprises a suite of computational tools that explore, measure, and calculate various physical properties of porous and granular materials.

Although the initial research was specifically focused on applications in the oil and gas industry, experience has shown that these tools allow the characterization and investigation of materials in general. Consequently, new collaborative research has steered the group into fields such as bone and soft tissue engineering, ceramic composites, fiber-reinforced composites, foams, wood, pharmaceuticals, and paper.

A complete review is beyond the scope of this article, so we present here a description of the data-processing pipeline we use, followed by

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the description of a few case studies that illustrate the capabilities of this technology.

While many researchers are aware of synchrotron-based tomography, laboratory-based methods often yield equivalent data fidelity, but with greater accessibility. In practice, tomographic data (*tomograms*) can be accepted from any imaging modality, however, our group predominately generates data from an in-house built X-ray attenuation micro-computed tomography facility[1–3]. This facility routinely collects data comprising of 2048[3] (8 billion) data points (*voxels*). Such large data sets are paramount to understand multiscale effects on the properties of materials. Currently, these data sets are imaged with a resolution down to a few microns. Even though there are synchrotron and laboratory systems capable of resolutions in the 100 nm range, the trade-off is that the specimen size is smaller (<200 μm). Ultimately, the desired resolution is defined by the need to capture a volume representative of the material heterogeneity. Unfortunately, this leads to conflict for materials with fine and large scale heterogeneity.

Data exploration – three-dimensional visualization

The first step in understanding the properties of a specimen is to explore the configuration of materials (*phases*) using computer visualization. The most basic method is to traverse the data volume serially along user-defined two-dimensional cross sections, helping one to build a mental picture of the structure in the specimen. While still the most convenient approach for the clinical presentation of patient data, this method is disrespectful of three-dimensional phase connectivity and fails the viewer for large complex data sets. A more percipient method is to explore the data using *direct volume rendering*[4]. Although more time consuming, this engages the viewer to study in detail the compositional variation in terms of connectivity, distribution, and relative densities. This form of rendering takes advantage of density gradients in the material and is more flexible than traditional *indirect volume rendering* in which a surface is used to delineate phase boundaries. To illustrate the advantage of direct volume rendering, Fig. 1 shows how a user selects a region based on density and density gradients to render both the interface and volume of a plastic toy selectively. The ability to merge both simulation and data volumes visually becomes an essential part of this technique. To assist collaborators, a multiplatform tool *Drishti*[5] has been written in-house and is now available as freeware‡. Thanks to a keen research community, the functionality of *Drishti* is continuously evolving.

Data segmentation

The main goal of the Virtual Materials Laboratory is the quantitative calculation of physical properties, for which the composition of each voxel in a tomogram must first be deduced. In an X-ray tomogram, the value at each voxel is related to the average X-ray attenuation and depends on the substance located in each voxel. For micro-tomography, one can assume the material is homogenous within regions much larger than the voxel size. This assumption, that voxels are predominantly composed of a single substance, is the chief difference between micro-tomography, which tries to observe structure directly, and standard tomography, which estimates material distributions. Using this assumption reduces the task of determining composition to segmentation: classifying each voxel into components (or phases) according to the value it contains, for which a single gray-scale image should be perfectly adequate, as long as there is sufficient contrast between the image value of the different substances present. This task is complicated by the fact that materials are inhomogeneous, they have complex absorption spectra, laboratory-based X-ray sources are strongly polychromatic, and images have noise. Although segmentation is inherently imperfect at component boundaries – where voxels may be composed of several substances – it nonetheless represents the best starting point for quantitative analysis. Once identified, each component is assigned material properties using *a priori* knowledge, sometimes refined with experimental measurements.

Prior to segmentation, we have found that image quality can be significantly improved by the application of an edge-preserving

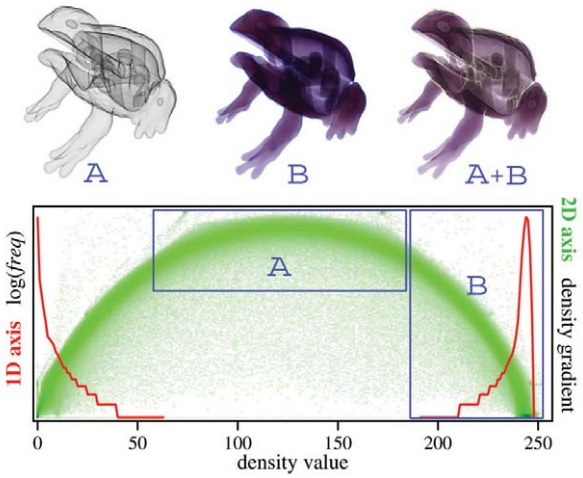

Fig. 1 The red trace shows a one-dimensional histogram of densities in a tomogram containing a void and a solid phase. The green image is a two-dimensional histogram of density gradients versus density values. The arch spans and links the two peaks in the one-dimensional histogram and shows that a continuous variation of density values and gradients exists at the interface between the two phases. The sharpness of the arch relates directly to the diffuseness of the interface; in this case, a result of the resolution of the tomogram. However, other materials could have diffuse or distributed interfaces. To visualize only the interface, the voxels within region A of the two-dimensional histogram are used, resulting in rendering A. To visualize the solid plastic, the voxels within region B are used, resulting in rendering B. In contrast to surface rendering, it is trivial to composite both regions A and B, resulting in the rendering A+B. In this way diffuse or buried structures can be easily explored.

‡Download available at: http://sf.anu.edu.au/Vizlab/drishti