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

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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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\(^6\). 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 grayscale 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 \textit{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

\footnote{\#Download available at: http://sf.anu.edu.au/Vizlab/drishti}

\begin{figure}[h]
\centering
\includegraphics[width=\linewidth]{fig1.png}
\caption{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.}
\end{figure}
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Denoising filter, and that best results are obtained with the three-dimensional anisotropic diffusion filter\(^6\), particularly the hybrid method of Frangakis et al.\(^7\). To perform the segmentation itself, we have found that classifying voxels purely according to their local intensity values (i.e. thresholding by intensity) is sufficient only for very high quality images containing two substances. Therefore, nonlocal and gradient information needs to be incorporated into the segmentation process. There are many published image segmentation techniques, mainly tailored to medical imaging to identify particular features\(^8\)–\(^11\). These methods invariably have the same basic principle: identify seed regions, grow the seed regions based on some rules, and finally terminate at a suitable point. To analyze large tomograms routinely, segmentation must be computationally efficient and allow for data-parallel execution.

We have developed a region-growing algorithm that uses the fast-marching method\(^12\),\(^13\) to achieve a good compromise between segmentation quality and computational efficiency\(^14\). This algorithm cannot automatically segment a tomogram; on the contrary, some user skill is required and there tends to be some uncertainty in the outcome. To identify multiple components, the algorithm is applied repeatedly by masking all previously identified components. To demonstrate the technique, examples of two- and three-phase segmentation are shown in Figs. 2 and 6, respectively.

Morphological and geometrical analysis

Once a tomogram is segmented into two or more components, one can begin a morphological and geometrical structural analysis of these components. Questions that spring to mind are: how well connected is it? Is it a single connected labyrinth, a foam-like structure, or a number of isolated pieces? What are the shapes of the structural or porous elements? These questions can be roughly broken into two categories: questions of connectivity (topology) and questions of shape. The classical toolkit to quantify forms of arbitrary shape include averaged statistical information (volume fractions and two-point correlation functions)\(^15\), stereology\(^16\), integral\(^17\),\(^18\), and differential\(^19\) geometry.

The main difficulty in analyzing the shape of complex labyrinthine structures that emerge in materials science is their sheer complexity. One method to deal with this is to apply a classic reductionist approach: partition the object into morphologically simple building blocks. This separates the connectivity information – now contained in the network of connections between building blocks – from the local shape, which is contained in the distribution of building block shapes. This approach has been used by many groups\(^20\)–\(^26\), mainly

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Fig. 2 A magnified region in one slice of a phase-contrast tomogram of timber, with a voxel size of 280 nm. The experimental data (a), filtered with anisotropic diffusion (b), and the initial thresholding to identify seed regions for the segmentation (c). Blue is the void phase seed and red is grain phase seed. The final segmentation (d) is overlaid on the tomogram; regions of wood phase have been colored green.

Fig. 3 The top row shows a magnified region in one slice of an unconsolidated sand pack. The original gray-scale tomogram (a), a false-color labeling of grains identified by partitioning the solid phase (b), and a false-color labeling of the pore volumes identified by partitioning the void phase (c). The bottom row shows the networks taken from a subvolume surrounding the above images. The grain network (d), the pore network (e), and the combined networks (f) are shown. In (d–f), the sphere sizes are proportional to the volume of the grain or pore body being represented, and the tube diameters indicate the cross-sectional area of the relevant grain-grain contact or pore throat. To ease visualization, the size of the spheres and the diameter of the tubes are reduced by a factor of two.
in the context of studying the multiphase flow properties of porous materials. The usual way to decompose an object is to break it at its locally narrowest points, or necks. We identify true necks by a two-stage method\textsuperscript{14,27}: first applying the watershed transform\textsuperscript{28} and then merging regions separated by necks that are not significant constrictions. One can use the three-dimensional medial axis transform\textsuperscript{20,29} to assist in seeding the watershed transform. In Fig. 3, we show the results of partitioning a granular material into local grains and pores and illustrate the interwoven network of connections of grains and pores within a granular material.

### Numerical analysis

Previous processing steps provide partitions of space into distinct constituent phases, pores, and grains. Making a measurement of a physical quantity on a tomogram involves defining a measurement volume, assigning relevant constituent material properties using those partitions, and solving the particular equation considered under appropriate boundary conditions. When large tomograms are considered, parallel computing is a necessity. Agreement with experiment can be expected if the physics of the problem is captured in the equation solved, scales are compatible, and the discretization of the problem (and resolution of the tomogram) is sufficient.

### Permeability to fluid flow

The permeability calculation on tomograms is typically based on a lattice Boltzmann (LB) method\textsuperscript{30,31}. LB methods are computationally expensive, but handle complex geometric boundary conditions effectively and can be parallelized easily if long-range interactions can be neglected. Consequently, LB remains the method of choice for flow and transport at the pore scale\textsuperscript{32–38} including dispersive\textsuperscript{39}, multiphase\textsuperscript{40,41}, and basic reactive flow\textsuperscript{42,43}. The fluid permeability of simple sandstones can be derived directly from tomograms and presents a benchmark case for comparison of numerical predictions with experimental data\textsuperscript{38,40,44–46}. In Fig. 4a, we compare numerically derived permeability to experimental data; the match is good over four orders of magnitude in permeability.

### Diffusive transport

Steady-state diffusive transport caused by an electrical, thermal, or chemical potential gradient across a specimen is numerically modeled by a Laplace equation with appropriate boundary conditions at material interfaces. For problems with complicated internal boundaries, finite difference\textsuperscript{47–51} or random walk solution methods\textsuperscript{52,53} are typically used. Good agreement with experiment has been obtained for sandstone\textsuperscript{45,49} (Fig. 4b) and polymer foams\textsuperscript{54}. Another class of diffusive transport, which has been considered for three-dimensional model materials and tomograms, is self-diffusion with trapping\textsuperscript{55,56}, important for the simulation of transport-limited chemical reactions or nuclear magnetic resonance (NMR) responses in porous media\textsuperscript{57–60}.

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**Fig. 4** Comparison of numerically derived and experimentally measured values of the absolute permeability (a), the effective conductivity $\sigma_{\text{eff}}$ normalized by the fluid conductivity $\sigma_{\text{fluid}}$ (b), and the effective bulk modulus (water saturated) (c) for Fontainebleau sandstone, as a function of porosity, $\phi$. The simulation data are calculated from four different specimens of Fontainebleau: each specimen is subdivided into 64 domains allowing data to be generated as a function of $\phi$. The agreement is good over a wide range of $\phi$. The results illustrate the feasibility of combining three-dimensional images with accurate numerical simulations to predict the properties of complex materials.

### Elasticity

Elastic properties on images are typically calculated using a finite element method (FEM). FEM uses a variational formulation of the linear elastic equations and finds the solution by minimizing the elastic energy using a fast conjugate-gradient method\textsuperscript{51–63}. Each voxel is taken to be a trilinear finite element. A strain is applied, with the average stress or the average elastic energy giving the effective elastic modulus. This technique has been applied to solve the elastic properties
of a range of composite materials and good agreement with experiment has been obtained, as shown in Fig. 4c.

Case studies

The following case studies illustrate the feasibility of combining tomograms with numerical calculations to predict useful material properties. This work has the potential to free materials scientists from the use of overly simplistic models that fail to capture essential topological and geometric features of real-world materials, from biological skeletons to rocks and paper. Although the numerical laboratory approach does not replace physical measurement nor theoretical insight, it has been shown that numerical measurements can be performed directly on images with similar accuracy and considerably reduced complexity and cost than corresponding laboratory measurements. Numerical experiments can be performed at conditions where experimental difficulties and uncertainties make it impossible to perform actual laboratory measurements. Understanding how the mechanical and transport properties of natural and synthetic materials are governed by structure and composition at varying length scales has potential applications in a wide range of materials science applications. In this section, we highlight a small subset of applications: the medical diagnosis of bone disease, the development of advanced industrial composites and biocomposites, and the design of advanced biomaterials.

Development of optimized industrial foamed materials

Many materials can be foamed, a process that dramatically extends the range of accessible properties. Porous foams exhibit a wide variety of complex microstructures. It is important to link the physical properties of foams to their density and complex microstructure, and to understand how such properties can be optimized for a given application. Tomograms of a range of cellular polymeric foamed materials have been obtained at sufficient resolution to measure local structure and connectivity, and over a sufficient field of view to calculate a range of structural and mechanical properties. Comparisons with experiment and common correlations are excellent. Moreover, numerical ‘experiments’ can also give important local information that cannot be measured experimentally, e.g. mapping local stress distributions during elastic deformation and fluid flow pathways within a porous specimen at the pore scale.

Design of tissue-engineered implants

Bone and cartilage generation by tissue transplantation is a promising clinical approach in orthopedic surgery. Almost all tissue-engineering concepts require the use of some form of porous scaffold serving as a template for cell proliferation and ultimately tissue formation. Three-dimensional control of pore size and morphology, mechanical properties, flow and diffusion properties, and degradation and re-absorption kinetics are critical for controlling mechanical stability, cellular colonization rates, and the organization within an engineered scaffold/tissue construct. Tomograms of porous scaffold materials and bone regeneration within these implants, Fig. 6, are helping researchers understand which scaffold designs work best and why, and will assist in the design of optimal scaffold architectures for bone in-growth.

Medical diagnosis of bone disease

Age-related bone fractures resulting from osteoporosis and other conditions impose a significant social and economic cost on our increasingly aging population. The assessment of bone quality is important in the diagnosis of bone fragility and for studying the success of bone therapeutic interventions. This assessment requires an understanding of the role of bone micro-architecture and mineralization. Micro-computer tomography (CT) imaging studies have shown the importance of bone micro-architecture in determining bone strength. In recent work, network representations of bone microstructure have been developed and may be a robust indicator of bone health. Imaging of bone ultrastructure in the femoral neck, shown in Fig. 7, allows one to calculate the full set of (anisotropic) elastic properties of the hip. This research will advance the problem of how to characterize bone quality in an accurate manner.

Granular materials: static and dynamic properties

Granular materials are ubiquitous in nature and in human activity. The worldwide annual production of cereals and aggregates of...
various kinds is gigantic, reaching around ten billion tonnes. Coal and cement account for over half of this value. They span the lowest technology sectors through to the most highly advanced\(^8\). Advanced manufacturing of high-technology materials relies heavily on the processing of mixed granular materials. The complex static structure of these materials immediately lends itself to three-dimensional analysis of geometrical structure and local densities\(^8\). NMR has also found application in generating three-dimensional data sets \(^9\) and particularly in dynamic studies. These types of study typically rely on a statistical mechanical approach to understand local configurations and packing parameters. Central to this approach is the accurate determination of both grain centers and contacts and many of the tools are common to those discussed above. For some time there has been promise for the detailed study of dynamic properties in these materials\(^9\)–\(^9\), although the scale of analysis required rapidly becomes enormous. The sequential collection of tomograms is straightforward, although it is fair to state that exhaustive analysis of singular static data sets is still a trial not only computationally but also for the theoretical understanding required. Fig. 8 shows a series of volumetric snapshots of a rod penetrating a granular pack in an attempt to study shear in granular materials. While insightful as an animation, detailed analysis is still required\(^9\). In a simpler application, X-rays have also been used to map density fluctuations in flowing granular systems radiographically\(^9\)–\(^9\).

Tomographic imaging also allows one to quantify the contribution of various compaction processes\(^9\). In studies of granular compaction, each grain must be identified uniquely in the tomogram, allowing one to analyze grain rotation and translation, ductile and elastic grain deformations, and grain failure. To achieve this, data segmentation is an important first step; the next step requires a complex process of identifying monophasic convex bodies. It is important to note that the geometry of the grains assists in the grain identification. In Fig. 9, we
show the results of a grain partitioning of a pack (a) before and (b) after compression to failure. The central grayscale image shows the original tomographic data. In this sequence, two mineral phases are present with sufficient contrast that they can be individually identified. Note that one phase has fractured more readily under load than the other, so much so that fragments are at the limits of resolution. With the identification of each grain, statistics and networks of grain size distribution, grain contacts, and evolution of the grain and pore structure can be directly analyzed in three dimensions.

Discussion

The path to the construction of a Virtual Materials Laboratory from tomographic images has been demonstrated. Complex structural, transport, and mechanical properties of real-world porous and granular materials are notoriously difficult to measure at the individual grain/pore scale; tomography provides the resolution required to probe a wide variety of complex materials at appropriate length scales. Tomographic data sets are rich in detail and parallel software developments have been required to allow researchers comprehensive and timely access to this data. We have described the development of highly optimized and massively parallel algorithms for image reconstruction, novel phase identification, structural characterization, and property prediction on these large data sets. Now other directions and the process of consolidation must be explored. There is also the need to incorporate other types of data of into the tomographic set to aid interpretation. Complementary three-dimensional modalities such as microscopic magnetic resonance imaging (μMRI) will give important functional meaning to data sets, but equally two-dimensional information from electron and optical microscopy will improve material identification. Dynamic CT places enormous emphasis on streamlining data analysis, and a heightened demand on faster and more sensitive X-ray detector technology. The interplay between increased field-of-view and spatial resolution exposes a tension between detector and X-ray source technologies. The injection of tangible materials science applications is helping to lead this conflict. In all these directions, in the near term, the fastest growth will need to be in more advanced computational tools. Clearly, new innovations in this field will be the result of ongoing multidisciplinary union between mathematicians, physicists, computational and materials scientists.

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