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Review article

Computational challenges in the analyses of petrophysics using microtomography and upscaling: A review

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A B S T R A C T

Microtomography provides detailed 3D internal structures of materials in micro- to tens of nano-meter resolution and is quickly turning into a new technology for studying petrophysical properties of rocks. An important step is the upscaling of these properties as micron or sub-micron resolution can only be achieved on the sample-scale of millimeters or even less than a millimeter. We have developed a computational workflow for the analysis of microstructures including the upscaling of material properties. Computations of properties are first performed using conventional material science simulations at micro to nano-scale. The subsequent upscaling of these properties is done by a novel renormalization procedure based on percolation theory. In this paper we discuss the computational challenges arising from the workflow, which include: 1) characterization of microtomography for extremely large data sets; 2) computational fluid dynamics simulations at pore-scale for permeability estimation; 3) solid mechanical computations at pore-scale for estimating elasto-plastic properties; 4) Extracting critical exponents from derivative models for scaling laws. We conclude that significant progress in each of these challenges is necessary to transform microtomography from the current research problem into a robust computational big data tool for multi-scale scientific and engineering problems.

Contents

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1. Introduction

Microtomography provides detailed 3D internal structures of materials in micro- to tens of nano-meter resolution and is quickly turning into a new technology for studying petrophysical properties of rocks. Such high resolution can only be achieved on the sample-scale of millimeters or even less than a millimeter, thus to scale up the properties from micro-scale to macro-scale is essential. Consequently this problem is the subject of many microtomography studies (Arns et al., 2001, 2002; Knackstedt et al., 2006; Fredrich et al., 2006; Chai et al., 2010; Derzhi et al., 2010; Grader et al., 2010; Liu and Regenauer-Lieb, 2011; Liu et al., 2014, 2015; Dernaika et al., 2015). The available literature has provided an in-depth account of the basic theory and methodology underpinning the upscaling workflows. However, computational issues arising from big data of microtomography, intensive computations of petrophysics and upscaling, and appropriate strategies for dealing with this challenge have not been discussed yet.

These computational issues include (but are not limited to): 1) characterization of microstructures of very large data – how to characterize, how large are the data sets we can handle, and how fast is the procedure; 2) determination of the size of a representative volume element (RVE) – the size of RVE sets the quanta of computations of properties and the procedure of determination may be very time consuming itself, thus the reliability, complexity and computing costs of the methods must be considered; 3) computations of petrophysical properties – the key problems are which method is used, how accurate the method is and how much it costs in computing resources; 4) extracting critical exponents for upscaling based on percolation theory – there are similar problems to the computations of properties and some additional problems related to the critical model of percolation where the connectivity, such as the width of the channel for fluid flow, is very small. The determination of the size of RVE is a relatively important issue related to the methodology and theory. As we are concerned here with the computational aspects we refer to the cited literature and focus on the problems related to the computations of properties and upscaling. We will also give a brief description about current capability of the characterization of microstructures. Readers that are interested in the topic of RVE size can refer to relevant contributions (Kanit et al., 2003; Terada et al., 2000; Liu et al., 2009; Regenauer-Lieb et al., 2013a). We refer to the same literature for the discussion of the upscaling methodologies which is a complex and much debated issue. It is beyond the scope of this paper, which restricts itself to the important computational problems related to the percolation theory.

While the process described is generic we will discuss derivation of upscaled properties such as permeability, elastic modulus and Poisson's ratio, plastic yielding stress, electrical conductivity. More efforts have been focussed on the analyses of permeability and elastic properties, and less on plastic properties.

Fluid transport and elastic properties have been studied with respect to consideration of microtomographic characterization (Roberts and Garboczi, 2002; Arns et al., 2002, 2005; Knackstedt et al., 2006; Moreno-Atanasio et al., 2010; Lopez et al., 2012; Dvorkin et al., 2012; Shulakova et al., 2013). Numerical methods such as the finite element method (FEM) (Arns et al., 2002; Shulakova et al., 2013), random walk methods, network models (Blunt et al., 2002; Pereira, 1999), smoothed particle hydrodynamics (SPH) (Pereira et al., 2011,2012) and Lattice–Boltzmann (LB) methods (Chai et al., 2010; Narvaez et al., 2010; Ahrenholz et al., 2008; Pan et al., 2006) have been used in the past. Numerical computations on microtomographic data have shown good agreement, to some extent, with experimental data for fluid flow and elastic properties (Arns et al., 2001, 2002, 2005; Knackstedt et al., 2006; Fredrich et al., 2006). New methods have been presented for the derivation of scaling relationships of plastic properties based on percolation theory as well as entropic uncertainty principles which provide sound theoretical bounds for the upscaling of properties from microtomographic data (Liu et al., 2012, 2015; Regenauer-Lieb et al., 2013a, 2013b).

Scientific and technical applications were fully discussed in these publications. Computational and technical aspects have, however, not yet been described. In this contribution, we are concerned with the challenges related to the computations in studying petrophysics and upscaling from microtomographic data. Computational challenges primarily stem from the enormous data size of microtomography. Highly configured computers and parallelized computing are essential but not enough. We introduce here the problems/difficulties and the computational solutions/expectancy based on our practical experience.

An important prerequisite in our approach is that the suggested solutions need to be fully scalable as we anticipate a dramatic increase in computational challenge for future developments. These include amongst others – time-lapse X-Ray microtomography data, significantly larger cameras, data fusion with state-of-the-art equipment such as Focus Ion Beam Scanning Electron Microscope FIB-SEM, Transmission Electron Microscope TEM, Saturated Excitation SAX Microscope, Electron Microscope EMP, more images from nano- to centimeter scales are available. In addition, the computational workflows should be designed as modules for a cyber-infrastructure including data assimilation techniques through mathematical forward and inverse modelling for the upscaling from nano- to reservoir scale. The following workflow and computational approach is designed to tackle current challenges as a preparation for future developments.

2. Workflow and computational methods

Before going into the description of the computational approach we need to summarise the workflow and associated computational method used (Fig. 1). For a complete description and worked examples we refer to the literature (Liu and Regenauer-Lieb, 2011; Regenauer-Lieb et al., 2013a, 2013b; Liu et al., 2014, 2015). A prerequisite to all X-Ray microtomography is segmentation, which in the discussed examples resolves a binary spatial database of pores and solid from gray-scale microtomography images. Andrä et al. (2013a) gave a through introduction and comparison of the techniques of image processing and segmentation. After segmentation is performed the starting model for the following analysis is a digital rock equivalent. This digital rock equivalent is then analyzed in three main components of the workflow. The processing of the segmented binary data is grouped in the left, middle and right columns.

The left column deals with a geometrical analysis, which accomplishes the characterization of geometry (of pores) of the model. Stochastic analyses are also carried out and its outputs are probabilities of porosity, percolation and anisotropy of different sized samples (Liu et al., 2009). The size of a representative volume