REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
03-09-2021	Final Report	1-Nov-2017 - 31-May-2021

4. TITLE AND SUBTITLE
Final Report: Scale Dependence of Governing Laws in Earth Materials

5a. CONTRACT NUMBER
W911NF-18-1-0008

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

6. AUTHORS

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
70866-EV.1

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Tapan Mukerji
UU	UU	UU	UU		19b. TELEPHONE NUMBER 650-721-1263

RPPR Final Report
as of 21-Oct-2021

Agency Code: 21XD

Proposal Number: 70866EV **Agreement Number: W911NF-18-1-0008**
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DUNS Number: 009214214 EIN: 941156365
Report Date: 31-Aug-2021 Date Received: 03-Sep-2021
Final Report for Period Beginning 01-Nov-2017 and Ending 31-May-2021
Title: Scale Dependence of Governing Laws in Earth Materials
Begin Performance Period: 01-Nov-2017 **End Performance Period:** 31-May-2021
Report Term: 0-Other
Submitted By: Tapan Mukerji Email: mukerji@stanford.edu
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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 1 **STEM Participants:** 2

Major Goals: The focus for the last year of the project was be on porous media property relations and their scale dependence. The tasks to be completed include: computation of elastic, electrical and single-phase permeability in porous digital rocks as a function of evolving geometry of the pore. What are the transport properties across different scales as the pore microgeometry evolves? The micro geometry will be computationally evolved simulating precipitation and dissolution, using level-set methods. At different stages of the simulated precipitation and dissolution, physical property relations will be computed using finite-element and lattice-Boltzmann solvers.

Accomplishments: See uploaded PDF document.

Training Opportunities: Training of two PhD graduate students.
J. P. Daza was able to finish and defend his PhD dissertation, thanks to ARO funding.
Daza wass able to develop professionally by presenting at the InterPore international conference.
A. Kashefi was supported for one quarter for his ongoing PhD training.

Results Dissemination: Two conference presentations and one accepted manuscript to the journal "Physics of fluids" published by the American Physical Institute.

Honors and Awards: Manuscript submitted to Journaal of Physics selected as a "featured" article, as the Editors felt that the article was one of the journal's best.

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Faculty
Participant: Tapan Mukerji
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

RPPR Final Report
as of 21-Oct-2021

Participant Type: Graduate Student (research assistant)
Participant: Juan Pablo Daza
Person Months Worked: 9.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Graduate Student (research assistant)
Participant: Ali Kashefi
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Partners

,

I certify that the information in the report is complete and accurate:
Signature: Tapan Mukerji
Signature Date: 9/3/21 5:07PM

Final Report

Proposal Number: 70866-EV
Agreement Number: W911NF-18-1-0008

Prepared for the Army Research Office

August 25, 2021

Tapan Mukerji

Stanford University

Summary

This report describes the work done on research in digital porous media and computational rock physics, as part of the PhD work of Juan Pablo Daza at Stanford University, who was supported on this project, and successfully completed his PhD in March 2021. The following sections constitute a summary of his final dissertation. In addition Ali Kashefi was also supported for a few months. His work on deep learning applications for predicting permeability in porous media has been selected as a featured article in the journal Physics of Fluids, published by the American Institute of Physics. The manuscript is also summarized in the following.

Summary of the PhD dissertation of Juan Pablo Daza:
CHANGES OF GEOMETRY AND PROPERTIES OF POROUS MEDIA

This work introduces and new methodology to analyze 2D and 3D imaging data to predict and model physical processes in porous media. The primary focus is on geometry, as it defines the essential quantities needed to numerically solve PDEs, which aid in predicting and computing material properties. Geometry defines the domain and boundary conditions. Thus, it is essential to define a standard method to process the geometry available in real data such as CT-scan and thin-sections.

Chapter 2 introduces how geometry is measured using robust mathematical tools derived from the Level Set method. This new geometrical representation is compatible with already available methods for numerical simulations.

Chapter 3 describes the mathematical theory for a 2D to 3D transform for porous media that can be used to create 3D representation of porous media from 2D thin sections, enabling us to compute physical properties such as permeability, bulk modulus, and conductivity from 2D sections. Obtaining 2D section images are more widely available, economical and are often at a higher resolution than 3D scans.

Chapter 4 of the dissertation describes application of the transform to real rocks, including sandstones, carbonates, and glass bead packs. Details of actual numerical implementation of the algorithm are described followed by the application to real rocks. In general it is

found that the transform gives good results for the carbonates and sandstones, with low to intermediate porosity but performs worse for very high porosity artificial glass bead packs. Physical properties calculated include permeability, elastic moduli, and electrical conductivity.

In the fifth chapter (Ch. 5), the Level Set method is used to simulate rocks' diagenetic processes. This chapter introduces numerical models that depend only on the porous medium's geometry. Numerical results and experiments are compared with good matches in experimental trends observed in sandstones. This chapter highlights the importance of focusing on geometry, as shown in the figure below from the dissertation.

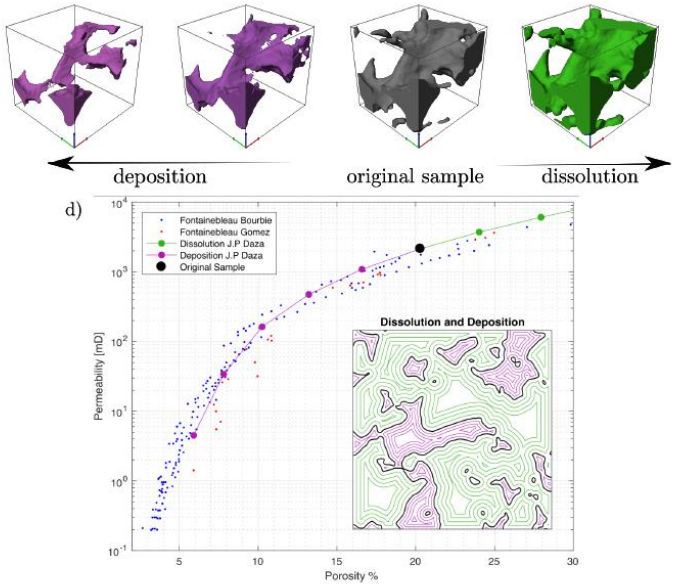


Figure 5.2: Permeability as function of the different levels of ϕ. Upper volumes correspond to different stages of the pore space. Permeability for original CT-scan is in black, the trend of the different isolevels of ϕ matches the porosity-permeability trend studied by Bourbie in Sandstones.

Chapter 6 moves on to simulating natural processes, starting with dissolution and followed by dissolution dependent on anisotropic stress. This chapter opens the door to explain diagenesis and any process that can change the rock structure. These processes are quantified following physical laws and equations. This work will enable the study of diagenetic processes computationally. Moreover, this can be helpful for providing useful predictions for any industry dealing with porous media.
The complete dissertation is available at:
https://searchworks.stanford.edu/view/13826070

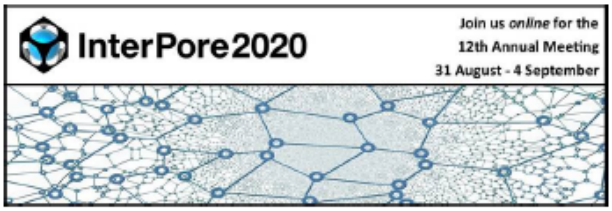
This work led to two presentations at the Interpore 2020 conference:

Simulating Diagenesis: Computing Temporal Pore Structure and Physical Properties Changes Due to Dissolution/Precipitation Under Stress and Reactive Fluid Flow

Primary authors: DAZA, Juan Pablo (Stanford University); MUKERJI, Tapan (Stanford University); NUR, Amos (Stanford University)
Presenter: DAZA, Juan Pablo (Stanford University)
Track Classification: MS 9 - (MS9) Pore-scale modelling
Contribution Type: Pre-Recorded Oral Presentation 1

2D to 3D Transform: Material Properties from 2D Images

Primary authors: DAZA, Juan Pablo (Stanford University); NUR, Amos (Stanford University); MUKERJI, Tapan (Stanford University)
Presenter: DAZA, Juan Pablo (Stanford University)
Track Classification: MS 10 - (MS10) Advances in imaging porous media: techniques, software and case studies
Contribution Type: Pre-Recorded Oral Presentation 3



Abstract ID : **1024**

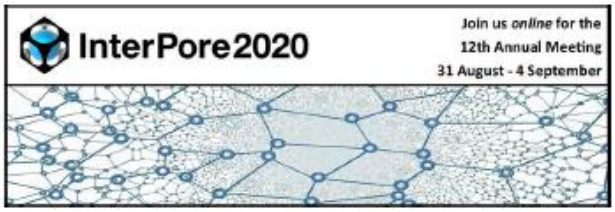
Simulating Diagenesis: Computing Temporal Pore Structure and Physical Properties Changes Due to Dissolution/Precipitation Under Stress and Reactive Fluid Flow

Content

Understanding thermo-chemo-mechanical processes with fluids in porous media and rocks is important. Because of the likelihood of fluid-rock chemical interactions, and our limited ability to decipher the mechanical, and fluid flow effects of these coupled processes. One of the missing links is understanding the evolution of elastic and transport properties together with reactive transport. Because the properties of porous media evolve as a result of chemical reactions and vice versa. Capturing this coupling experimentally and theoretically is one of the missing elements in the existing literature. We describe here recent advances in theoretical modeling and simulation of reactive fluids processes in rocks with complex pore structure, in order to understand the effects of dissolution-induced changes on acoustic velocity, porosity, permeability and electrical properties.

To deal with the problem of modeling the effects of reactive fluids in porous media properties, we adopt the approach by Osher and Sethian (1988) - a conceptual framework for using level sets as a tool for numerical analysis of surfaces and shapes - together with 2D and 3D scanned and segmented pore structure images. The advantage of the level-set approach is that one can perform numerical computations involving complex curves and irregular surfaces on a fixed Cartesian grid without having to parameterize these objects. With this we have already shown how material evolution problems can be mathematically/computationally solved accurately, efficiently (fast), while honoring the coupling between physics and chemistry.

We can get different versions of the pore geometry by using the Osher's approach with the simplest velocity field to change the pore-space interface. Properties such as permeability are then calculated using the Lattice-Boltzmann method (Keehm, Mukerji, and Nur 2001), for each change in the geometry. The results of the calculated permeability are compared with the experimental observations (Bourbié 1985) for Fountainebleau sandstone. Thus the method used in our work is the enabling technology to model and simulate the structural changes of the different components of the porous media, under different physical and chemical processes.



Abstract ID : **1022**

2D to 3D Transform: Material Properties from 2D Images

Content

Recent advances in 3D imaging allow us to get high resolution geometry of different porous media. However, 3D imaging is expensive and time consuming compared with 2D imaging. 2D imaging gives us high resolution and quality, quickly and with little economical investment.
In this work we propose a geometrical transformation of thin slices to a 3D volume. This transformation is unique, isotropic, analytical, and given that we obtain a 3D volume with the same geometrical characteristics as the 2D image, it enables us to compute physical properties such as permeability, bulk modulus, and conductivity.

We rely completely in the geometrical information available in 2D images, and use this information to construct a 3D volume that preserves the geometrical measurements in 2D. The result is a 3D volume that has the same porosity as the 2D image, as well as a pore-space, well connected and geometrically isomorphic to the pore space of the original sample.

We test the success of this 2D to 3D transform in its ability to predict the physical properties of the sample, in our case the bulk and shear modulus, conductivity and permeability. Obtaining and excellent match of properties computed in volumes obtained from micro-CT, and those properties obtained just from 2D thin slices. For instance in the figure we can see permeability estimates just from a 2D image, compared with the permeability estimates obtained from the original 3D CT-scan, for REV samples the results from 2D images are comparable to those from 3D images.

In conclusion, we have created a transform that creates a 3D volume from a 2D image, with the same geometrical characteristics, reproducing space connectivity, and providing reliable estimates of properties as permeability using only one thin section.

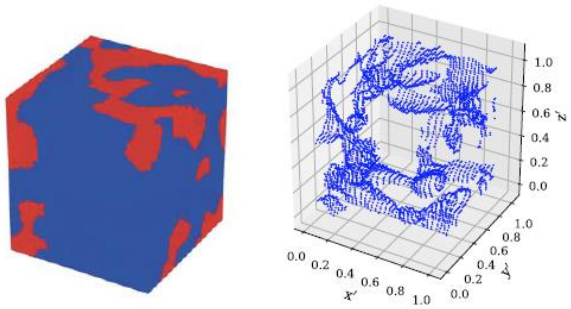
Point-Could Deep Learning of Porous Media for Permeability Prediction

Ali Kashefi & Tapan Mukerji

Accepted to *Physics of Fluids*

A novel deep learning framework is proposed for predicting permeability of porous media from their digital images. Unlike convolutional neural networks (CNN), instead of feeding the whole image volume as inputs to the network, the boundary between solid matrix and pore spaces is modeled as point clouds and used as inputs to a neural network based on the PointNet architecture. This approach overcomes the challenge of memory restriction of graphics processing units and its consequences on the choice of batch size, and convergence. Compared to convolutional neural networks, the point-cloud based network provides freedom to select larger batch sizes. The proposed deep learning methodology significantly reduces the size of network inputs. As a test case, two and three dimensional synthetic digital rock images are considered, to investigate the effect of different components of the neural network on its performance. The pointnet deep learning strategy is compared with a convolutional neural network from various perspectives, specifically for maximum possible batch size. The generalizability of the network is tested by predicting the permeability of real-world rock samples as well as synthetic digital rocks that are statistically different from the samples used during training. The network predicts the permeability of digital rocks times faster than a Lattice Boltzmann solver and requires much less GPU memory than a CNN based network.
The complete manuscript is available at:

arXiv:2107.14038



Voxel representation (left) versus point cloud representation of the geometry of a porous rock.