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Rock physics for multiscale, multiphysics data assimilation from molecular to laboratory scale

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SUMMARY

Exploration geophysics and reservoir production strategies rely on a robust knowledge of reservoir petrophysical properties and their uncertainties. We have developed a new approach that not only quantifies uncertainties of petrophysical properties in a static scenario but also assesses their dynamic changes under tectonic, chemical and production loads. We address this challenge with a new Multi-scale and Multiphysics data assimilation approach integrating experiments, numerical simulations and rock physics theory. This paper focusses on data integration from molecular to laboratory scale to provide a solid physics foundation for the multiscaling approaches presented in companion papers for the larger scales.

Key words: 4th research paradigm, Integrated Computational Materials Engineering ICME, data-intensive science

INTRODUCTION

Measuring empirical laws for predicting Multiscale and Multiphysics rock physics behaviour on time scales ranging from milliseconds to millions of years and from quantum to planets transcends by far our capability in the laboratory. Yet, with the 4th research paradigm (Bell et al. 2009) of data-intensive science and discovery this restriction is starting to slowly fade away. Digital rock physics is becoming one of the first wave of industry applications that have become available using the data-intensive paradigm. Carefully calibrated experiments with digital rocks allow assessment of in-situ properties and their changes on the spatial and time scale of fluid flow through a chemically reacting and deforming core specimen to the scale and lifetime of operating an entire reservoir.

To this end we propose to extend a digital rock physics approach that enables coupled virtual computer simulations that are able to assimilate data dynamically during a reservoir operation, provide input into the full cycle from exploration through production and abandonment, while providing guidance on appropriate stimulation and reservoir management protocols as well as quantitative uncertainty analyses for economic assessments and fast management decisions.

METHOD AND RESULTS

The current paper tackles the first step of molecular-micrometre scale data assimilation, which is at the heart of this new approach through focusing on rock physics innovations. We propose to obtain a fundamental understanding of the physics of reservoir rocks through:

[1] Data acquisition from molecular (ångström) to cm-scale through an integrated X-Ray Microscopy (XRM) facility allowing multiscale imaging of flow through porous media from molecular-scale using Small Angle X-Ray or Neutron Scattering SAXS and SANS to sub-micron tomographic resolution with Neutron and X-Ray micro-CT;
[2] Data Analysis by using objective segmentation and co-registration methods of micro-CT images with additional 2-D analyses and feature identification via artificial intelligence supported by Grey Level Co-occurrence Matrix (GLCM) technology (Singh et al. 2018);
[3] Data Compression by using massively parallel codes for upscaling of material properties using percolation theory and calculating thermodynamic bounds of digital rock physics experiments using computational homogenization techniques;
[4] Data Assimilation via open source multiscale numerical forward and inverse simulations built around a Python driven Object-Oriented Multiscale Simulation Environment MOOSE (Gaston et al. 2015). Its parallel capability allows direct coupling of multiscale simulations up to reservoir scale.

The particular innovation of our approach is that we start with experiments at [1] to identify molecular scale processes and enrich the next scale by assimilation through [5] to obtain a robust multiscale physics-based data integration framework (Figure 1).

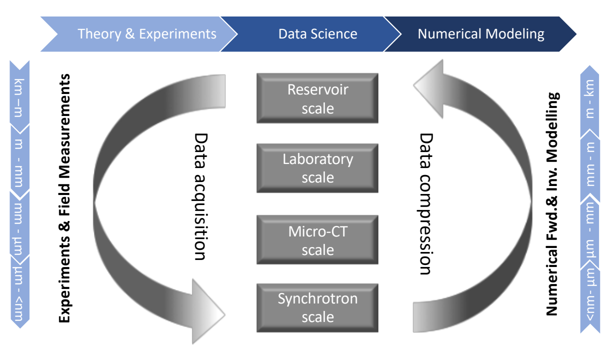

Figure 1. Multiscale/physics Data Assimilation Framework

We start at molecular scale because of the risk of losing the important driving physics of the problem if empirical relations obtained from larger scale laboratory measurements of effective material constants are used. Physics based upscaling is the key to obtain the lowest necessary dimension for microstructurally enriched continuum simulation defining the tensorial coefficients of the partial differential equations for the next scale up.

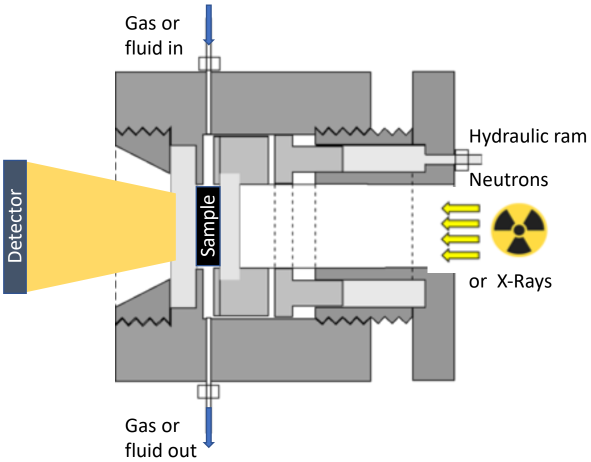

Figure 2. Example of a portable cell for SAXS/SANS allowing measurement of open and closed pore sizes seamlessly from 0.5 nm scale to cm scale. The picture shows an in-house design by Blach in operation on D11 in ILL (Institue Laue Langevin, Grenoble, the world's largest 47 MW Neutron Source); Specifications: fluid pressure (up to ca. 100 MPa); uniaxial stress (up to 100 MPa); temperature (up to ca. 500°C); exchangeable windows (Ti, TiZr, Sapphire, secondary, explosion resistant safety windows); fluids used (CD_4, He, CO_2) (Blach et al. 2018)

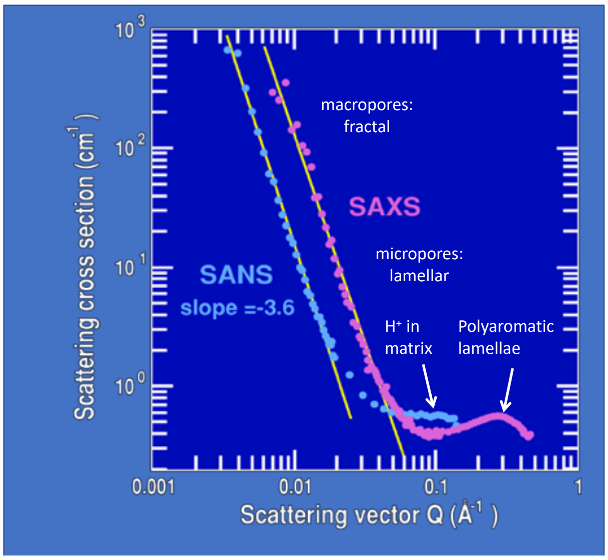

Figure 3. Small Angle X-Ray Scattering (SAXS) and Small Angle Neutron Scattering (SANS) multiscale imaging of pores in a coal sample. SAXS and SANS absolute scattering cross sections differ due to different scattering mechanisms for X-rays and Neutrons.

Small and Wide-Angle X-Ray Scattering (WAXS) imaging are ideal tools for this approach as they allow real time data acquisition of pores with sizes between 10^{-9} to 10^{-7} m and the crystal lattice on the scale of 10^{-10} m information at each irradiation point volume (Figures 2 and 3). The information is augmented through SEM imaging and inverse modeling with a polydisperse sphere model (Hinde 2004).

In order to investigate the physics of submicron processes in reservoir conditions bespoke flow through and deformation cells have been built (T. Blach) which allow for new insights into the dynamic processes from the lowest scale onwards (Figure 2 and 3). An example of the new insights into the physics of the processes gained by experiments with the SAXS/WAXS cell is the multiscale quantification of dynamically evolving drainage and fluid expulsion patterns accommodated by deformation mechanisms of the matrix during dehydration of a poly-crystalline gypsum sample (Schrank et al. 2019). The experiment provides the missing link to understand observations obtained for the same problem at the next scale up through time-series μ-CT experiments (Fusseis et al. 2012). The analysis confirms that the fluid expulsion and porosity evolution can indeed be identified as proxy for the reaction progress as claimed earlier (Fusseis et al. 2012). However, the upscaled reaction is obviously also a function of the dynamic pore evolution network and needs insights from the sub-micron physics in order to derive meaningful parameters for in-situ conditions.

The SAXS/WAXS investigations of these processes (Schrank et al. 2019) clearly show that gypsum dehydration reactions obtained from standard laboratory experiments are inappropriate for reservoir simulators. Carefully designed experiments under in-situ conditions must be performed to obtain a micro-structurally enriched framework providing meaningful results for reactions triggered by thermal changes due to e.g. fluid flow in a reservoir.

Having characterized the sub-micron physics by SAXS/WAXS in situ experiments, it is now possible to use the insight for the next scale of experiments for which triaxial flow and deformation cells have been developed to replicate in-situ conditions (Figure 4).

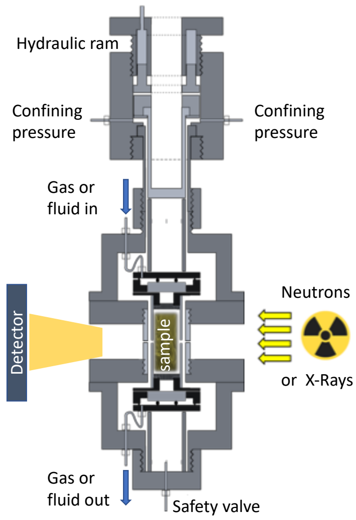

Figure 4. Example of a prototype X-Ray and Neutron tomography cell design by T. Blach which has been successfully tested in 2018 in the NIST Centre for Neutron Research in Gaithersburg, US and in the Institute Laue Langevin (ILL) in Grenoble, France. Specifications: fluid pressure (up to ca. 100 MPa); hydraulic ram (up to 100 MPa); temperature (up to ca. 300 °C, dual heaters); exchangeable windows (Ti, TiZr, Be, Al); cores (up to

20mm diameter and 100mm long); fluids used (CD_4, He, CO_2).

Triaxial deformation μ-CT experiments in conjunction with the step [5] of the workflow are now being investigated to understand the hydraulic homogenization (Figure 5) under an applied reservoir stress using a Navier-Stokes fluid solver and a Lagrangian solid-solver for the coupled deformation of the solid matrix (Lesueur et al. 2017).

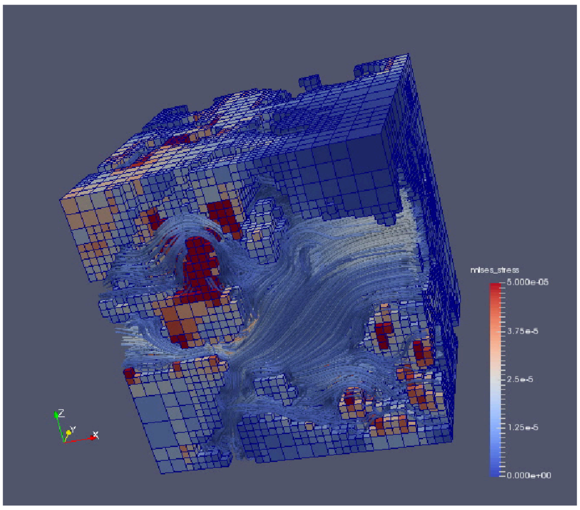

Figure 5. Example of an automated MOOSE-based (Gaston et al. 2015) Octree meshing of a μ-CT experiment and implementation of an Eulerian flow solver that is coupled to a Lagrangian solid mechanics solver, both in a sequential or tight manner. The flow simulator is successfully benchmarked for permeability computation on a digital rock that has been previously used for other code validations (Lesueur et al. 2017)

CONCLUSIONS

We have showcased here the first steps of development of a laboratory scale workflow for molecular- micrometre scale data assimilation. The project leverages on a long track record of developing the fundamental theory for cross-scale multiphysics interactions and computational modelling of their feedbacks (Regenauer-Lieb et al. 2013; Regenauer-Lieb et al. 2013) and presents a seed for the full scale of geophysical data assimilation from the molecular to the field scale.

The full framework consists of multiscale and multiphysics rock physics theory allowing combination of multiscale artificial intelligence assisted rock physics characterization, laboratory experiments and forward numerical models with geophysical inversion to enable a microstructurally enriched rock physics property database for static and dynamic conditions from sub-nm to field scale.

This paper briefly presents technological innovations in each of the four areas [1] data acquisition, [2] data analysis, [3] data compression, [4] and data assimilation. Figure 1 shows the concept for what is known as an Integrated Computational Material Engineering (ICME 2008) framework which has already revolutionized the automotive and aerospace industry.

We claim that this approach is necessary for the 4th industrial revolution in the energy and mineral industry. It provides new simulation techniques exploration, reservoir characterisation and exploitation with multiscale uncertainty quantification (Wellmann and Regenauer-Lieb 2012). Coupled with geophysical imaging the novel framework allows the resource industry to intelligently predict where to best look for particular resources, how to characterise and upscale the material behaviour, how to best stimulate the reservoir and how to develop the optimal production protocol.

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