Near Surface Geophysics at Synchrotron and Neutron User Facilities

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Motivation

Near surface geophysics seeks to characterize the top hundreds of meters of Earth's surface remotely using geophysical techniques such as seismic, radar, gravity, electrical and magnetic imaging; although it could be extended to include the topmost layer of the crust directly affected by human activities, the anthropogenic near surface. This top layer of the Earth's surface is often of critical importance to environmental and industrial activities. Connecting geophysical data to subsurface properties entails applying a physical model which often contains explicit geometric assumptions. Applying these models accurately is a persistent challenge due to the heterogeneous nature of the near surface, which is often characterized by complex mineralogy and pore structure as well as the presence of multiphase fluids. The ability to image samples while measuring their physical properties makes beamline science an invaluable tool for the advancement of near surface geophysics.

The purpose of this white paper is to highlight the value of in-situ experimental capabilities and propose areas of investment that will lead to significant scientific advancements over the next decades. The previous decade has seen significant progress in beamline geophysics in the fields of multiphase flow, chemo-mechanical coupling and granular mechanics. The development of more sophisticated beamline-compatible cells and data analysis tools facilitates multiphysics experiments for which in-situ imaging capabilities add significant value (e.g. Mancini et al., 2020).

Multiphase and Reactive Flow

The study of multiphase flow on the beamline has advanced our knowledge of the fundamental mechanisms responsible for multiphase flow processes such as capillary pressure evolution, relative permeability behavior and drainage/imbibition hysteresis. Consideration of the pore-scale dynamics of multiphase flow is important to a full understanding of vadose zone processes, oil and gas recovery, geological storage of carbon dioxide and other underground energy storage technologies. Direct knowledge of pore geometry is invaluable in the investigation of multiphase flow in porous materials. Early in-situ work on drainage and imbibition in sand has helped understand capillary pressure-saturation curves, pointing to preferential drainage from large pores as the source of discrepancies between fast and slow drainage (Wildenschild et al., 2005). Pore geometry and wettability have been shown to be central to the dynamics of capillary trapping in both oil and gas as well as geological storage scenarios (Singh et al., 2017). High resolution imaging allows for the quantification of heterogeneous capillary pressure at reservoir conditions in a variety of materials (Garing et al., 2017) and flow paths during drainage and imbibition (Voltolini et al., 2017). High quality 3D data also increases the fidelity of models, allowing them to capture dynamic relative permeability during complex processes such as dissolution and exsolution of gasses in pore spaces (Zuo et al., 2017). These unique data sets also allow for unprecedented insight into multiphase flow in heterogeneous materials such as shale, highlighting the role of preferential flow paths (Peng and Xiao, 2017). There are some limitations to using x-rays as an imaging source given low attenuation coefficients. One common solution to this issue is the use of contrast agents (typically iodides) to improve the contrast on samples where fluids with similar attenuation are present (e.g. Voltolini et al., 2017), but recently interferometry-based techniques are gaining attention, since they do not require any modification to the chemistry of the fluids (Yang et al., 2014). Another approach for imaging water in geological samples is the use of a different probe, more sensitive to H, such as neutrons. Neutrons readily penetrate centimeters of metal, yet strongly scatter from water and other light elements. Neutrons are effective in imaging water (and hydrocarbons) by absorption contrast alone without the need of using additional elements to use as contrast agents (Perfect et al., 2014 for a review). A neutron analog to Hooke's microscope will soon be available at NIST that will provide 3-micron spatial resolution with >1 s temporal resolution (tomography in a minute), a factor 10,000 reduction in time over state of the art (Hussey et al, 2021). With a meter-long focal length, high spatial resolution images will be maintained even when the sample sits in a pressure or flow vessel. Coupled with high energy x-ray imaging for simultaneous Neutron/X-ray tomography (LaManna et al, 2017), this imaging capability will greatly facilitate the analysis of multiphase flow in complex geological systems at the core scale. Another neutron source-based technique of interest for the Earth scientist working on flow in microporous materials is small angle neutron scattering (SANS). This is especially appealing since it allows to measure (in bulk, typically) very small pores in large samples, thus avoiding the hard rule resolution vs. field of view typical of the measurements in the direct space: an example of SANS applied to study how different fluids occupy micro- and nanopores can be found in Zhang et al. (2020).

In-situ investigation of chemical-mechanical processes has yielded insight into the ways that chemical and mechanical driving forces are coupled in the near subsurface. Reactive flow leading to dissolution and precipitation in the subsurface is important for the characterization and design of high-tech engineering projects such as enhanced geothermal systems and geological carbon storage. These processes are also central to the evolution of faults and aid proper assessment of dynamic seismic hazard for both natural and induced seismicity. Reactive flow experiments are extremely helpful in characterizing the evolution of the pore space in reservoir rocks, e.g. in a CO2 subsurface sequestration scenario (Menke et al., 2015, Voltolini and Ajo-Franklin, 2017). In addition to reservoir rocks, similar approaches have been successfully used to investigate reactive transport in fractured caprocks (Deng et al., 2016). Performing flow through experiments in situ allows for the characterization of channelized dissolution in fractures and the assessment of associated changes in strength and compressibility (Ajo-Franklin et al., 2015). 4D imaging of precipitation in reactive samples can shed light on heterogeneous pore clogging and the production of fractures due to the force of crystallization (Zhu et al., 2016) and the associated data can be used to fingerprint mechanisms of porosity evolution (Xing et al., 2018). Solid-state phase transitions can also lead to porosity and permeability evolution such as during the dehydration of gypsum (Bedford et al., 2017; Schrank et al., 2020). X-ray microCT can adapt miniaturized setups aimed at coupling micromechanical testing with 4D imaging, such as indentation (Voltolini et al., 2020). In the field of mechanical testing coupled to imaging, neutrons show the advantage of being able to allow for larger samples and bulkier in situ cells (Tengattini et al., 2020 for a review).

Geomechanics

In situ imaging of granular mechanics experiments allows for the ability to track the mechanics of individual grains, which has helped unravel some long-standing issues in granular mechanics. Developing reliable constitutive laws for granular materials at a range of conditions is integral to many projects in civil and environmental engineering. X-ray 4D imaging allows to monitor the development of deformation structures such as shear bands and measure fabric evolution of the grain pack (Andò et al., 2012; Wiebicke et al., 2017). Using in situ imaging coupled with 3D X-ray diffraction, beamline experiments can be used to measure full stress and strain tensor for individual grains, effectively allowing the construction of constitutive laws based on true geometries (Cil et al., 2014). The extension of this type of analysis allows for the characterization of force chains in larger grain packs, beginning to bridge the gap between grain-scale and continuum-scale mechanics (Hurley et al., 2017). At higher strains, in situ experiments can shed light on the dynamics of grain fracturing (Hurley et al., 2018), strain localization (Baud et al., 2019) and fabric development (Imseeh et al., 2018). The incorporation of ultrasonic sensors has added an addition source of data on fracturing processes in crystalline rocks (Cartwright-Taylor et al., 2020) and has the potential to enhance the study of granular mechanics as well. Beamline experiments can also be used to image the deformation in sedimentary materials where grain sizes are beyond current resolution capabilities. These materials represent critical components of subsurface engineering projects, acting as barriers to flow (aquatards, cap rocks) and energy/storage reservoirs. Although strains in fine-grained materials may be orders of magnitude less than coarse granular materials, the application of digital volume correlation algorithms to 4D image data has enabled quantification of sample-scale strain fields (Sone et al. 2017; Beck et al. 2018).

Opportunities for future investment

Significant improvements can be made in the practice of beamline near surface geophysics with relatively modest investments. As the experimental setups for near surface deformation experiments are quite general, there is immense opportunity for developing cells and sample assemblies across the national beamline infrastructure similar to the COMPRESS consortium. In particular, the development of modular cells with interchangeable pressure vessels and plumbing could enable the use of different techniques over a broad range of conditions and promote the growth of experimental programs at the beamlines. This organization of beamline resources would need to involve investments in personnel and infrastructure to support users. In general, an engineer to assist with cell modification and maintenance, a software engineer to assist with reconstruction of large amounts of 4D data and a data scientist or image analysis expert to assist with data analysis are clearly needed. This staffing model is employed at many international beamline facilities to great success, allowing for highly productive science output.

The improvement of in situ cells through the inclusion of additional sensors systems for measuring, dielectric properties, electrical resistivity and acoustic velocities would greatly enhance the possibilities for beamline experimentation. The incorporation of acoustic sensors in an x-ray transparent triaxial pressure vessel has already started yielding insights into rupture processes in crystalline rocks and could be easily transitioned to operate at near surface conditions (Butler et al., 2020).

One of the major assets of synchrotron X-ray and neutron imaging to the near surface community is the ability to capture processes over a wide range of temporal resolution. Rapid X-ray radiography can be acquired over 100s of nanoseconds, allowing 3D visualization (2D space and time) high energy deformation events such as hydraulic fracturing (Renard et al., 2009), mechanical indentation (Ma et al. 2021), and impact events (Farbaniec et al., 2021). Slow deformation processes are easily characterized by 4D imaging. However, often the rates of geologic processes are so slow that they cannot be measured within the course of a single beamline session (3-5 days). This motivates the need for modular, possibly transportable cell designs across the national beamline infrastructure that would allow users to pursue longer term experiments.

The combination of different techniques for simultaneous measurements is one of the current trends at the current beamlines; given the flexibility in the building of conventional cone-beam X-ray microCT setups, those can be easily coupled with other techniques to add a 3D imaging capability. This has been used to couple X-ray microCT with XRD to couple fabric and crystallographic properties (Suuronen et al., 2014; tabletop setup), with neutron imaging to take advantage of the very different cross sections of important elements (as the aforementioned H, but also Li, Cl, etc.) when using the two sources (Zambrano et al., 2019; Stavropoulou et al., 2019).

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