

MONet 2nd XCT Working Group meeting

Attendees (Total 16 participants): Carl, Cassandra Miller, Derek Detweiler, Garystinchcomb, Jared Lee Wilmoth, Julie Jastrow, Michael Ricketts, Phillip Owens, Rachel Berner, Ruifang Hu, Sharon Billings

- Review XCT MONet data types (Tamas)
 - Highlighting the various XCT data types collected, particularly focusing on lower resolution scans for overall core visualization and higher resolution scans for detailed porosity analysis.
 - Discussion of the data collection methods: lower resolution scans (core overview) and higher resolution scans (pore network analysis).
- Quick overview of topics discussed in the first meeting and GitHub (Tamas)
 - Meeting notes and meeting recordings available on the GitHub
- How do we do XCT segmentation? (Maruti)
 - Segmentation of XCT data
 - Focused on differentiating between solid and pore spaces.
 - Use computer vision and machine learning techniques for segmenting XCT images.
 - Showcased the Jupyter notebook workflow for segmenting and visualizing XCT data in a 3D context using tools like Paraview.
 - Important links to reference:
 - https://github.com/EMSL-MONet/XCT_Working_Groups
 - Visualizing 3D data towards modeling:
 - <https://www.paraview.org/download/>
 - XCT (sub-volume) Google Colab Notebook:
 - <https://colab.research.google.com/drive/1Tbm49gRwDpvYKg5ukrrtfSo8yshRLil7?usp=sharing>
 - Complete XCT data and associated analysis are available through Jupyter Lab notebooks.
 - Please see `XCT_FullDataAnalysis_Notebook.ipynb`
 - https://github.com/EMSL-MONet/CommSciMtg_Nov23/blob/main/XCT/XCT_FullDataAnalysis_Notebook.ipynb
 - Download ParaView software for visualization:
 - <https://www.paraview.org/download/>
- Review Jupyter notebook workflow (Maruti)
 - How do we run PFLOTTRAN workflows for analyzing bulk data and how to extend to 3D format?
 - PFLOTTRAN Model focusing on C degradation
 - Use Google Colab and Jupyter Notebooks for exploring XCT data
 - FLOTTRAN workflows for analyzing bulk data.
 - Overview of extension of these workflows to 3D data formats.
 - Examples of how to construct meshes for modeling purposes and provided an overview of PFLOTTRAN input decks.

- Discussed the integration of chemical imaging data for advanced modeling of flow, transport, and energy balance scenarios.
- PFLOTTRAN EMSL Integration
 - PFLOTTRAN input files for modeling more complex reactions
 - Reaction Sandbox
 - https://www.pflotran.org/documentation/theory_guide/reaction_sandbox.html
 - Some resources to get started
 - <https://bitbucket.org/pflotran/pflotran/src/master/shortcourse/>
 - https://bitbucket.org/pflotran/pflotran/src/master/regression_tests/default/batch/
 - PFLOTTRAN developers and users at PNNL are happy to help EMSL users on using PFLOTTRAN on Tahoma
 - Questions regarding PFLOTTRAN installation (i.e. not answered in the installation tab), bug reports: pflotran-dev@googlegroups.com
 - Questions regarding running PFLOTTRAN: pflotran-users@googlegroups.com
 - <https://groups.google.com/g/pflotran-users>
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- Questions and discussion (All)
 - Is there a R studio workflow as well? Or with XCT data is python better?
 - Choice of thresholds for segmenting XCT images: Is 10 a good number or would we need to play around a bit with threshold?