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Pore2Chip: All-in-one python tool for soil microstructure analysis and micromodel design

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Software

- Review
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Summary

The `Pore2Chip` Python package is designed to create 2D micromodels using extracted data from 3D X-ray computed tomography (XCT) images. This package helps analyze soil structure and function, allowing for the investigation of hydro-biogeochemical processes that impact mineral extraction and reactivity, oxygen concentrations, and nutrient availability in disturbed or managed soils. Key metrics encompass pore size distributions, pore throat size distributions, and connectivity (pore coordination numbers). The final output is a 2D scalable SVG design representing a core or aggregate. Designs can be fabricated with methods such as laser etching, 3D printing, and photolithography.

Statement of need

The resilience of agricultural and natural landscapes is intrinsically connected to soil structure. Land management (e.g., tillage, grazing, and fire) and associated impacts (e.g., compaction, pore-clogging) can transform soil microstructure (Feng et al., 2020; Liu et al., 2018; Oliveira et al., 2022; Rooney et al., 2022; Stoof et al., 2016). These changes in the soil microstructure determine the flow of water, solutes, and gasses as well as mineral retention, transport, and distribution (Bailey et al., 2017; Hamamoto et al., 2010; Waring et al., 2020). Simplified, homogeneous pore networks provide innovative demonstrations of how water, solutes, and microbes interact (Bhattacharjee et al., 2022) but need more accurate representations of soil properties. Creating realistic heterogeneous habitats is time-consuming and does not include pore network characteristics, such as pore connectivity. Incorporating pore dynamics into soil models such as chemical species degradation enables dynamic predictions for soil responses under changing pore networks (Davidson et al., 2012; Moyano et al., 2018).

The need for software that can generate various micromodel designs that researchers can test and validate with minimal computational cost (Dentz et al., 2023; Oostrom et al., 2014) is increasing. `Pore2Chip` allows this functionality by providing the intended users, such as earth scientists and lab-on-chip instrument specialists, with easy-to-use research software for lab-on-chip designs. Specifically, the Pore2Chip-based information analysis of XCT images allows researchers to fill this experimental design gap by enabling the ability to build a representative quasi-2D pore network along with first-order, fast, and reasonably accurate flow models that can be linked with experiments. These flow models are built using recent advances in physics-informed neural networks (New et al., 2024), laying the foundation to accelerate numerical simulations and improve the fidelity of predictions in microscale environments. Moreover, `Pore2Chip` allows one to assess the impact of various system parameters, such as pore structures, fluid properties, and flow conditions, needed to develop optimal micromodel experiments. Such a capability can guide model-experiment-data (ModEx) integration at the microscale, allowing for upscaling microscale processes and predictions of dynamic soil properties and functions (see Figure 1).

Main features and differences with other tools

`Pore2Chip` addresses complex pore structures by representing pore networks as connected shapes, unlike older sphere packing algorithms. This enables users to easily create and control pore networks representing various real-world conditions. `Pore2Chip` offers experimental design capabilities that cannot be achieved by existing software such as epyc (Dobson, 2022). `Pore2Chip` provides support and reproducibility for developing lab-on-chip experimental designs uniformly across different soil datasets with fast, reasonably accurate, first-order flow modeling capabilities. Microscale experiments using `Pore2Chip` micromodels may target both abiotic and biotic processes and be integrated into modeling efforts such as water flow modeling, reactive transport modeling, and microbial activity simulations.

Implementation details and support libraries

Using `Porespy` (Gostick et al., 2016), `OpenPNM` (Gostick et al., 2016) and various graphics rendering libraries (e.g., drawsvg, ezdxf, svglib, cairosvg, reportlab), `Pore2Chip` renders SVG or DXF micromodel designs of the generated network. Output designs are scalable and adjustable based on the target porosity of the micromodel. It can also be exported as micromodel data in VTK formats for visualization in Paraview or microfluidic simulations with open-source software such as `PFLOTRAN` (https://www.pflotran.org), `OpenFOAM` (https://www.openfoam.com), and other physics-informed neural network modules. If the user wants to extract data from XCT images, `Pore2Chip` has image filtering and network extraction modules utilizing Otsu thresholding and `PoreSpy`. Though, generation function can also work with data extracted by other software as long as it is an array of values that Python can read.

Figure 2 provides a high-level overview of the repository structure and example use cases (Figure 1) within the `Pore2Chip` repository.

Figures

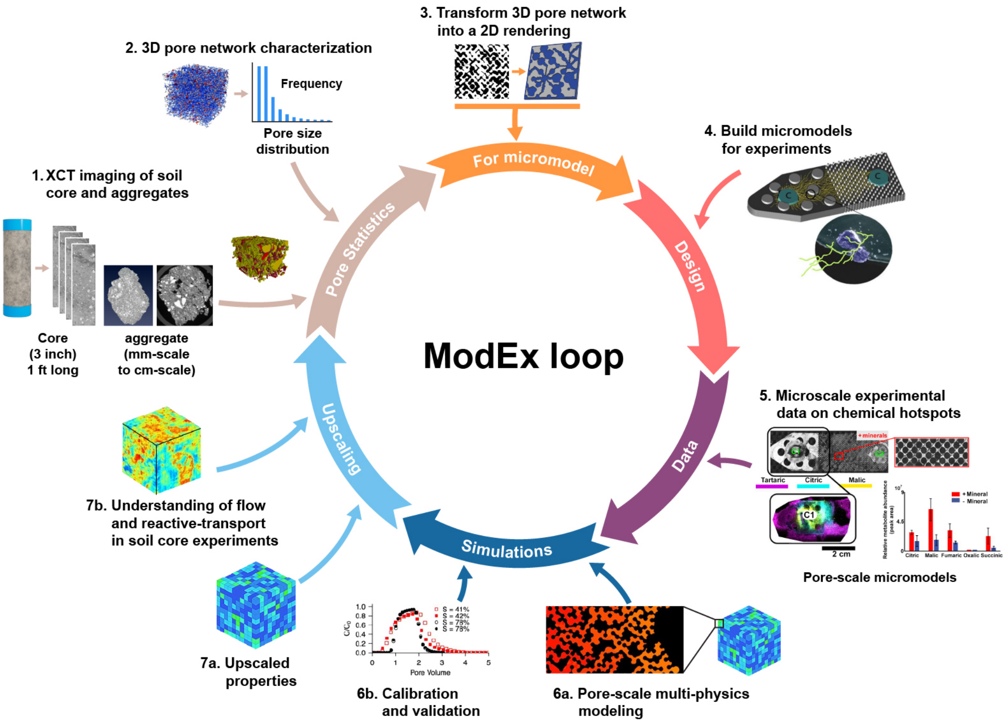

Figure 1: A high-level overview of essential steps in Pore2Chip-based micromodel designs informed by soil dataset. The iterative ModEx loop continuously improves multi-physics process models by integrating experimental data, leading to more accurate predictions for fluid flow, reactive-transport, and rhizosphere function applications.

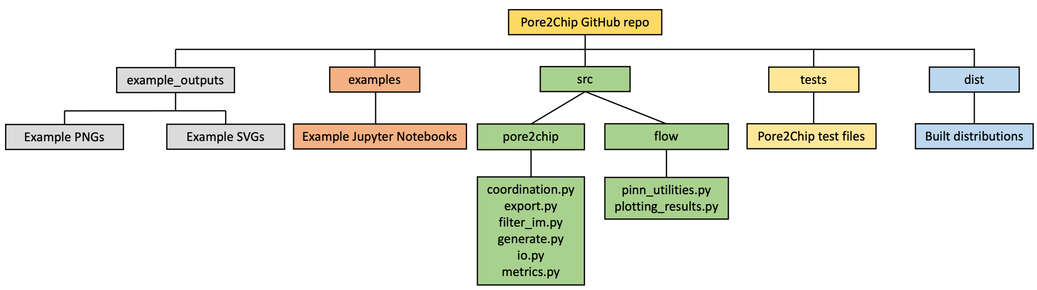

Figure 2: An overview of the Pore2Chip repository structure, detailed example notebooks, and built distributions.

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References

Bailey, V. L., Smith, A., Tfaily, M., Fansler, S. J., & Bond-Lamberty, B. (2017). Differences in soluble organic carbon chemistry in pore waters sampled from different pore size domains. *Soil Biology and Biochemistry*, *107*, 133–143. https://doi.org/10.1016/j.soilbio.2016.11.025

Bhattacharjee, A., Qafoku, O., Richardson, J. A., Anderson, L. N., & al., K. S. et. (2022). A mineral-doped micromodel platform demonstrates fungal bridging of carbon hot spots and hyphal transport of mineral-derived nutrients. *mSystems*, *7*(6), e00913–22. https://doi.org/10.1128/msystems.00913-22

Davidson, E. A., Samanta, S., Caramori, S. S., & Savage, K. (2012). The dual arrhenius and michaelis–menten kinetics model for decomposition of soil organic matter at hourly to seasonal time scales. *Global Change Biology*, *18*(1), 371–384. https://doi.org/10.1111/j.1365-2486.2011.02546.x

Dentz, M., Hidalgo, J., & Lester, D. (2023). Mixing in porous media: Concepts and approaches across scales. *Transport in Porous Media*, *146*(1–2), 5–53. https://doi.org/10.1007/s11242-022-01852-x

Dobson, S. (2022). Epyc: Computational experiment management in python. *Journal of Open Source Software*, *7*(72), 3764. https://doi.org/10.21105/joss.03764

Feng, Y., Wang, J., Bai, Z., Reading, L., & Jing, Z. (2020). Three-dimensional quantification of macropore networks of different compacted soils from opencast coal mine area using x-ray computed tomography. *Soil and Tillage Research*, *198*, 104567. https://doi.org/10.1016/j.still.2019.104567

Gostick, J., Aghighi, M., Hinebaugh, J., Tranter, T., Hoeh, M. A., Day, H., Spellacy, B., Sharqawy, M. H., Bazylak, A., Burns, A., & Lehnert, W. (2016). OpenPNM: A pore network modeling package. *Computing in Science & Engineering*, *18*(4), 60–74. https://doi.org/10.1109/MCSE.2016.49

Hamamoto, S., Moldrup, P., Kawamoto, K., & Komatsu, T. (2010). Excluded-volume expansion of archie's law for gas and solute diffusivities and electrical and thermal conductivities in variably saturated porous media. *Water Resources Research*, *46*(6). https://doi.org/10.1029/2009wr008424

Liu, Z., Ma, D., Hu, W., & Li, X. (2018). Land use dependent variation of soil water infiltration characteristics and their scale-specific controls. *Soil and Tillage Research*, *178*, 139–149. https://doi.org/10.1016/j.still.2018.01.001

Moyano, F. E., Vasilyeva, N., & Menichetti, L. (2018). Diffusion limitations and michaelis–menten kinetics as drivers of combined temperature and moisture effects on carbon fluxes of mineral soils. *Biogeosciences*, *15*(16), 5031–5045. https://doi.org/10.5194/bg-15-5031-2018

New, A., Gearhart, A. S., Darragh, R. A., & Villafañe-Delgado, M. (2024). Physics-informed neural networks for scientific modeling: Uses, implementations, and directions. *Artificial Intelligence and Machine Learning for Multi-Domain Operations Applications VI*, *13051*, 492–502. https://doi.org/10.1117/12.2611234

Oliveira, J. A. T. de, Cássaro, F. A. M., Posadas, A. N. D., & Pires, L. F. (2022). Soil pore network complexity changes induced by wetting and drying cycles—a study using x-ray microtomography and 3D multifractal analyses. *IJERPH*, *19*(17), 10582. https://doi.org/10.3390/ijerph191710582

Oostrom, M., Mehmani, Y., Romero-Gomez, P., Tang, Y., Liu, H., Yoon, H., Kang, Q., Niasar, V., Balhoff, M., Dewers, T., Tartakovsky, G., Leist, E., Hess, N., Perkins, W., Rakowski, C., Richmond, M., Serkowski, J., Werth, C., Valocchi, A., & Zhang, C. (2014). Pore-scale and continuum simulations of solute transport micromodel benchmark experiments. *Computational Geosciences*, *20*, 1–23. https://doi.org/10.1007/s10596-014-9424-0

Rooney, E. C., Bailey, V. L., Patel, K. F., Dragila, M., & al., A. K. B. et. (2022). Soil pore network response to freeze-thaw cycles in permafrost aggregates. *Geoderma*, *411*, 115674. https://doi.org/10.1016/j.geoderma.2021.115674

Stoof, C. R., Gevaert, A. I., Baver, C., Hassanpour, B., & al., V. L. M. et. (2016). Can pore-clogging by ash explain post-fire runoff? *International Journal of Wildland Fire*, *25*(3), 294. https://doi.org/10.1071/WF15037

Waring, B. G., Sulman, B. N., Reed, S., Smith, A. P., & al., C. A. et. (2020). From pools to flow: The PROMISE framework for new insights on soil carbon cycling in a changing world. *Global Change Biology*, *26*(12), 6631–6643. https://doi.org/10.1111/gcb.15365