canarie

OpenPNM
Advancing materials science to safeguard society

The study of porous materials is an important sub-discipline of materials science. Learning how liquids and gases flow through permeable materials is critical to researchers who are safeguarding the future of our society, whether it's optimizing batteries for more efficient electric vehicles, ensuring aquifers have adequate supplies of fresh water, finding new sources of energy, or slowing the weathering of buildings and bridges.

However, a comprehensive computational framework is needed for analyzing, simulating, and visualizing porous materials. These tools are often reinvented from scratch by each new researcher working in their own specific field. Lacking a shared open source package for studying permeable substances, each researcher spends significant time designing, writing, and debugging software, introducing extra cost and engineering into each project as well as reducing the time available for quality research.

Solving problems rather than creating new frameworks

Mitigating this repetitive rebuilding is what OpenPNM is all about. A package written in Python that models porous materials, it draws upon a rich community of scientists already using the popular programming language, leveraging many existing numerical, scientific, and visualization packages.

This approach to building on top of existing code has other benefits as well: OpenPNM is maintained, debugged, and refined by many researchers, ensuring that optimal code gets incorporated back into computational models. It also means that researchers already

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familiar with the well-known Python language can more easily adopt and customize OpenPNM methods. And because it is customizable for new materials, fluid models, and material structures to suit any problem, researchers are able to focus on solving problems rather than creating new frameworks.

OpenPNM was created by a team now at the University of Waterloo, who has designed it to address data-intensive problems with computational ease. This makes the software suitable for simulating liquid or gas flow throughout an entire system, unlike traditional numerical simulations that are only able to reproduce very small portions of a material.

Software Evolution

Funded through the CANARIE Research Software Program, OpenPNM was originally developed and maintained for studying electric vehicle battery efficiency but has since found applications in many different areas such as oil exploration, hydrogen fuel cell fabrication, and desalination plants.

Filling a much-needed gap in materials science

OpenPNM is filling a much-needed gap in the materials science community by providing a rich, adaptable open-source framework for the study of porous materials. Montreal company DragonFly is currently using it in tomography visualization software for the international instrumentation giant, ZEISS. As many of our technological advances come through the understanding, fabrication, and refinement of porous materials – such as more powerful batteries, or more efficient water filters – OpenPNM is directly contributing to accelerated research in many critical areas that impact Canadians.

Platform: OpenPNM

Description	OpenPNM is an open source project aiming to provide porous media researchers with a ready-made framework for performing a wide range of pore network simulations.
Contributor(s)	University of Waterloo
Research Subject	Materials structure, properties and testing
Supports Separate Projects	Yes
Software License	MIT License
To Learn More	https://science.canarie.ca/res/101