

Gas Flow in Mesoporous Media

Opportunity

Transport of gases in mesoporous media is a fundamental process involved in unconventional natural gas production from tight sandstones, shale formations, and deep coal beds, as well as in engineered energy systems such as fuel cells.

Meso Challenge

- Gas flow in mesoporous media is in the slip or transitional flow regimes, where the continuum description of fluids requires empirical slip boundary conditions or is no longer valid.
- Molecular Dynamics or DSMC method simulation is prohibitively expensive due to the large number of molecules.
- A mesoscopic approach is highly desirable to develop scientific understanding of gas flow in mesoporous media.

- Suga, K., S. et al., 2010. "Evaluation of a lattice Boltzmann method in a complex nanoflow." *Physical Review E*, 82, (1), 10.
- <https://software.lanl.gov/taxila/trac>

Approach

- High performance computation using Taxila LBM, an open source, massively parallel software package developed in an ongoing LANL LDRD-DR project will be fully utilized.
- The Taxila LBM will be enhanced (by increasing the number of discrete velocities and keeping higher-order moments in the LB equation) to simulate flow in slip and transitional regimes.

Impact

- LBM mesoscopic modeling can provide unique insights into the problem of gas flow in mesoporous media.
- Potential applications include unconventional gas production, Geological CO₂ sequestration, chromatography, ultrafiltration, chemical vapor deposition, fuel cells, and MEMS.



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