# **A fractional PDE and molecular dynamic modeling of anomalous diffusive transport in heterogeneous nano-scale digital rock**

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Fluid flows confined in nano-pore structures exhibit physical behaviors that are not observed in large-scale structures. Molecular dynamics simulation has been used for modeling nano-scale fluid flows at nanoscale, but is deemed to be computationally very expensive and is often limited to problems with simple geometry.

We develop an integrated fractional partial differential equation and molecular dynamics upscaling modeling of anomalously diffusive transport in heterogeneous nano-pore structures, which has a significantly improved computational efficiency and memory requirement over the molecular dynamics simulation. Representative applications demonstrate the usage of the new model.