Many-GPU Simulation of Nanopore Flow on the Summit Supercomputer

Presentation · August 2019

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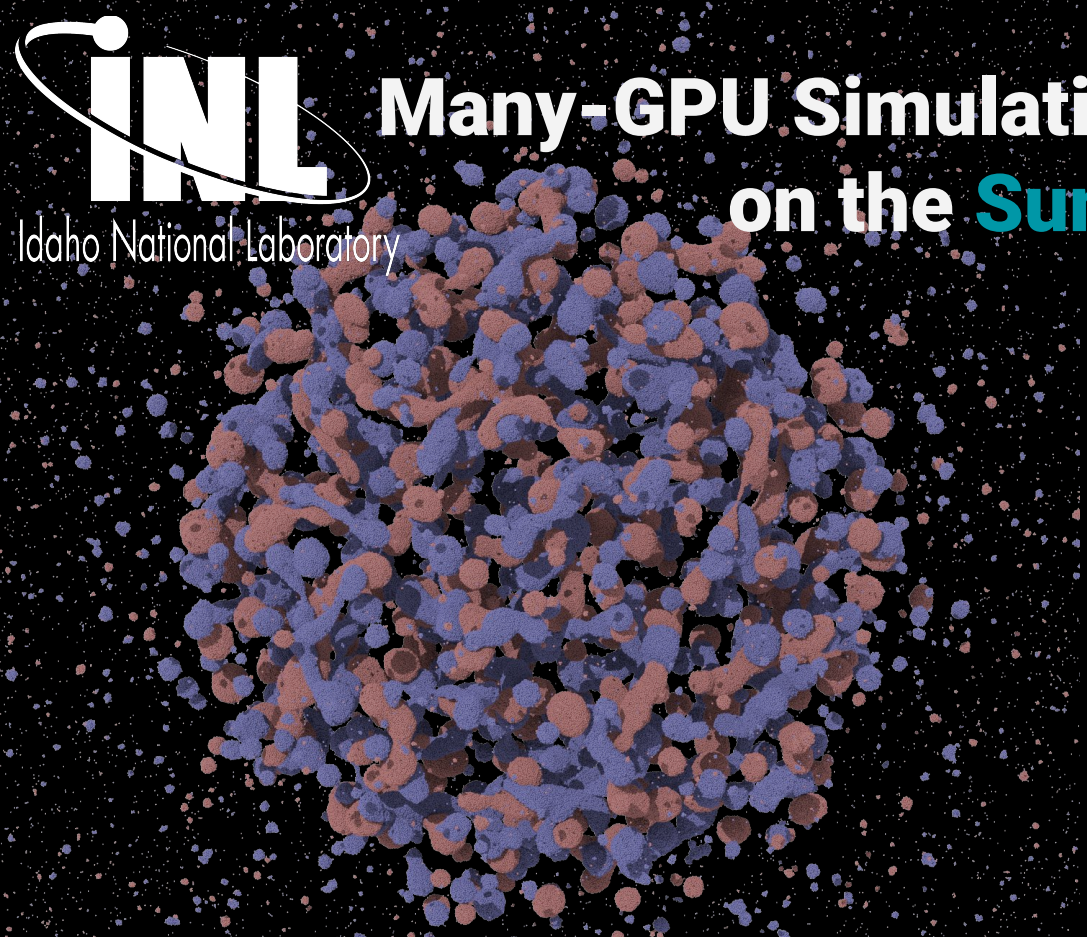
Many-GPU Simulation of Nanopore Flow on the Summit Supercomputer



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The **Summit Supercomputer** @ Oak Ridge National Laboratory

Processor: IBM POWER9 (2/node; 42 “usable” cores/node)
GPUs: 27,648 NVIDIA Tesla V100s (6/node; 5120 CUDA cores/GPU)
Nodes: 4,608
Node Performance: 42TF
Memory/node: 512GB DDR4 + 96GB HBM2
NV Memory/node: 1600GB
Total System Memory: >10PB DDR4 + HBM + Non-volatile
Interconnect Topology: Mellanox EDR 100G InfiniBand, Non-blocking Fat Tree
Peak Power Consumption: 13MW

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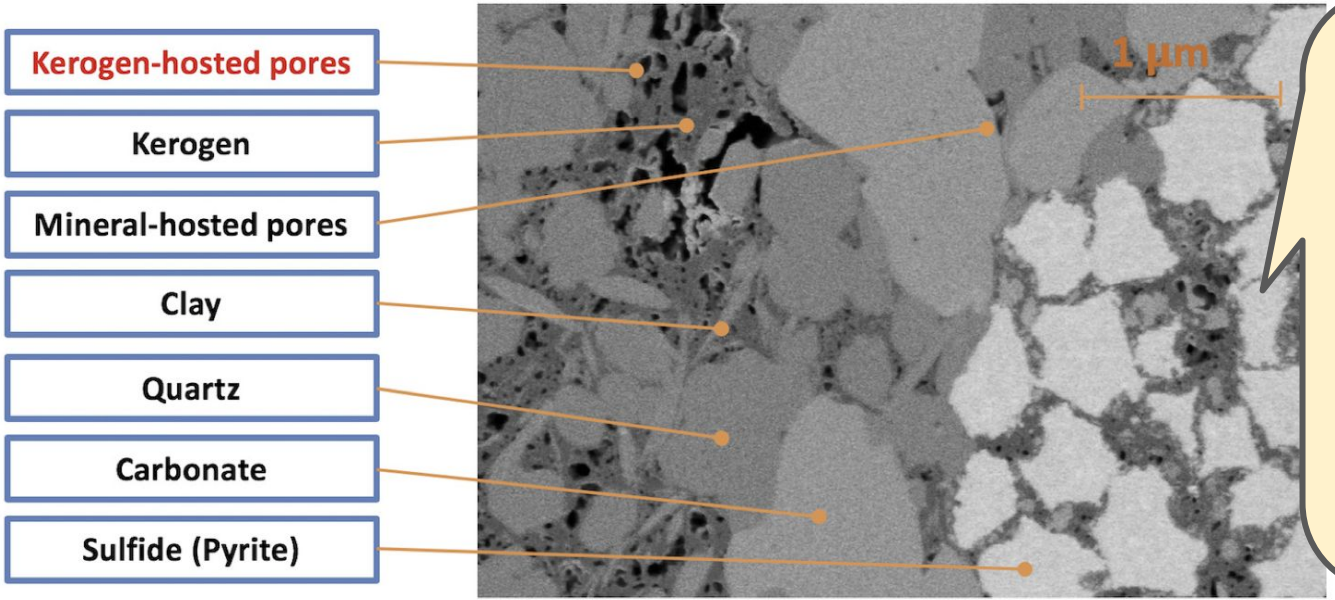
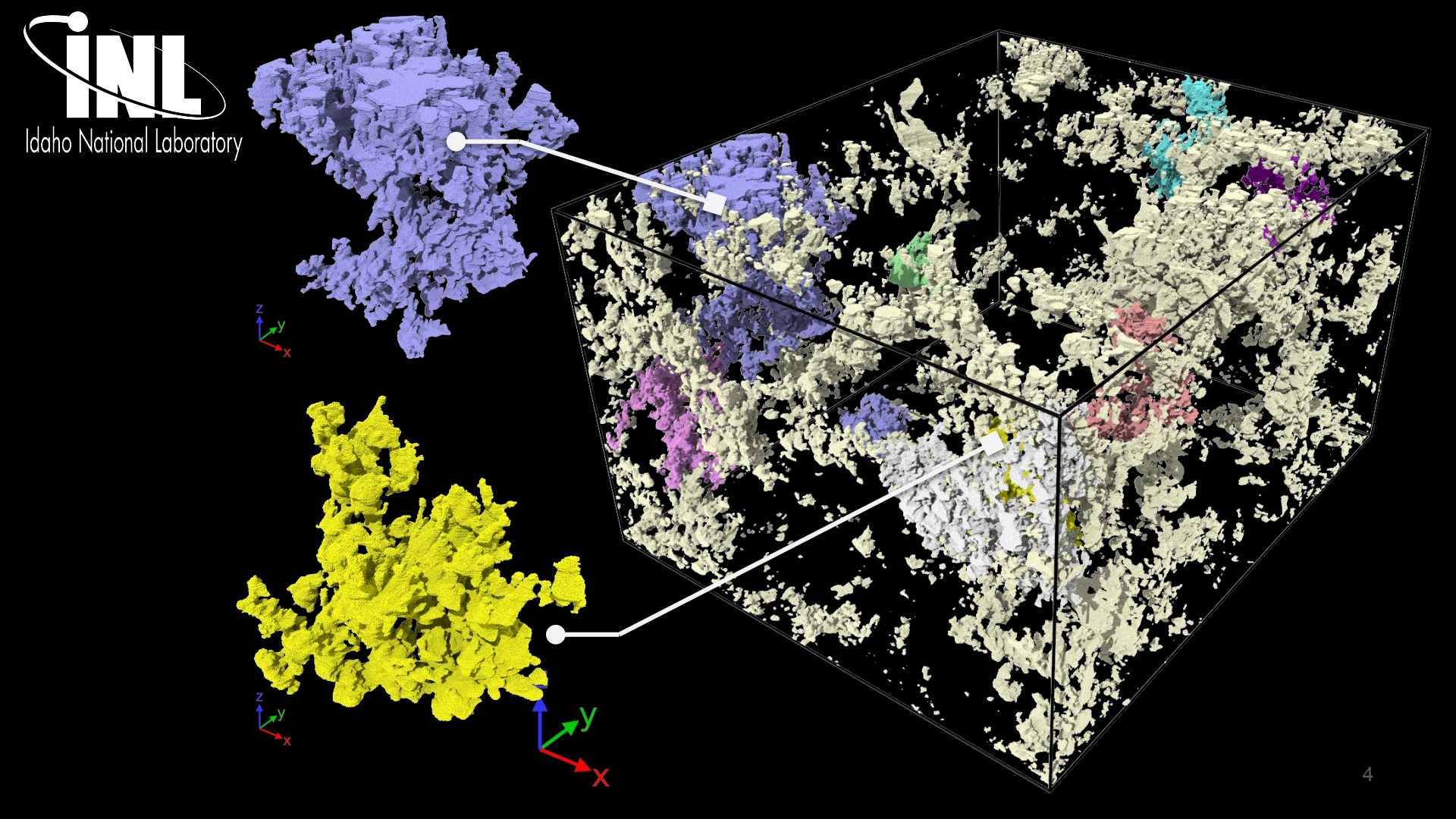
Understanding of **Hydrocarbon Recovery** in **Low-Permeability, Tight Shale** ???



Challenges

- **Multiscale pore sizes (10^{-9} - 10^{-6} m)**
- **Heterogeneities in physical & chemical properties**
- **Continuum fluid mechanics models no longer valid**

Credit: Y. Xia et al. "A GPU-accelerated package for simulation of flow in nanoporous source rocks with many-body dissipative particle dynamics", Computer Physics Communications (accepted), arXiv preprint, arXiv:1903.101341, 1 (2019)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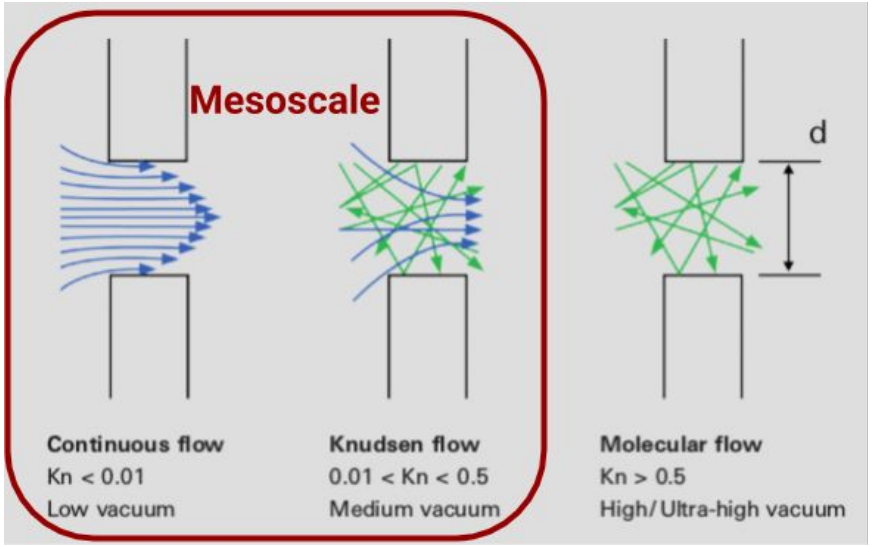
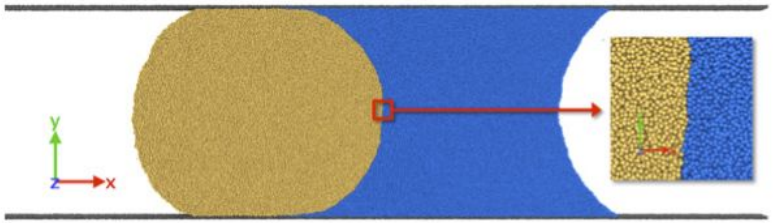
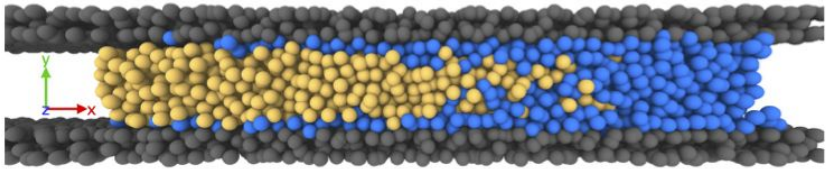
Dissipative Particle Dynamics (DPD)

- A class of **mesoscopic** particle dynamics method (**LAMMPS USER-MESO**)
- For both **discrete** & **continuum** flow behaviors





a) Fluid-fluid and fluid-solid interfaces in a **100-nm**-wide pore are stable.



b) Thermodynamic fluctuation and diffusion in a **2-nm**-wide pore are profound.

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userMESO 2.5 DPD Flow Simulator a GPU Extension Package to LAMMPS

V2.5 is the latest release [Xia et al 2019] to **userMESO** [Tang et al 2014, Blumers et al 2017]

- I/O related tasks such as inter-rank host-to-host comm are attended by **LAMMPS**.
- All computations and host-device comm are handled by **userMESO**.
- Notable innovative features are discussed in [Tang et al 2014].
- New feature: the **many-body DPD model** [Li et al 2013, Xia et al 2017].
- New feature: an **impenetrable wall** model for **arbitrary geometries** [Li et al 2018].

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References

[1] Y. Xia et al. Computer Physics Communications (accepted), arXiv preprint, arXiv:1903.101341, 1 (2019).

[2] Y. Tang et al. Computer Physics Communications 185, 11 (2014), 2809–2822.

[3] A. Blumers et al. Computer Physics Communications 217 (2017), 171–179.

[4] S. Plimpton. Journal of Computational Physics 117, 1 (1995), 1–19.

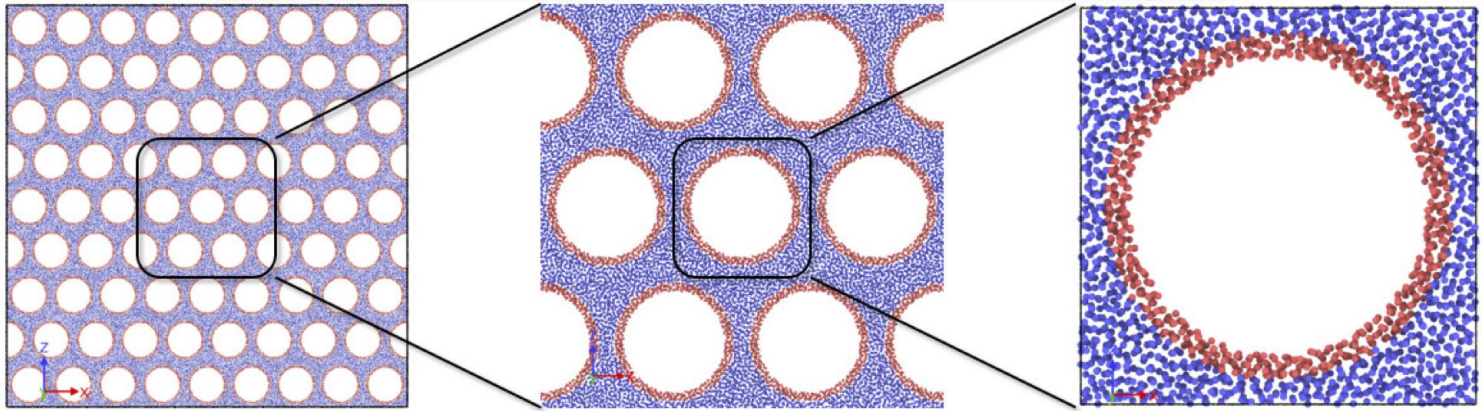
[5] Z. Li et al. Physics of Fluids 25, 7 (2013), 072103.

[6] Y. Xia et al. Physics of Fluids 29, 5 (2017), 056601.

[7] Z. Li et al. Journal of Computational Physics 355 (2018), 534–547.

userMESO 2.5 Code Readiness on Summit

Benchmark problem
a body-force driven flow in a quasi-2D domain



- Strictly uniform porosity distribution with periodic BC in all the 3 directions.
- Pore channel size: **narrowest gap = 4 nm**; circle size: **14 nm in diameter**.
- An impenetrable wall BC at wall surfaces

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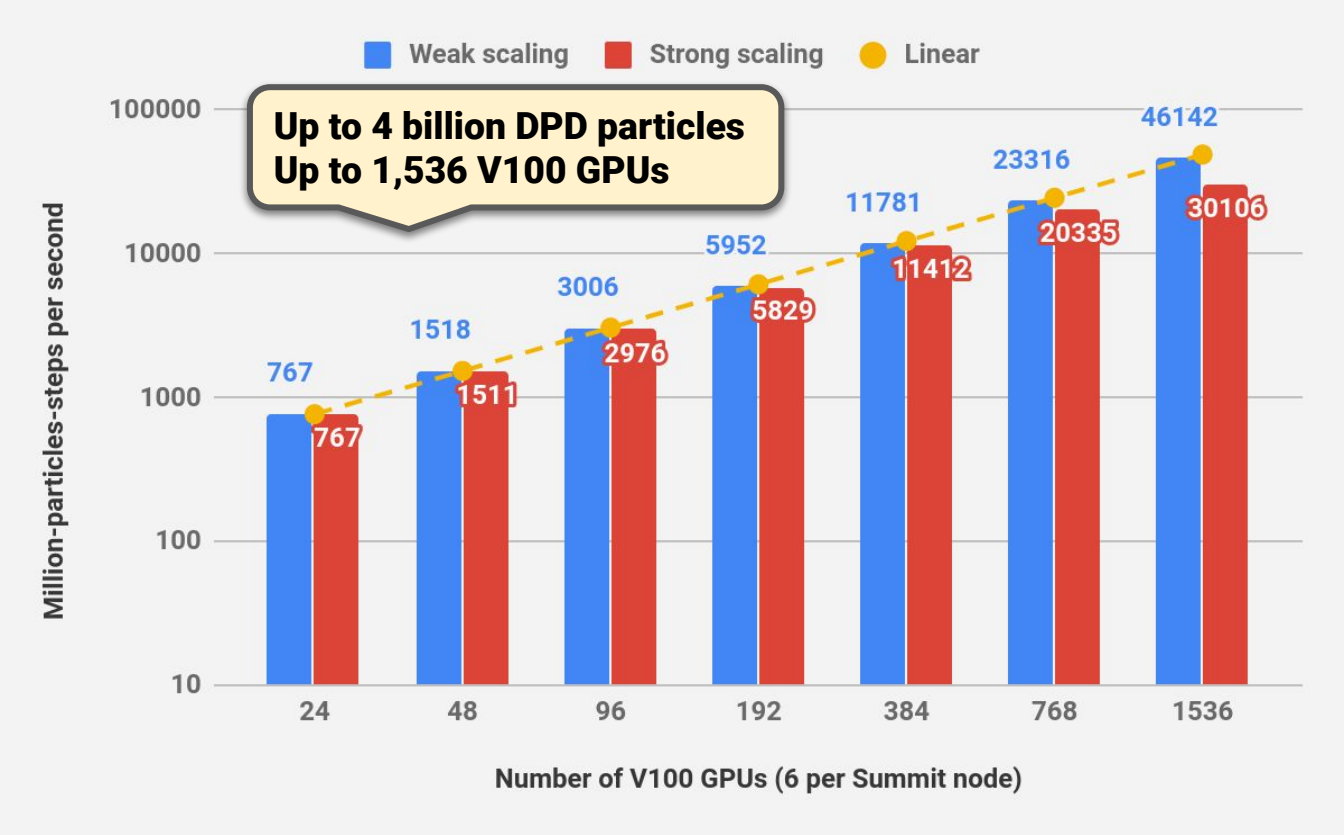
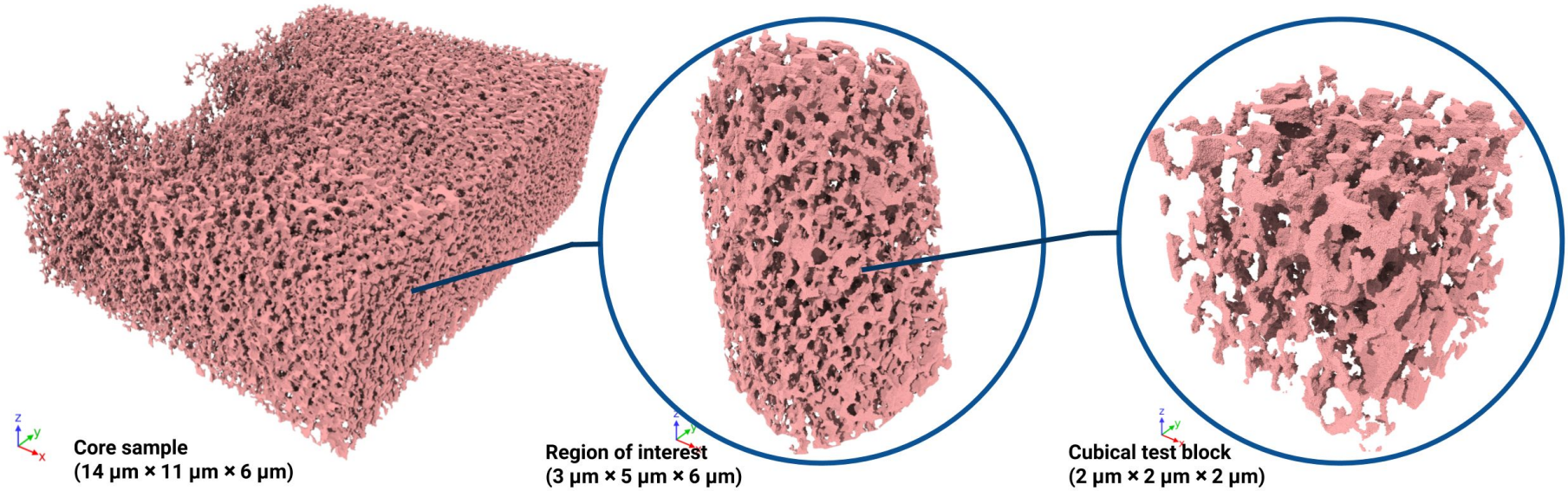
userMESO 2.5 Code Readiness on Summit



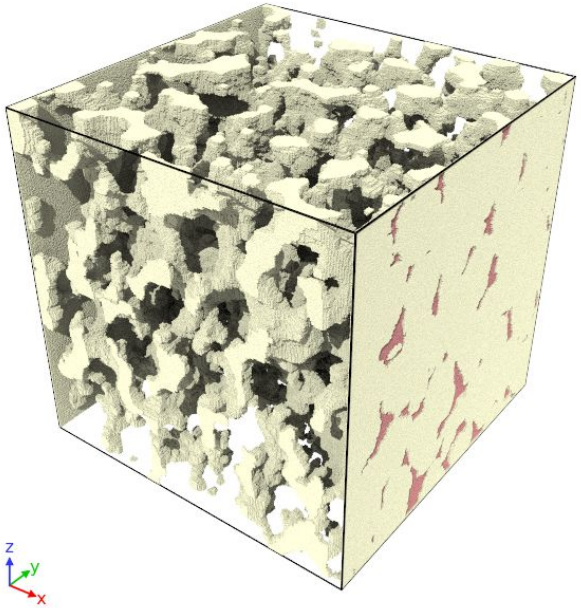
DPD for Flow in **Synthetic Nanoporous Silica**

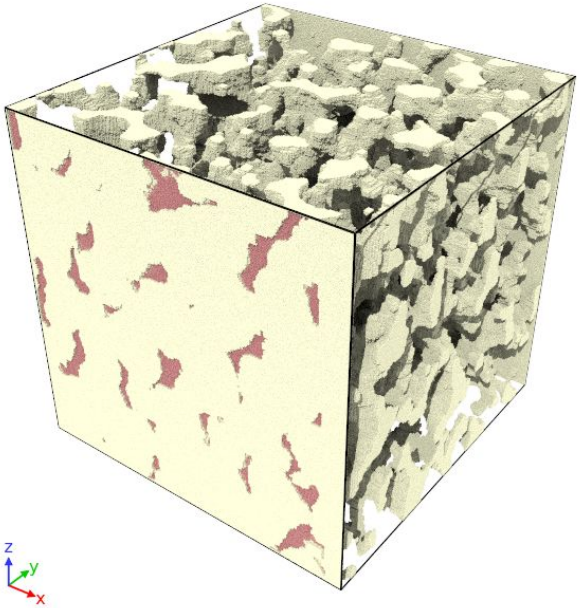


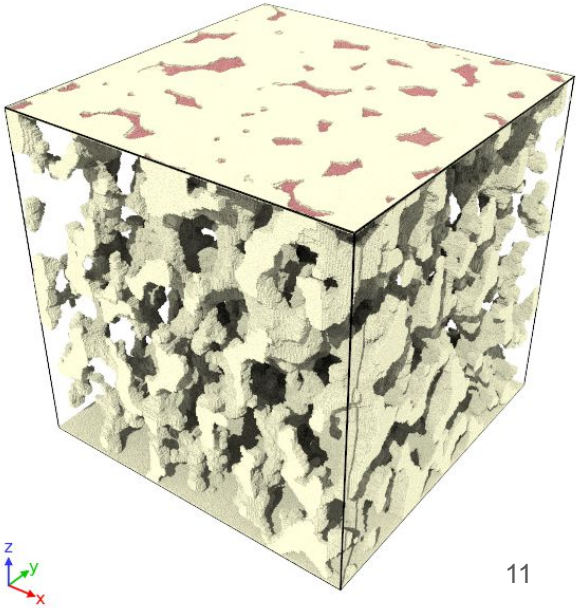
* Processed stack images of sample provided by
Joshua Kane (Materials and Fuel Complex, INL)

A **Strong-Scaling** Test (~ 70 million DPD particles): Pore Channel Flow in Three Directions

Domain: 2 x 2 x 2 (micrometer^3)







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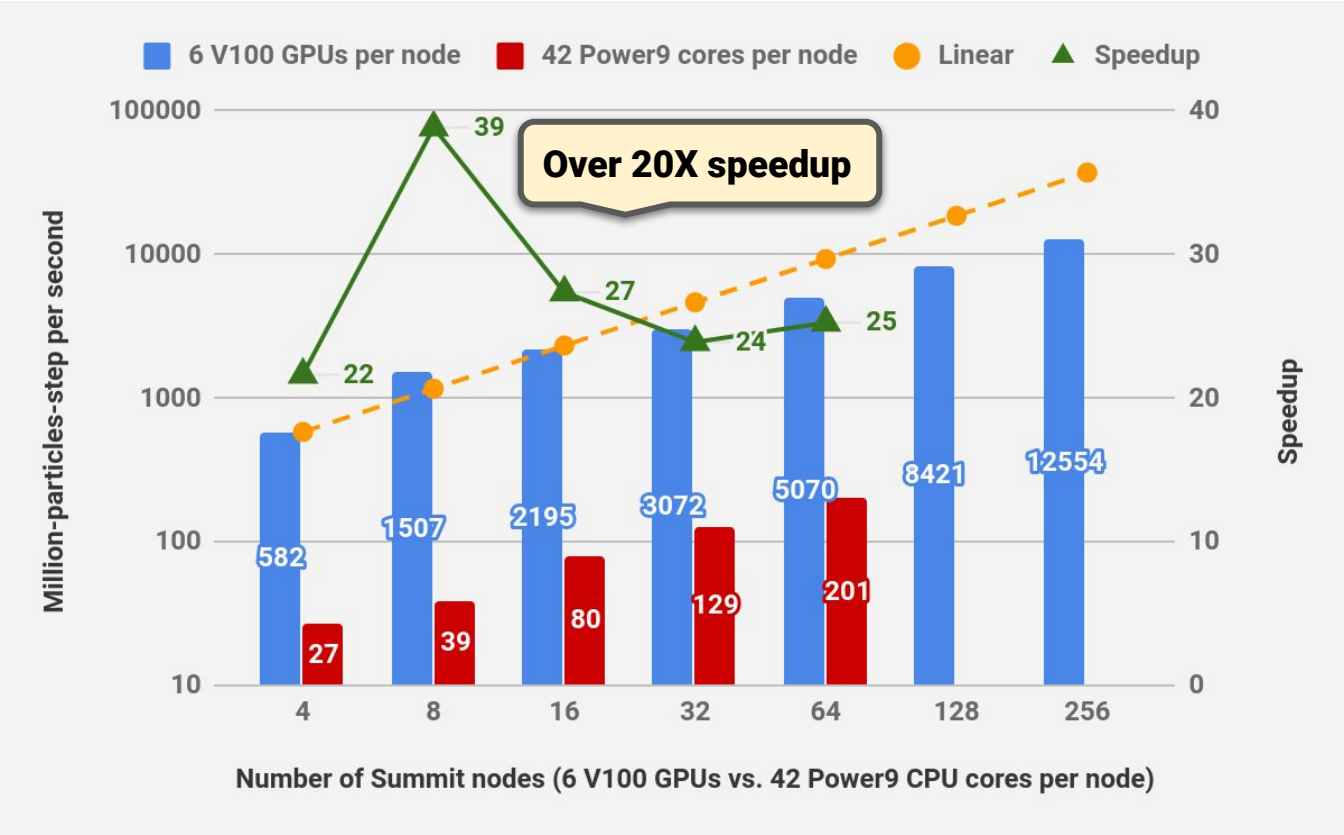
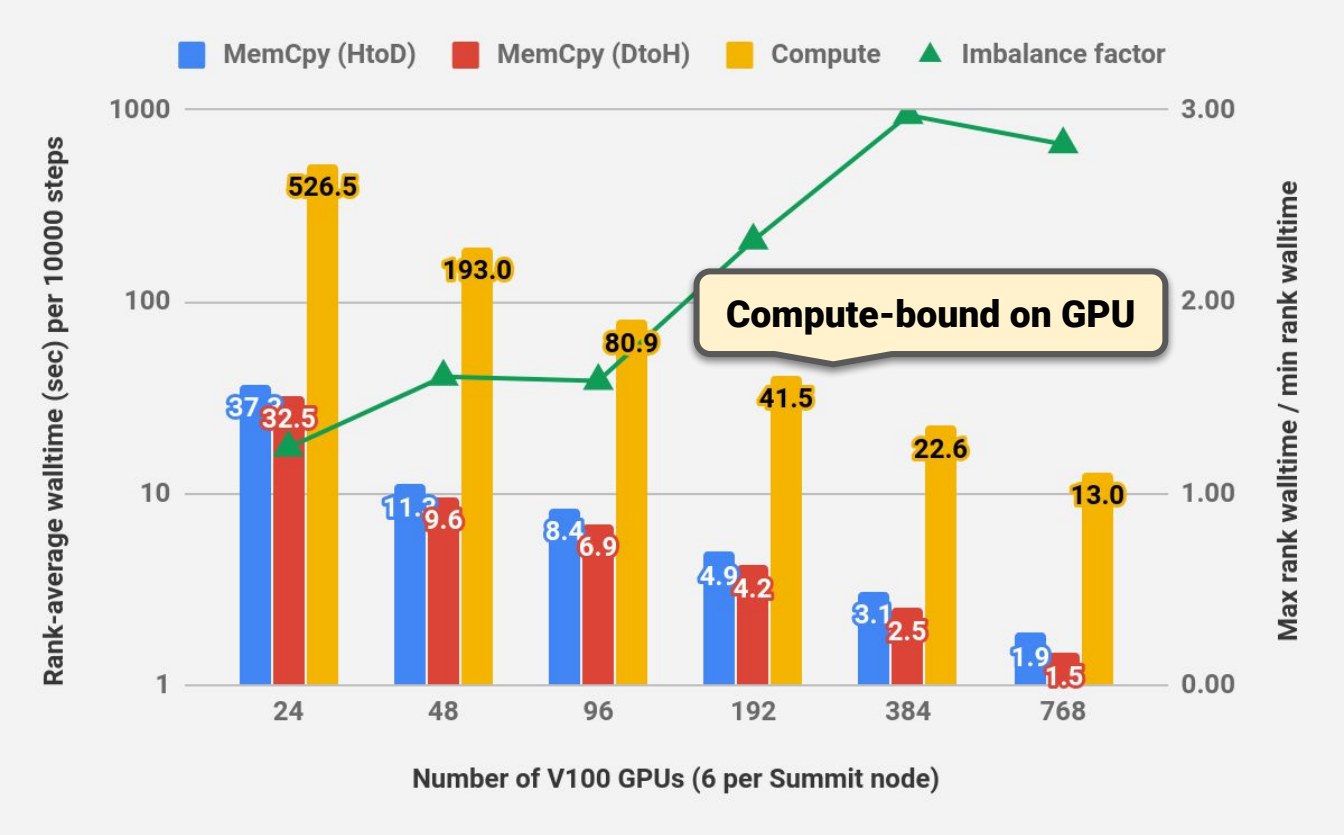
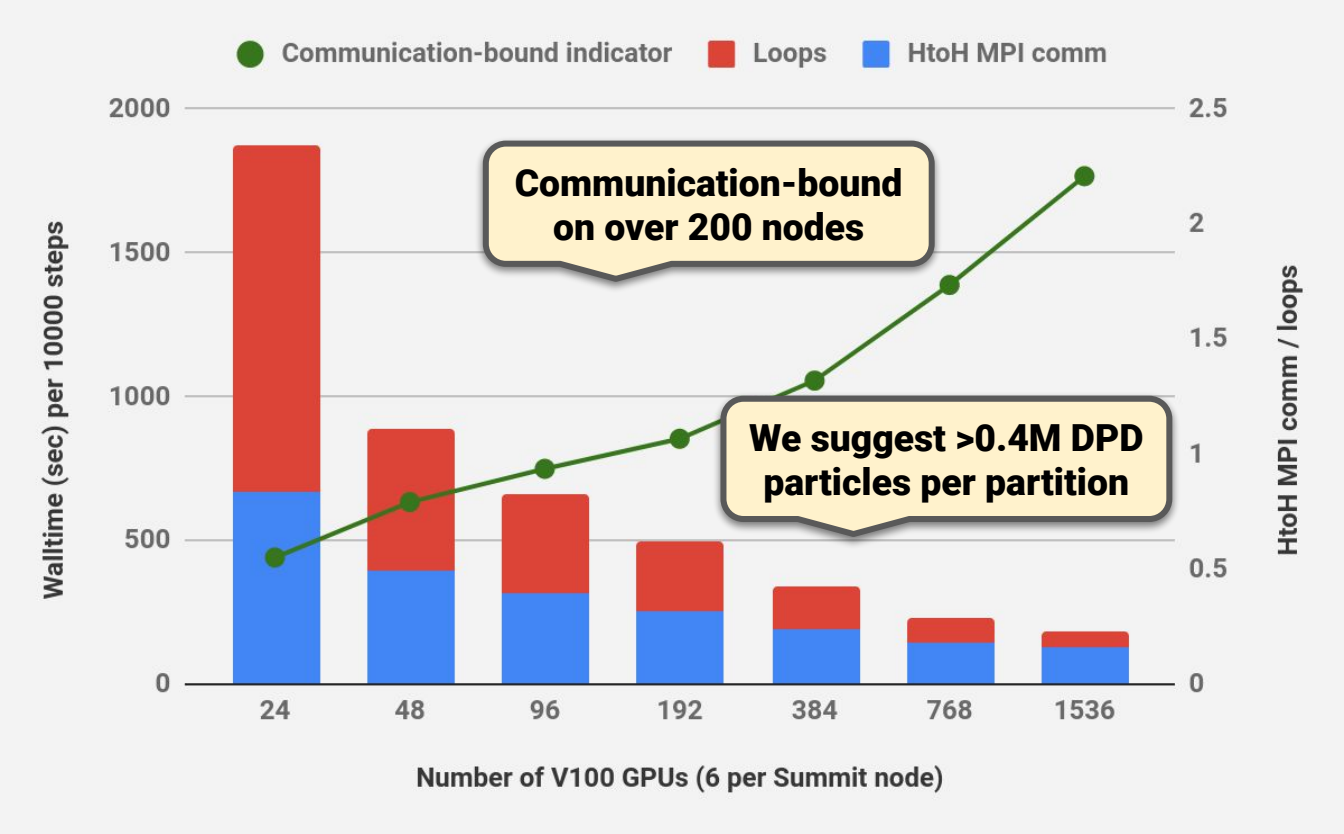
V100 GPUs vs. Power9 CPUs on Summit Nodes



Breakdown of GPU Activities on **Summit** Nodes



Breakdown of Walltime on **Summit** Nodes



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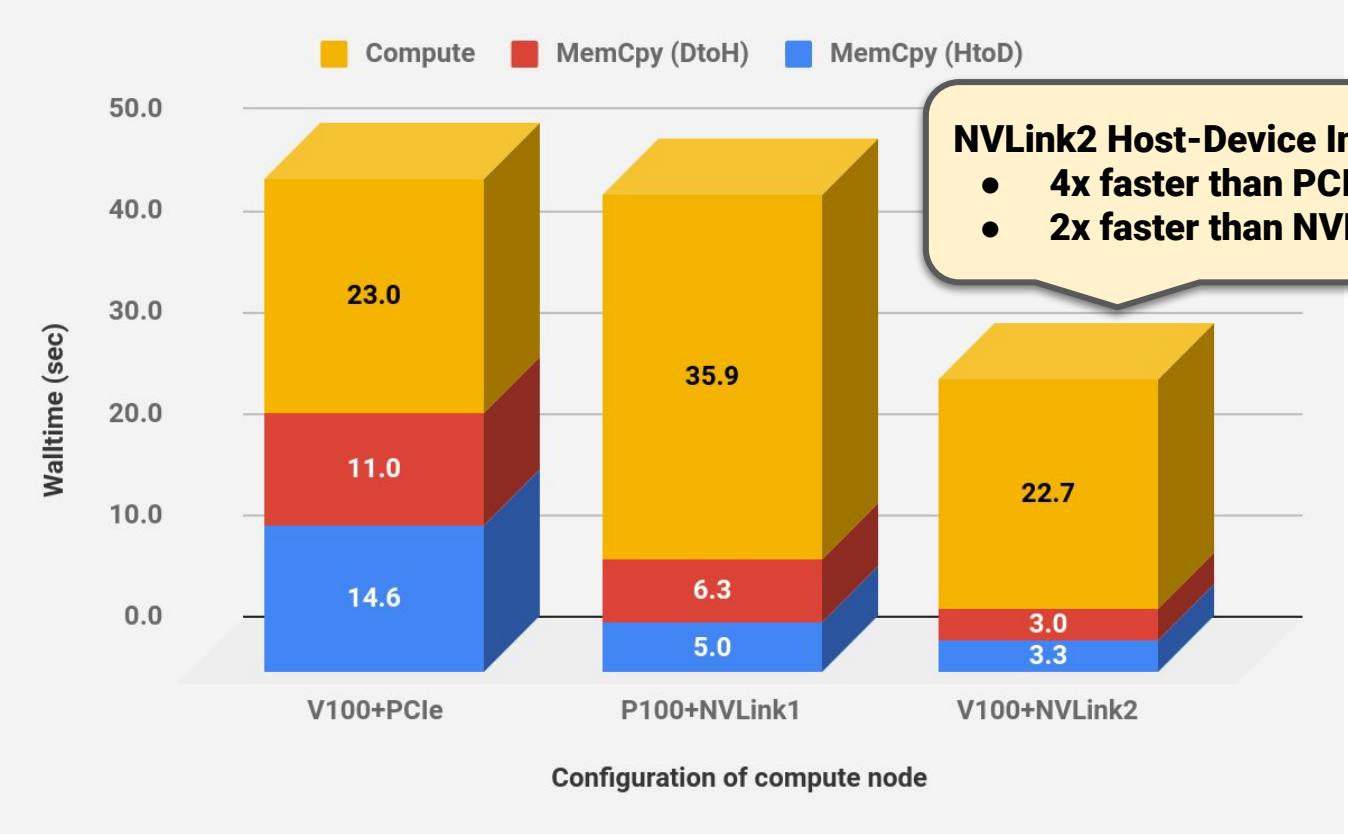
V100+PCIe vs. P100+NVLink1 vs. V100+NVLink2



DPD for Flow in Nanoporous Shale

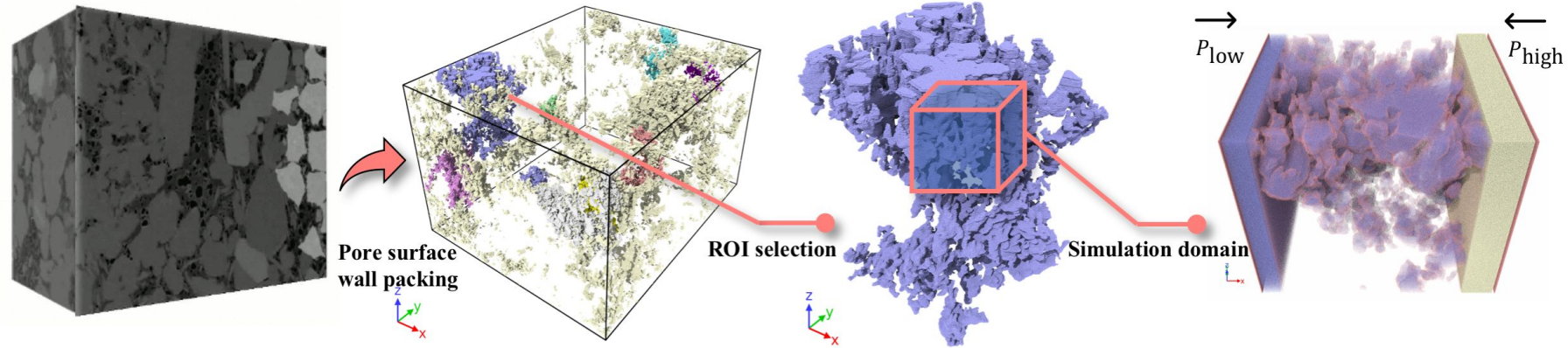
A new Digital Rock Physics workflow
From digital imaging to DPD pore flow simulations

a) A shale micro core sample with size 5 μm × 4 μm × 3 μm

b) DPD particle representation of kerogen-hosted nanopores

c) A region of interest selected (ROI) for nanopore-flow study

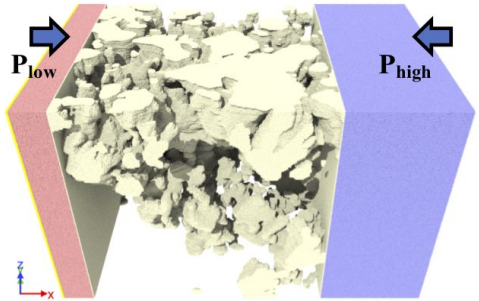
d) Snapshot of nanopore-scale flow simulations with 10^8-10^9 particles



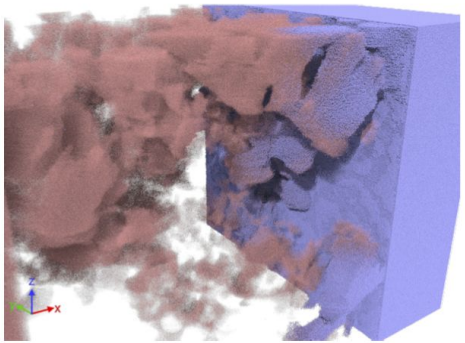
Credit: Y. Xia et al. "A GPU-accelerated package for simulation of flow in nanoporous source rocks with many-body dissipative particle dynamics", Computer Physics Communications (accepted), arXiv preprint, arXiv:1903.101341, 1 (2019)

Research Capability Demonstration

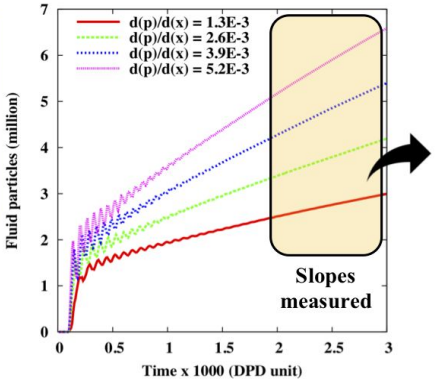
Flooding simulations (**about 240 million DPD particles**)
for permeability characterization
in a micro shale domain
with realistic nanometer-resolution pore geometries.

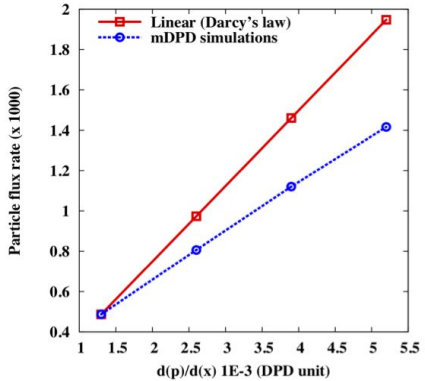


Block size: 957.5 × 952.5 × 945.0 nm³



Snapshot of flooding in nanopores





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Code Repositories

CPU version: LAMMPS USER-MESO (in my fork)

<https://github.com/yidongxiainl/lammps/tree/inl>

GPU version: userMESO 2.5 (as an GPU extension package for LAMMPS)

<https://github.com/AnselGitAccount/USERMESO-2.0-mdpd>

Acknowledgement

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- The scaling benchmarks were performed at the **Oak Ridge Leadership Computing Facility (OLCF) through the OLCF Director's Discretion Program** under project GEO133, which is supported by the Office of Science of the U.S. Department of Energy under Contract DE-AC05-00OR22725.
- The digital imaging & processing of silica sample was supported as part of the **EFRC-MUSE, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences** under Award No. DE-SC0019285.