

Reproducibility Description Appendix

for “A Parallel-efficient GPU Package for Multiphase Flow in Realistic Nano-pore Networks”

The legacy versions of the *USERMESO* code are hosted as open-source software on GitHub

USERMESO <https://github.com/yhtang/MESO>

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

USERMESO 2.5 <https://github.com/AnselGitAccount/USERMESO-2.0>

These repositories contain the relevant software source code, user’s instruction for installation, and script for verification test. Users are able to reproduce benchmark test results by following the step-by-step instructions in the README file in each repository.

Each version was rigorously tested on a regular desktop computer with an Nvidia GPGPU card and on Oak Ridge National Laboratory’s Titan supercomputer. Relevant references are below:

- [1] Tang, Y. H., & Karniadakis, G. E. (2014). Accelerating dissipative particle dynamics simulations on GPUs: Algorithms, numerics and applications. *Computer Physics Communications*, 185(11), 2809-2822.
- [2] Blumens, A. L., Tang, Y. H., Li, Z., Li, X., & Karniadakis, G. E. (2017). GPU-accelerated red blood cells simulations with transport dissipative particle dynamics. *Computer Physics Communications*, 217, 171-179.

USERMESO 2.5 is the new version to be presented in the poster. Since a further advanced feature (implementation of a Voronoi-inspired partitioning algorithm) is a work-in-progress, the source code is hosted in a private branch on GitHub. We’ll release it once finished by November.