GPU Teaching Kit: Accelerated Computing

Molecular Dynamics Demo Project

CoMD

Classical molecular dynamics proxy application.

Building this project is more difficult than the other demo projects, as it started as real-world code. See the readmes in `src-mpi`.

This is CoMD version 1.1

CoMD is a reference implementation of typical classical molecular dynamics algorithms and workloads. It is created and maintained by The Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx). http://codesign.lanl.gov/projects/exmatex. The code is intended to serve as a vehicle for co-design by allowing others to extend and/or reimplement it as needed to test performance of new architectures, programming models, etc.

To view the generated Doxygen documentation for CoMD, please visit exmatex.github.io/CoMD/doxygen-mpi/index.html.

To contact the developers of CoMD send email to exmatex-comd@llnl.gov.

Building CoMD

Please see `src/README.TXT` for more information.