

High performance computing (HPC) in chemical engineering

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Experiment and theory have a new partner, simulation. Supercomputer simulations have become essential to making discoveries and advancing science. PLSI (Partnership & Leadership for the national wide Supercomputing Infrastructure) having totally 94 teraflops in 19 systems. was constructed in Korea for the efficient usage of national -wide supercomputing resources of which the platform uses Linux cluster technology. Tachyon II (25,000 cores and 300 teraflops) which was deployed in NISN leads challenging and creative parallel supercomputings in Korea. Heterogeneous GPU (graphics processing units) computing will be realized soon with more powerful speed but lower cost.

HPC including computation, storage, and networking has been applied to quantum mechanics, molecular dynamics simulation, chemical reactions, bioinformatics, chemo -informatics, computational biology, multi -scale simulation, computational fluid dynamics (CFD), etc. Simulations on HPC will show insights and prove new things in Chemical engineering. In this study, an example of Linux clustering HPC (168 cores and 0.91 teraflops) is presented for realistic simulation of amine absorber with structured packing.