

Petaflops special-purpose computer for molecular dynamics simulations and its application to protein science

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We are developing a special-purpose computer for molecular dynamics simulations with petaflops performance (10^{15} operations/sec, 25 times faster than Earth Simulator), MDGRAPE-3. We also apply special-purpose machines to analysis of proteins. In the talk, we introduce our project and explain its merits and demerits. The new methodology which will be enabled by such massive molecular dynamics simulations will be also discussed.