Efficiency of ARM processors for classical molecular dynamics calculations

Vsevolod Nikolskiy¹, Vladimir Stegailov ^{1,2}

- 1. National Research University Higher School of Economics, 20 Myasnitskaya ulitsa, Moscow 101000, Russian Federation
- 2. Joint Institute for High Temperatures of the Russian Academy of Sciences (JIHT RAS), Izhorskaya st. 13 Bd. 2, Moscow 125412, Russian Federation

Supercomputing of the exascale era is inevitably limited by power efficiency. Nowadays different CPU architectures are considered as possible choices for these purposes. Recently the development of ARM processors has come to the point when their floating point performance can be seriously considered for a range of scientific applications. In this talk we present the analysis of the floating point performance of the latest ARM cores and their efficiency for the algorithms of classical molecular dynamics.