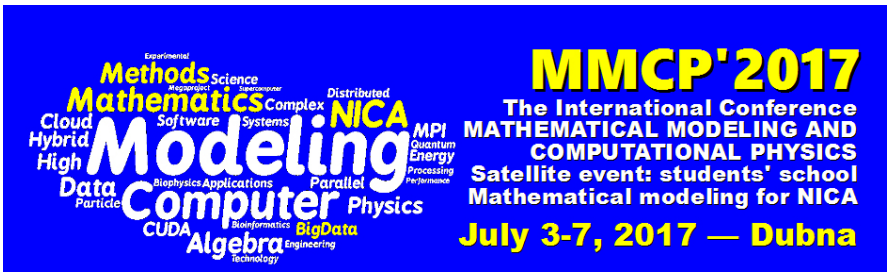

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Multiscale Multilevel Approach to Solution of Nanotechnology Problems

Friday, 7 July 2017 10:30 (30 minutes)

The multiscale multilevel approach for solution of nanotechnology problems by supercomputer systems is presented. The approach is based on combining the continuum mechanics models and the Newton's dynamics for individual particles. This combination includes three scale levels such as macroscopic, mesoscopic and microscopic levels. For gas - metal technical systems we use the following models. The quasihydrodynamic equations system is used as a mathematical model at the macrolevel. The system of Newton's equations is used as a mathematical model at the meso- and microlevels. Numerical implementation of the approach is based on the method of splitting into physical processes. The quasihydrodynamic equations are solved by finite volume method on grids of different types. The Newton's equations of motion are solved by the Verlet integration in each cell of grid independently or in groups of connected cells. Within the framework of this general methodology the four classes of algorithms and methods of their parallelization are offered. Parallelization technology is based on the principles of geometric parallelism and efficient partitioning the computational domain. Special dynamic algorithm is used for load balancing the solvers. The testing of developed approach was made by the example of the nitrogen outflow from balloon with high pressure to vacuum chamber through the micronozzle and microchannel. Obtained results confirm the high efficiency of the developed methodology.

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