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Mesoscale Simulation of Nanoparticle Production GIANLUCA ZUCCARO, Politecnico di Torino, GIOVANNI LAPENTA, LANL, GIOVANNI MAIZZA, Politecnico di Torino — We present a model to study complex physical systems composed by a set of clusters of different chemical species immersed in a matrix with which they interact. The overall model describes the transient of the basic mechanisms governing the processes of interaction in a two-dimensional micrometer size system. At each time step, the continuum (micrometer scale) model computes the macroscopic fields according to the prescribed boundary conditions. The continuum system is discretized with a desired number of uniform computational cells. Each cell contains a number of computational particles which represent the actual particles mixture. The particle-in-cell (discrete) model maps the macroscopic fields from the (continuum) cells to the particles. A molecular dynamics approach is used for computing the chemical reactions among the particles. We present results of a recent application of this approach to the simulation of nanoparticles formation in SHS reactors [1].
[1] G. Zuccaro, G. Lapenta, G. Maizza, Computer Phys. Commun., 162, 89 (2004).

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