Stochastic Kinetic Mean Field model - a new, low-cost, atomic scale simulation technique

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We introduce a new model for calculating the change in time of three-dimensional atomic configurations. The method is based on the kinetic mean field (KMF) approach [1], however we have transformed that model into a stochastic approach by introducing dynamic Langevin noise. The result is a stochastic kinetic mean field model (SKMF) which produces results similar to lattice kinetic Monte Carlo (KMC). SKMF is, however, more cost-effective and the algorithm is easier to implement. [2] The group made the software and the program code (together with tutorials) freely available to the scientific community at the http://skmf.eu webpage. We plan to keep this open source approach with the model's further developments, too. [3]

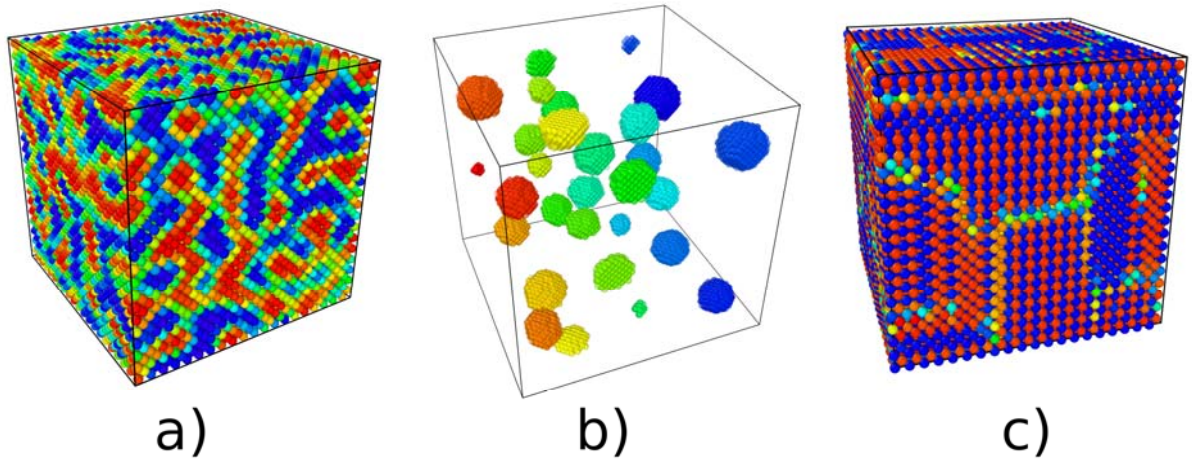

Figure 14: Demonstrations of a) spinodal decomposition, b) nucleation and growth and c) ordering in SKMF simulations

References

[1] G. Martin, Atomic mobility in Cahn's diffusion model, Phys. Rev. B **41**, 2279-2283 (1990)

[2] Z. Erdélyi, M. Pasichnyy, V. Bezpalchuk, J.J. Tomán, B. Gajdics, A.M. Gusak, Stochastic Kinetic Mean Field Model, Computer Physics Communications **204**: pp. 31-37. (2016), http://dx.doi.org/10.1016/j.cpc.2016.03.003.

[3] http://skmf.eu