Analysis and Numerical Experiments of a Variance Reduction Technique for Effective Energies of Random Atomic Lattices

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We discuss the calculation of effective energies of random materials modeled by the Thomas–Fermi–von Weizsäcker (TFW) equations in the framework of the method of representative volume elements (RVEs). The TFW equations constitute a coupled system of nonlinear elliptic equations and describe the distribution of electrons in the presence of a prescribed nuclear charge density. The representative volume approximation is subject to a systematic error (due to the restriction to finite material samples) and a random error (due to material differences in different RVEs). Our emphasis lies on the reduction of the variance of the energy when evaluated for the RVE, as the systematic error decreases exponentially as a function of the diameter of the RVE. This variance reduction can be achieved by selecting the RVE in such a way that it represents the statistical properties of the underlying material particularly well, an approach proposed by Le Bris, Legoll, and Minvielle in the numerical homogenization of linear elliptic equations. A rigorous analysis of this strategy has been carried out recently by Fischer for linear elliptic PDEs.

For establishing the variance reduction in the case of the nonlinear TFW equations, we need a locality result which ensures that perturbations of the nuclear density inside a bounded region result in a change of the electronic density decaying exponentially away from this region. We prove the required locality by extending a recent result by Nazar and Ortner for smeared nuclear charges to the case of point nuclei represented by Dirac measures. We finally illustrate the performance of the proposed selection method for RVEs compared to the standard RVE approach by calculating the energy per atom of random AlTi lattices on RVEs of different size.