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Examination of nanoparticle dispersion using a novel GPU based radial distribution function code . THOMAS ROSCH, National Institute of Standards and Technology, MATTHEW WADE, Case Western Reserve University, FREDERICK PHELAN, National Institute of Standards and Technology — We have developed a novel GPU-based code that rapidly calculates radial distribution function (RDF) for an entire system, with no cutoff, ensuring accuracy. Built on top of this code, we have developed tools to calculate the second virial coefficient (B_2) and the structure factor from the RDF, two properties that are directly related to the dispersion of nanoparticles in nancomposite systems. We validate the RDF calculations by comparison with previously published results, and also show how our code, which takes into account bonding in polymeric systems, enables more accurate predictions of g(r) than current state of the art GPU-based RDF codes currently available for these systems. In addition, our code reduces the computational time by approximately an order of magnitude compared to CPU-based calculations. We demonstrate the application of our toolset by the examination of a coarse-grained nanocomposite system and show how different surface energies between particle and polymer lead to different dispersion states, and effect properties such as viscosity, yield strength, elasticity, and thermal conductivity.

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