Configurationally resolved methods at elevated temperatures

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Over the past decades, atomistic simulations have become a viable and useful tool in materials design. A variety of different computational approaches exists, though they commonly determine the properties of some material as a function of the atomic coordinates of its components. However, even at a fixed composition, there are many inequivalent ways to distribute different atomic species on a given lattice. A priori, it is often unknown which configuration is realized in thermodynamic equilibrium. This gives rise to so-called computationally exhaustive methods, which directly solve this problem by considering all possible atomic configurations simultaneously, filtering for the thermodynamic groundstates among them. I will outline some of the commonly used methods and talk about selected applications in the design of Ni-rich superalloys, the theory of shape memory alloys at finite temperatures and the computation of intermetallic phase diagrams.