

Peter Piper Picked a Problem Trickier than most. Can Computer Science Solve the Problem Peter Piper Picked?

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Modern materials of scientific and technological interest are notoriously complex. This is exemplified by efforts to control the atomic organization of materials on the nanoscale to give them directed functionality. Clearly it is necessary to be able to characterize the structure of these materials. This is a difficult problem. In a crystal there is a good match between the information required to solve the problem (atomic positions, symmetry and unit cell metrics) and the information in the data (Bragg peak positions and intensities). We are all aware of the power of crystallography. In a nanostructured material the peaks broaden and become overlapped resulting in diffuse scattering which contains much less information. On the other hand the number of degrees of freedom needed to specify the model increases (in principle of order the number of atoms in the nanoparticle). This is the pesky problem Peter Piper picked.

In this talk I will illustrate the problem and discuss some efforts we are taking to overcome these difficulties. I will describe some developments inspired by computer science that could be brought to bear on problems like this. We are not currently able to answer the question posed in the title, but even thinking about it is proving to be a lot of fun.

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