Discovering complete pressure-temperature phase diagrams with Hamiltonian Monte Carlo nested sampling ROBERT BALDOCK, University of Cambridge, NOAM BERNSTEIN, Naval Research Laboratory, LIVIA BARTÓK-PARTÁY, GÁBOR CSÁNYI, University of Cambridge — Nested sampling is a Monte Carlo algorithm that can be used to efficiently calculate the complete configurational density of states in a material that undergoes multiple first-order phase transitions. From the density of states one can calculate the partition function as an explicit function of temperature and perform statistical mechanics from first principles. Indeed, we have shown how nested sampling can be used to automatically discover complete pressure-temperature phase diagrams with no prior knowledge of the locations of phase transitions or the structures of phases. In this talk I will present a new version of the nested sampling algorithm, based on a modified Hamiltonian ("Hybrid") Monte Carlo scheme. This new scheme reduces the scaling of a general nested sampling calculation. In particular the new algorithm expedites the sampling of atomic configuration spaces in condensed phases, and permits one to perform nested sampling calculations at a fraction of the cost required by ordinary nested sampling with standard Monte Carlo.

Robert Baldock
University of Cambridge

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