Nested sampling for high-throughput computational thermodynamics

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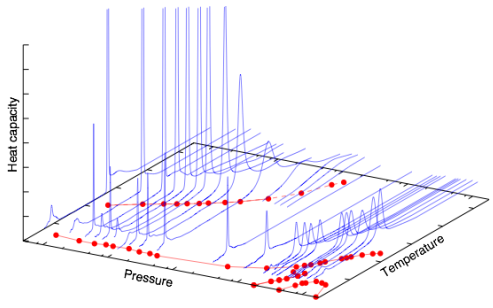
In recent years we have been working on adapting a novel computational sampling technique, called nested sampling, to study the potential energy surface of atomistic systems [1]. Nested sampling automatically generates all the relevant atomic configurations, unhindered by high barriers, and one of its most appealing advantages is that the global partition function can be calculated very easily as a simple post-processing step, thus thermodynamic properties become accessible. Nested sampling explores the potential energy surface starting from the high energy region, hence no prior knowledge of the potentially stable structures is needed. This means that unlike other methods, nested sampling may be fully automated, allowing high-throughput calculations of phase transformations and phase diagrams of different materials [2,3,4].

[1] L. B. Pártay, A. P. Bartók, and G. Csányi, J. Phys. Chem. B **114**, 10502 (2010)
[2] R. J. N. Baldock, L. B. Pártay, A. P. Bart´ok, M. C. Payne, and G. Csányi, Phys. Rev. B **93**, 174108 (2016)
[3] R. J. N. Baldock, N. Bernstein, K. M. Salerno, L. B. Pártay, and G. Csányi, Phys. Rev. E **96**, 043311 (2017)



[4] L. B. Pártay, Comp. Mat. Sci. **149**, 153 (2018).

Figure 1 : Calculating the phase diagram with Nested Sampling: calculations can be performed at a series of pressures, and phase transitions are located by peaks of the heat capacity curves (blue). Red lines show the evaporation, melting and solid-solid transition lines.