Calculating pressure-temperature phase diagrams of materials

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We extend the Nested Sampling algorithm to simulate materials under periodic boundary and constant pressure conditions, and show how it can be efficiently used to determine the phase diagram directly from the potential energy in a highly automated fashion. The only inputs required are the composition and the desired pressure and temperature ranges, in particular solid-solid phase transitions are recovered without any a priori knowledge about the structure of solid phases. We apply the algorithm to the Lennard-Jones system, aluminium, and the NiTi shape memory alloy.