

## Continuation and deflation methodologies in atomistic modelling

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High-throughput molecular and atomistic simulations depend on advanced optimisation tools to efficiently explore highly non-convex energy landscapes. Numerical continuation and deflation techniques—well-established in other nonlinear contexts [1],[2]—remain largely underused in atomistic and molecular modelling. A recent white paper [3] identified their broader adoption at particle and atomistic scales as one of the key opportunities. This talk will introduce these methodologies in the context of atomistic modelling, review their previous applications, highlight their potential, and present early results from new, tailored implementations. The aim is to set the stage for subsequent talks in the programme exploring this emerging theme.

### References

- [1] E Allgower and K Georg. Numerical continuation methods: an introduction. Vol. 13. Springer Science & Business Media, 2012.
- [2] P Farrell, A Birkisson, and S Funke. Deflation techniques for finding distinct solutions of nonlinear partial differential equations. *SIAM Journal on Scientific Computing* 37.4 (2015), A2026–A2045.
- [3] Bagchi et al. *New Mathematics for the Exascale: Applications to Materials Science*. Tech. rep. Institute for Pure and Applied Mathematics, UCLA, 2023.