

Software for Exploring and Visualising Landscapes

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- **GMIN**: [basin-hopping](#) global optimisation and global [thermodynamics](#).
- **OPTIM**: geometry optimisation, including a wide variety of minimisation schemes and [transition state](#) algorithms. Multi-step pathways exploit the Dijkstra [missing connection](#) algorithm (*J. Chem. Phys.*, **122**, 234903, 2005).
- **PATHSAMPLE**: discrete path sampling refinement of kinetic transition [networks](#). Recursive [regrouping](#) (lumping) based on free energy barriers. Extraction of [committor](#) probabilities and overall [rate constants](#).
- **disconnectionDPS** and **manipulate**: creation and transformation of potential and free energy [disconnectivity graphs](#) from **PATHSAMPLE** output files.

Current [svn](#) tarball image: <http://www-wales.ch.cam.ac.uk>. Direct access to the svn source tree can be arranged for [developers](#).