



On parallelization of structure optimization via “local heat pulse” - quench cycles



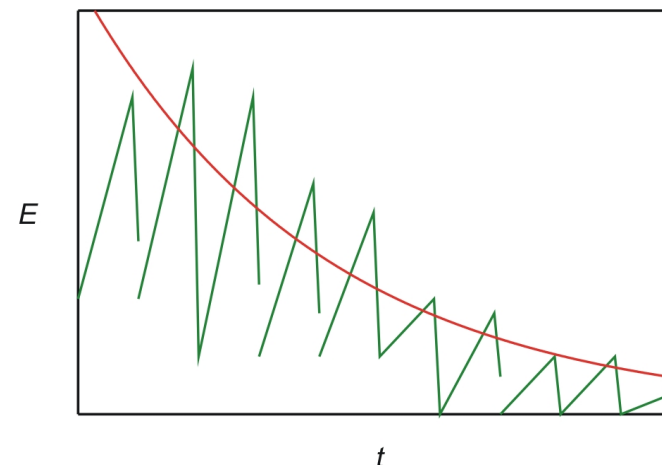
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Aim of algorithm: modify simulated annealing
making use of current altitude above ground.

Realization: **cyclically heating and quenching**
with decreasing amplitude instead of slowly
cooling down, **starting from lowest state** found.

Additional feature: **Parallel search** treating set of local minima



Examination problem:

Periodic structure of $\text{Mg}_{10}\text{Al}_4\text{Ge}_2\text{Si}_4\text{O}_{18}$, where energy landscape is defined by Coulomb, Buckingham and three-body potentials

Local search:

General Utility Lattice Program (GULP), v. 3.4

Parallelization strategies:

- (a) Simple distribution of effort to independent runs,
- (b) consideration of ensemble,
- (c) mixed

