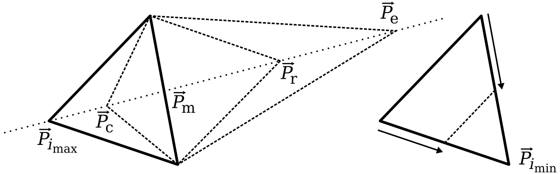
Local search

- Minimizing $f(X)$ which involves masses, radii, etc. calculated at the "HF(B)" level
  - ➡ Reuse fields from last iteration for speedup
  - ✘ Not a function : $E(X)$ depends (slightly) on last iterations
  - ✘ Numerical accuracy of a complicated self-consistent calculation ?
- Efficient gradient calculation ?
- Nelder-Mead ("Simplex") algorithm



If $f(X_{\mathrm{new}}) < f(X_{\mathrm{high}})$ keep X_{new}

- Local minima ? $\Rightarrow$ A Metropolis variant [1] : pick ε distributed $\propto \exp(-\varepsilon/T)$;
  If $f(X_{\mathrm{new}}) < f(X_{\mathrm{high}}) + \varepsilon$ keep X_{new} ; decrease T

➡ $T = 0$: Standard NM ; $T > 0$ explore uphill

✔ Avoids getting stuck in shallow local minima close to the best one

[1] www.nrbook.com/a/, Ch. 10.9

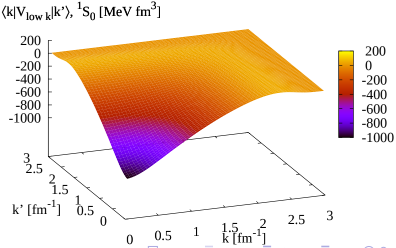
Global search

- Find absolute minimum of $f(X)$ in a domain of the parameter space
  - ➡ Simulated Annealing
  - ➡ Genetic Algorithms
- Simplex Coding Genetic Algorithm [2]
  1. Initialize a population of N simplexes
  2. Iterate (NM) each one
  3. Generate new population by crossover + mutations, iterate it
  4. Merge the populations (keep N best simplexes)
  5. Iterate each remaining simplex
  6. Loop to (3) until best simplex converges
- Probability of finding absolute minimum $\rightarrow 1$ as you increase N

✔ Scalable in N

✘ Computationally involved (HF(B)) functions $f(X)$ in large parameter spaces, large N : SMP/MMP...

➡ Fortran 95/MPI implementation : "fitpack" (V. Rotival, T.L.). First applications : building operator representations of $V_{\mathrm{low\ k}}$



[2] A. Hedar and M. Fukushima, *Optim. Meth. Soft.* **18** (2003) 265-282, `http://hedar.info/HedarFiles/SCGA.pdf`