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Set 08 - Parallel Tempering

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Question 1: Parallel Tempering

During last exercise, we used the Markov Chain Monte Carlo (MCMC) algorithm in an optimization setup. This algorithm is inherently sequential. In order to parallelize it, we can either parallelize the energy evaluation, which is not always easy, or take another approach: parallel tempering.

Parallel tempering consists in M systems with their own chains $\{x_k^i\}_{i=1}^M$ evolving at fixed temperatures $T_1 < T_2 < \cdots < T_M$. The high temperature chains lead to higher exploration ability while the low temperature chains aim to more accurate results. At each iteration, two chains i and j exchange their states with probability

$$p_{i,j} = \min\left[1, \exp\left\{(E_i - E_j)(\frac{1}{T_i} - \frac{1}{T_j})\right\}\right],$$

where E_i is the current energy in the system i. For simplicity, we only consider exchanges between neighboring systems $|i-j| = 1$. Furthermore, we consider exactly one swap at a given step.

The exchange selection is done as follow:

- compute weights $w_i = p_{i,i+1}$, $i = 1, 2, \ldots, M-1$
- compute exclusive prefix sum $s_i = \sum_{j=1}^{i-1} w_j$
- draw a uniform random variable $u \sim U(0, s_M)$
- find i such that $s_i \leq u < s_{i+1}$
- exchange i and $i+1$

In this exercise, we want to fit model parameters to given data $\{x_i, y_i\}_{i=1}^N$ (see `data.txt`). We consider the specific model $f(x) = A\sin(\omega x)$.

a) Formulate the problem as an optimization problem for A and ω using a simulated annealing approach.

b) We provide you a skeleton code `serial.cpp`. Implement the exchange procedure. Run the code with $M = 128$ chains and $N = 10000$ steps. What parameters do you obtain?

c) Parallelize the serial code using `MPI`. Each rank should take care of several chains. Verify the results.

d) Report the strong scaling for up to 12 processes with 1000 chains for 10000 iterations.