Monte Carlo methods as a means of scalability

Monte Carlo (MC) methods are a general class of computer algorithms that simulate a probability distribution for a system. A “random walker” generates a Markov chain of states in a phase space by performing a “random walk” stochastically with the use of pseudo-random number sequences.

In practice, a random walker is mapped to a computational thread. This enables Monte Carlo methods to provide a natural way of massive parallelism by increasing the number of random walkers working concurrently. This applies to the two distinct main branches of Monte Carlo approaches: (i) classical MC for the study of finite temperature properties through statistical mechanics; and (ii) quantum Monte Carlo (QMC) as an ab initio method for the study of electronic properties by solving the Schrödinger equation.

In the following, I demonstrate the feasibility of achieving improved strong and weak scaling by new algorithm designs and renovations, with an example in classical MC. I also discuss a few scalability challenges that I envision in future high performance computers.

Replica-exchange Wang-Landau sampling

Wang-Landau (WL) sampling\(^{[3]}\) is a classical Monte Carlo method that simulates the density of states, \( g(E) \), where \( E \) is the total energy of a system. The partition function is given by:

\[
Z(\beta) = \sum_{E} e^{-\beta H(E)} = \int g(E) e^{-\beta E} dE
\]

from which thermodynamic properties can be calculated. WL sampling was originally designed as a serial algorithm:

- Initialize: \( \beta(H_0) = 0, g(E_0) = \frac{1}{E_0} \)

2. Generate a trial configuration, accept with probability:

\[
p(E_{\text{new}} \rightarrow E_{\text{old}}) = \min\{\frac{g(E_{\text{new}})}{g(E_{\text{old}})}, 1\} E_{\text{new}} \rightarrow E_{\text{old}}, \text{ if accepted} \]

\[
E_{\text{new}} \rightarrow E_{\text{old}}, \text{ otherwise}
\]

3. Update \( g(E) \rightarrow g(E) \times f(E), H(E) \rightarrow H(E) + 1 \)

4. Repeat steps 2-3 until the histogram is “flat”: reset \( H(E) = 0, g(E) = \frac{1}{E} \)

To achieve greater fidelity of the Monte Carlo results and to enable the sampling of larger phase spaces, a more efficient and highly scalable parallel scheme, replica-exchange Wang-Landau (REWL)\(^{[2]}\) sampling, is recently developed:

\[
g(E) \rightarrow g(E) \times f(E)
\]

Acceptance probability:

\[
P(\text{X} \rightarrow \text{Y}) = \min\{\frac{g(\text{Y})}{g(\text{X})}, 1\} \frac{g(\text{Y})}{g(\text{X})} E_{\text{Y}} \rightarrow E_{\text{X}}, \text{ if accepted} \]

\[
E_{\text{Y}} \rightarrow E_{\text{X}}, \text{ otherwise}
\]

1. Splitting of entire energy range into smaller, overlapping windows

2. Ordinary Wang-Landau procedure within a window

3. Each walker updates its own density of states and histogram

4. Replica-exchange between neighboring windows at intervals to ensure ergodicity

REWL has demonstrated excellent strong and weak scaling. Superlinear speed-up is observed compared to serial, single walker WL sampling.

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