Improved Wang-Landau algorithm for the joint density of states of continuous models

Chenggang Zhou[1,2], T. C. Schulthess[1]
D. P. Landau[2]
[1] Computer Science and Mathematics Division, ORNL
[2] Center for Simulational Physics, UGA

The discrete WL algorithm

- F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
- Density of states $g(E_i)$: Number of microscopic states (configurations) at energy E_i , $i = 1,2,\ldots, N$
- Estimated density of states (histogram): $g'(E_i)$.
- The Random walker is guided by $P(E_i) \propto \dfrac{g(E_i)}{g'(E_i)}$
- Update $g'(E_i)$ by $f \cdot g'(E_i)$ "**once in a while**".
- **Convergence**: $g'(E_i) \to g(E_i) + O(\sqrt{\ln f})$ for arbitrary initial estimation.
- Then reduce the modification factor f to improve the accuracy

Continuous models and joint density of states

- Microscopic degrees of freedom: $\{s_1, s_2, \ldots s_N\}$
- Macroscopic observables: $O(s_1, s_2, \ldots, s_N)$
- For example, Heisenberg model of ferromagnet

$$H = -J \sum_{<i,j>} \mathbf{s}_i \cdot \mathbf{s}_j, \; M = \sum_i S_i^z \quad \text{or} \quad M = \left| \sum_i \mathbf{s}_i \right|$$

- Joint density of states:

$$\rho(M, E) = \int \delta\left(E - N^{-1} H(s)\right) \delta\left(M - N^{-1} M(s)\right) \prod_i ds_i$$

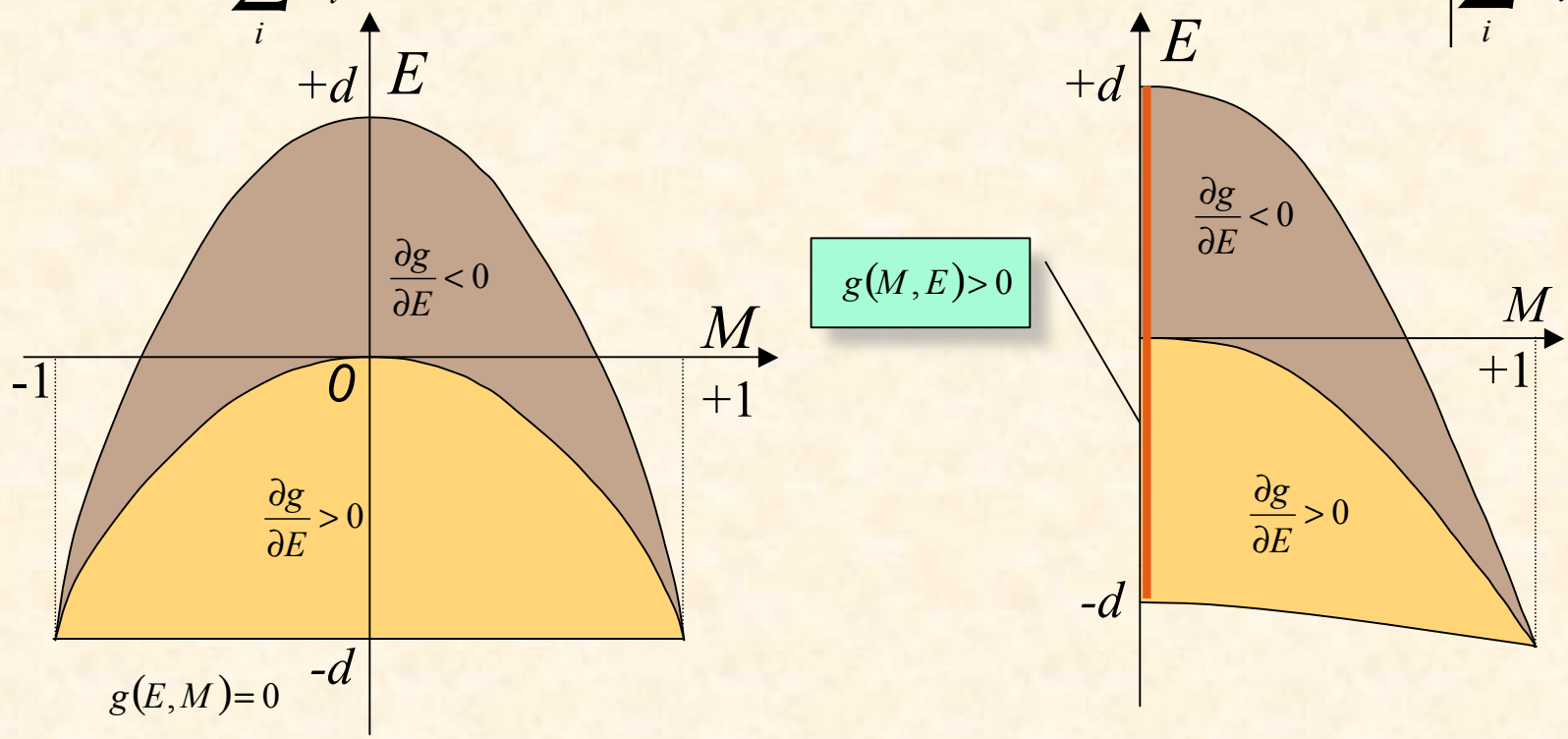
- (M, E) defines the macroscopic state

Support of joint density of states

$$Z = \int \rho(M,E) e^{-\beta(E-hM)N} dM dE$$

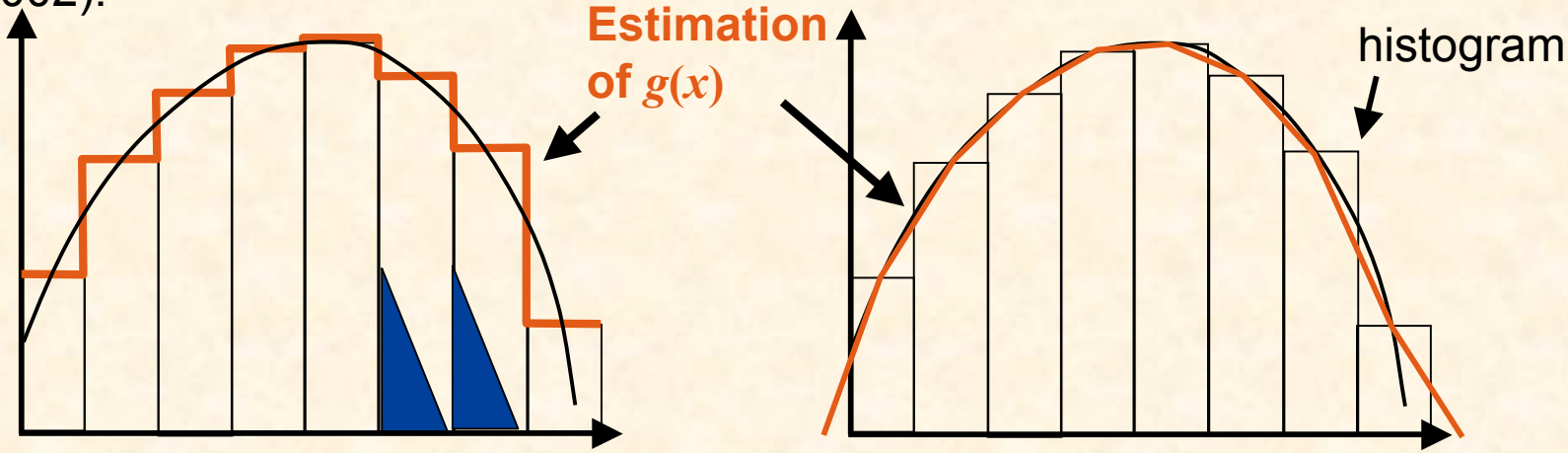
$$M = N^{-1} \sum_i S_i^z$$

$$M = N^{-1} \left| \sum_i \mathbf{S}_i \right|$$



Numerical representation of continuous density of states

- **Binning**
- **Binning + interpolation** M. S. Shell et. al. Phys. Rev. E 66,056703 (2002).



- **Kernel Density Estimation** Y. D. Wu J. Chem. Phys. 121, 1193 (2004).

$$g(x) = \sum_i f\left((x - x_i)/\sigma\right)$$

x_i: independent samples

$f(\ldots)$: kernel function, localized and smooth

Local update with kernel density estimation (KDE)

- **Let** $x = (M, E),\ w(x) = \log_\alpha \rho'(x)$

  $w(x) \rightarrow w(x) + \delta \cdot f((x - x_i)/\sigma)$

- **Kernel function:** Gaussian kernel: $f(x) = \exp(-x^2)$

  Epanechnikov kernel: $f(x) = [1 - x^2]_+$

- **Random walk acceptance ratio:**

$$A_{i \rightarrow f} = \min\{1,\ \exp[\alpha(w(x_f) - w(x_i))]\}$$

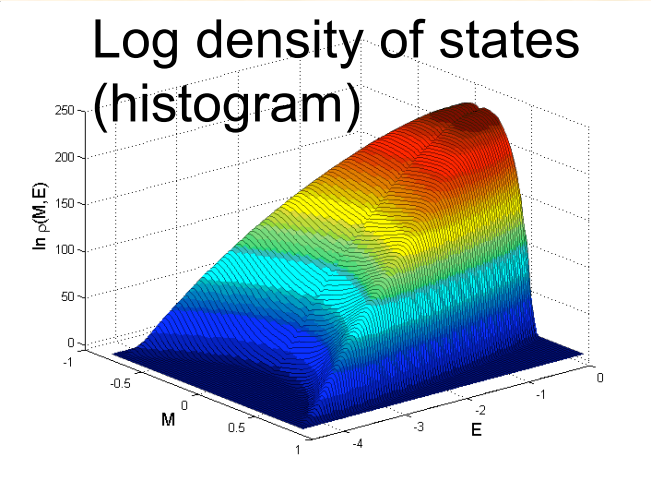
- **Accumulation:** $w_t(x) = [\log_\alpha \rho(x) + C(t) + O(\sqrt{\ln \delta})]_+$

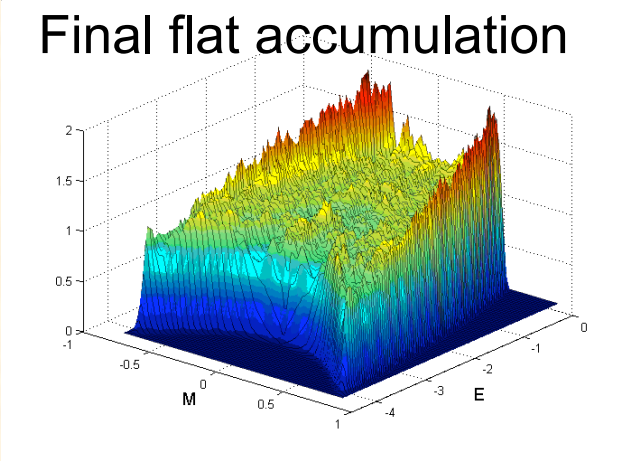
Difficulties in the simulation

- **Efficiency decreases due to the flat accumulation in the visited area.**

$$N \propto \int \log_{\alpha} g(M,E)\,dM\,dE$$

- **Continuous models usually has zero density of states on the boundary, leading to logarithmic divergence in $w(x)$**



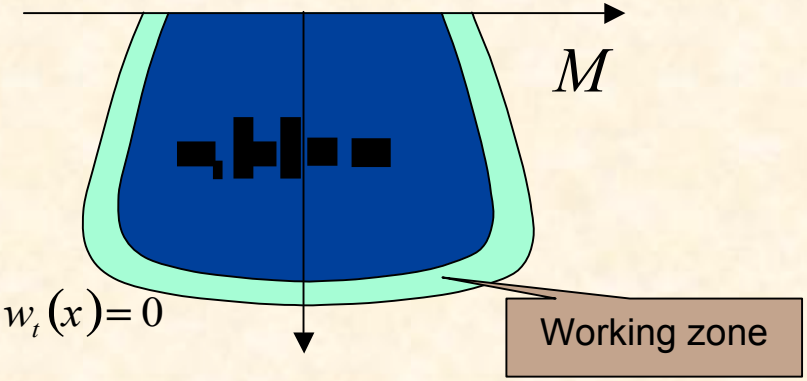


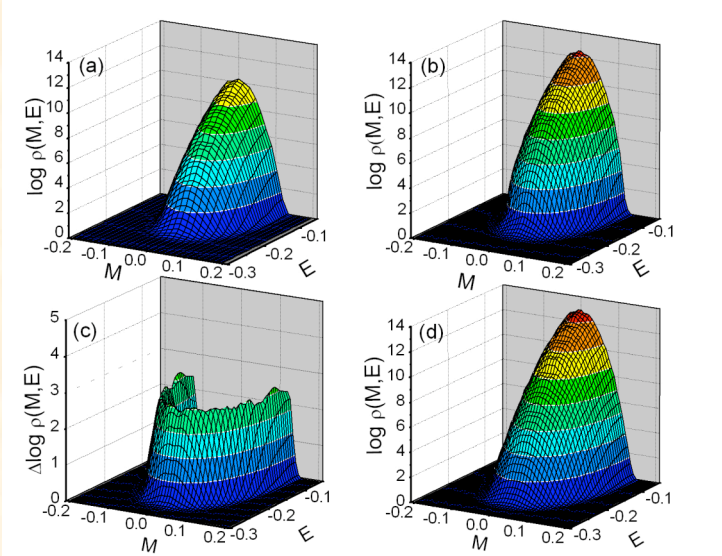
Global updates for efficiency

- **Add a constant shift to the interior of the known density of states**

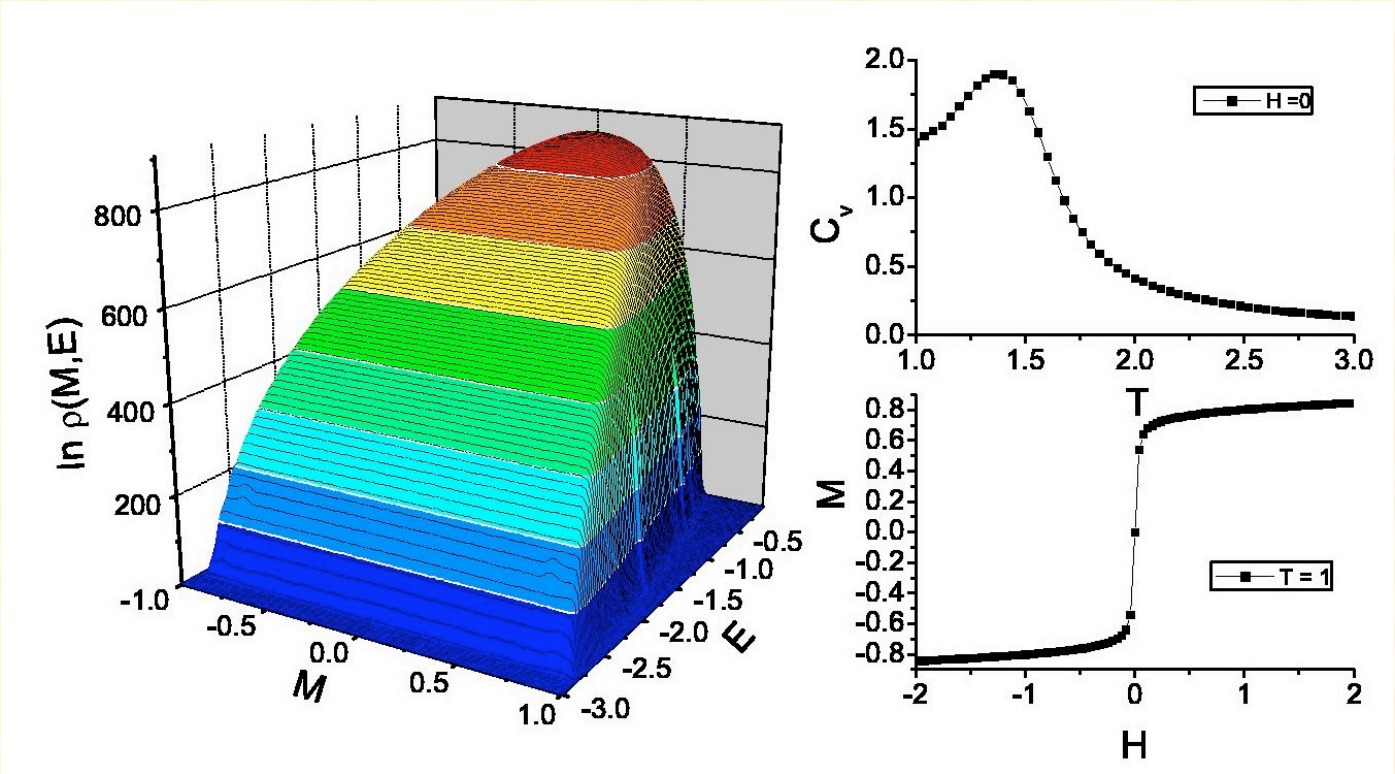
$$w_t(x) \rightarrow w_t(x) + \kappa \exp\left[\frac{-\lambda}{w_t(x) - \varpi}\right]\Theta\left(w_t(x) - \varpi\right)$$

- **Random walker is driven to the boundary.**





Heisenberg ferromagnet



- L = 5, 3D Heisenberg ferromagnet
- Density of states flat in M at low energies due to the rotational symmetry.
- Scaling to larger size: $\ln g_L(x) \approx \left(\frac{L}{L'}\right)^d \ln g_{L'}(x)$

Conclusions

- **Initial accumulation stage**
  - **Local updates that preserve the continuity of the model.**
  - **Global updates to save CPU time and increase the efficiency.**
- **Refining stage**
  - **Reduce the amplitude of the kernel function (modification factor) to increase the accuracy.**
- **Measure the observables by numerical integration.**

This research is sponsored by the Office of Basic Energy Science, U.S. Department of Energy. The Oak Ridge National Laboratory is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725.