A score-based small atomic model with application to stress calculation

Author1[a], Author2[b]

[a]*School of Mathematics and Statistics, Wuhan University, Wuhan, 430072, China*
[b]*Hubei Key Laboratory of Computational Science, Wuhan, 430072, China*

1. Problem setting

Consider a region Ω of N atoms, we divide the system into two subregions (see Figure 1). The inner system Ω_I with atoms position X, refers to the region of interest, and the surrounding region Ω_{II} with atoms position Y, can be regarded as an elastic medium surrounding the defects.

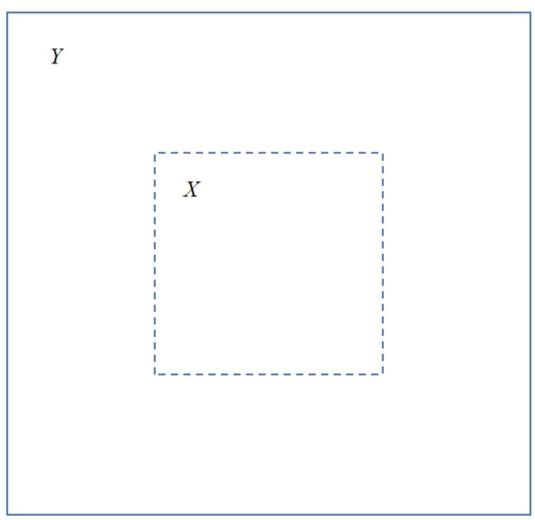

Figure 1: A region consists of inner atomic system X and outer atomic system Y.

Email addresses: A@whu.edu.cn (Author1), B@whu.edu.cn (Author2)

In principle, we could simulate the full atomic system $X \cup Y$ according to some ensemble distribution $\rho(X, Y)$, then calculate the macroscopic physical quantities A of interests using the inner atoms information X:

$$A = \int A(X)\rho(X, Y)dXdY. \tag{1}$$

Notice that we only concern the quantities inside Ω_I, the macroscopic quantity A depends only on inner atoms information X, while the simulation of outer atoms Y serves as a boundary condition of X.

When the freedom N is very large, a full simulation of $X \cup Y$ becomes expensive and we would just equip X with some artificial boundary conditions to approximate the effect of the large surrounding system Ω_{II}. In this article, we would propose a score-based small atomic model (SB-SAM) to learn some effective distribution $\rho_e(X)$, with which we have:

$$\int A(X)\rho_e(X)dX = \int A(X)\rho(X, Y)dXdY. \tag{2}$$

With such an effective distribution, we need only simulate the inner atoms X, which yields a statistical average equivalent to that of the entire system

2. Method: a score-based small atomic model

From equations (2), we know the exact formulation of ρ_e can be defined as the marginal distribution of ρ:

$$\rho_e^*(X) \triangleq \int \rho(X, Y)dY. \tag{3}$$

This indicates that we can first simulate the full system $X \cup Y$ to obtain samples $\{X_i, Y_i\}_{i=1}^n$, of which $(X_i, Y_i) \sim \rho(X, Y)$, then drop $\{Y_i\}_{i=1}^n$ to get samples $\{X_i\}_{i=1}^n$ distributed according to $\rho_e^*(X)$. Next, using the score matching techniques widely used int the generative learning, a score network $S(X, \theta)$ can be learned to approximate ρ_e as follows:

$$\begin{aligned}
\theta^* &= \arg\min_\theta \mathbb{E}_{X\sim\rho_e^*}\|S(X, \theta) - \nabla log\rho_e^*(X)\|_2^2, \\
&= \arg\min_\theta \mathbb{E}_{X\sim\rho_e^*}[\|S(X, \theta)\|_2^2 + 2\nabla \cdot S(X, \theta)]^2.
\end{aligned} \tag{4}$$

It should be pointed out that, DSM, SSM and diffusion progress can also be used here to improve the learning efficiency of $S(X,\theta)$. Furthermore, $S(X,\theta)$ can be used to generate samples by some classical sampling methods, like annealed Langevin Monte Carlo method.

In general, the distribution $\rho(X,Y)$ is defined to describe various ensembles under different constraints. For a canonical ensemble at temperature T, under deformation F, the ensemble distribution is written as

$$\rho(X,Y|F,T) = \frac{1}{\tilde{Z}} exp[-\beta\tilde{V}(X,Y;F)], \tag{5}$$

where $\beta = \frac{1}{k_B T}$, $\tilde{V}$ is some multi-body potential and $\tilde{Z}$ is the partition function. To ensure our score function $S(X,\theta)$ adapted to different F and T, we could further extend the score learning in (4) to the conditional generative learning. Since the joint distribution of (X,F,T) can be written as

$$\rho^*(X,F,T) \propto \rho(X|F,T)\rho(F,T), \tag{6}$$

Now we first generate samples $\{F_i,T_i\}_{i=1}^n$ according to some uniform distribution, with the size of density support being $N_{F,T}$. Then we draw $\{X_i,Y_i\}_{i=1}^n$ at different temperature T_i and deformation F_i according to (5). By keeping the $\{X_i,F_i,T_i\}_{i=1}^n$, we can learn the score for $\rho^*(X,F,T)$ as

$$\begin{aligned}\theta^* &= \arg\min_\theta \mathbb{E}_{(X,F,T)\sim\rho^*(X,F,T)}\|S(X,F,T,\theta) - \nabla log\rho_e^*(X,F,T)\|_2^2, \\ &= \arg\min_\theta \mathbb{E}_{(X,F,T)\sim\rho^*(X,F,T)}[\|S(X,F,T,\theta)\|_2^2 + 2\nabla\cdot S(X,F,T,\theta)]^2. \end{aligned} \tag{7}$$

Once we have learned the score $S(X,F,T,\theta^*)$ for the approximation of $\nabla log\rho_e^*(X,F,T)$, the score of conditional distribution $\rho(X|F,T)$ can be calculated by (6) as:

$$S(X|F,T,\theta) = S(X,F,T,\theta^*)\cdot \mathbf{e}_X, \tag{8}$$

in which $\mathbf{e}_X$ is a vector with first Nd elements being 1 and the rest elements are set to be zero.

3. Application to stress calculation

In this section, we shall apply SB-SAM to the calculation of the first Piola-Kirchoff stress.

Appendix A. Example Appendix Section

Appendix text.

Example citation, See [1].

References

[1] Leslie Lamport, *LaTeX: a document preparation system*, Addison Wesley, Massachusetts, 2nd edition, 1994.