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Using piecewise polynomials for faster potential function evaluation

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ABSTRACT

In many molecular dynamics simulation software packages and hardware implementations, piecewise polynomials are used to represent and compute pairwise potential functions efficiently. In this paper, we present three modifications applicable to most interpolations to increase their accuracy. The increased accuracy reduces the amount of data that needs to be stored for each interaction potential, making such interpolations more suitable for architectures with limited memory and/or cache or hardware implementations.

1. Introduction

In most molecular dynamics or Monte-Carlo simulations, the most expensive part of each time step is the evaluation of the non-bonded pairwise interactions [1–3]. Given a pair of particles p_i and p_j of the species A and B respectively, the *interaction energy*

$$e_{ij} = v_{AB}(r_{ij})$$

is computed from the *interaction potential* v_{AB} specific to the particle species A and B and the inter-particle distance r_{ij}. The resulting *interaction force* on the particles p_i and p_j is the gradient of the potential with respect to the particle coordinates

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Algorithm 1. Naive interaction of two particles p_i and p_j of species A and B respectively

$\mathbf{r}_{ij} \leftarrow \mathbf{x}_i - \mathbf{x}_j$ (*compute the inter-particle vector*)
$r_{ij} \leftarrow \|\mathbf{r}_{ij}\|_2$ (*compute the inter-particle distance*)
$\mathbf{f}_{ij} \leftarrow \mathbf{0}, e_{ij} \leftarrow 0$ (*initialize the force and energy*)
if AB interact with a Lennard–Jones 12-6 potential **then**
  $e_{ij} \leftarrow e_{ij} + 4\varepsilon_{AB}\left[\left(\frac{\sigma_{AB}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{AB}}{r_{ij}}\right)^{6}\right]$
  $\mathbf{f}_{ij} \leftarrow \mathbf{f}_{ij} + \mathbf{r}_{ij}\frac{24\varepsilon_{AB}}{\sigma_{AB}^2}\left[-2\left(\frac{\sigma_{AB}}{r_{ij}}\right)^{14} + \left(\frac{\sigma_{AB}}{r_{ij}}\right)^{8}\right]$
else if AB interact with a Morse potential **then**
  $e_{ij} \leftarrow e_{ij} + D_{AB}\left[1 - \exp\left(-\sqrt{k_{AB}/2D_{AB}}(r_{ij} - r_{AB})\right)\right]^2 + e_{AB}$
  $\mathbf{f}_{ij} \leftarrow \mathbf{f}_{ij} + \frac{\mathbf{r}_{ij}}{r_{ij}}\frac{\partial}{\partial r_{ij}} D_{AB}\left[1 - \exp\left(-\sqrt{k_{AB}/2D_{AB}}(r_{ij} - r_{AB})\right)\right]^2$
else if AB interact with a ... potential **then**
  $e_{ij} \leftarrow e_{ij} + \ldots$
  $\mathbf{f}_{ij} \leftarrow \mathbf{f}_{ij} + \ldots$
end if
if AB interact with a Coulomb potential **then**
  $e_{ij} \leftarrow e_{ij} + \frac{q_1 q_2}{r_{ij}}$
  $\mathbf{f}_{ij} \leftarrow \mathbf{f}_{ij} + \mathbf{r}_{ij}\frac{q_1 q_2}{r_{ij}^3}$
else if AB interact with an Ewald potential **then**
  $e_{ij} \leftarrow e_{ij} + \frac{q_1 q_2}{r_{ij}}\mathrm{erfc}(\kappa r_{ij})$
  $\mathbf{f}_{ij} \leftarrow \mathbf{f}_{ij} - \mathbf{r}_{ij}\frac{q_1 q_2}{r_{ij}^3}\left[\mathrm{erfc}(\kappa r_{ij}) - \frac{2\kappa r_{ij}}{\sqrt{\pi}}\exp(-\kappa^2 r_{ij}^2)\right]$
else if AB interact with a ... potential **then**
  $e_{ij} \leftarrow e_{ij} + \ldots$
  $\mathbf{f}_{ij} \leftarrow \mathbf{f}_{ij} + \ldots$
end if

$$\mathbf{f}_{ij} = -\nabla_{\mathbf{x}_i} v_{AB}(r_{ij}) = \nabla_{\mathbf{x}_j} v_{AB}(r_{ij}).$$

The computation of the pairwise energy and force can be implemented naively as shown in Algorithm 1. This naive computation has some obvious drawbacks:

(i) the relatively expensive evaluation of arithmetic operations such as $\sqrt{\cdot}$ or $(\cdot)^{-1}$, e.g. when computing the inter-particle distance r_{ij} or within the potentials themselves,
(ii) the relatively expensive evaluation of transcendental functions such as $\mathrm{erfc}(\cdot)$ or $\exp(\cdot)$ in the computation of the more complicated potentials,
(iii) the cascading conditional statements (**if-then-else** statements) can cause stalls on processors with long instruction pipelines or no branch prediction[1] and make exploiting SIMD parallelism more difficult,
(iv) the size of the interaction computation can cause problems on computers with small instruction caches or on hardware implementations where die surface and complexity are critical.

Problem (iii) can, in some cases, be avoided by implementing a separate interaction loop for each interaction type. This would, however, require the list of interacting particle pairs to be traversed more than once. This inefficiency can easily offset whatever advantage was obtained by avoiding conditional branches in the first place.

It is for these and other[2] reasons that several authors have opted to compute not the exact potentials, as is done in Algorithm 1, but to compute, store and evaluate an approximation of the potential function:

$$g_{AB}(r_{ij}) \approx v_{AB}(r_{ij})$$

The approximation $g_{AB}(r_{ij})$ is usually a function of r_{ij}^2 to avoid evaluating the $\sqrt{\cdot}$ to compute r_{ij}:

$$g_{AB}(r_{ij}^2) \approx v_{AB}(r_{ij}).$$

The approximated potential is then usually represented as a set of n piece-wise polynomials between a set of nodes $x_i,\ i = 0 \ldots n$:

[1] IBM's Cell Broadband Engine [4], for example, has no dynamic branch prediction capabilities, incurring a penalty of 18–19 cycles for each mis-predicted branch.
[2] GROMACS, for example, uses an interpolated potential only for tabulated user-supplied potentials.