Optimization of the AIREBO Many-Body Potential for KNL

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Introduction

The AIREBO [1] potential provides forces and energies for molecular dynamics (MD) simulations of carbon and carbohydrate structures. As opposed to more classical approaches, it also captures the bonding behaviour and allows bonds to break and appear. We develop an optimized AIREBO implementation for Intel's Xeon and Xeon Phi (co)processors [2] and integrate it into the open-source LAMMPS [3] molecular dynamics code. AIREBO consists of short and longer-ranged contributions that both depend on the bond-order.

Short-Ranged Contributions

$$E_{REBO} = \sum_{i,j} V_{ij}^R(r_{ij}) + b_{ij} V_{ij}^A(r_{ij}).$$

$$E_{TORSION} = \sum_{i,j,k,l} V_{kijl}^{tors}(\omega_{kijl}).$$

Bond-Order Calculation

$$b_{ij} = \tfrac{1}{2}[p_{ij}^{\sigma\pi} + p_{ji}^{\sigma\pi}] + \pi_{ij}^{rc}(N_{ij}, N_{ji}, N_{ij}^{conj}) + \pi_{ij}^{dh}$$

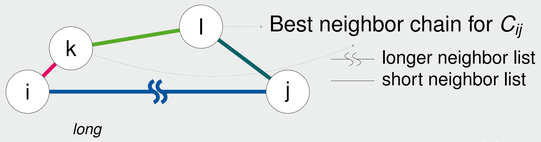
$$p_{ij}^{\sigma\pi} = \left[1 + \sum_k V_{jik}^{\sigma\pi}(r_{ij}, r_{ik}, \theta_{kij}) + P_{ij}(N_{ij}^C, N_{ij}^H)\right]^{-1/2}$$

$$\pi_{ij}^{dh} = T_{ij}(N_{ij}, N_{ji}, N_{ij}^{conj}) \sum_{k,l} V_{kijl}^{\omega}(r_{ik}, r_{jl}, \omega_{kijl})$$

$N_{\alpha\beta}$ = No. neighbors of α besides β

$$N_{ij}^{conj} = 1 + \left[\sum_k f(r_{ik}, N_{ki})\right]^2 + \left[\sum_l f(r_{jl}, N_{lj})\right]^2$$

Longer-Ranged Contributions

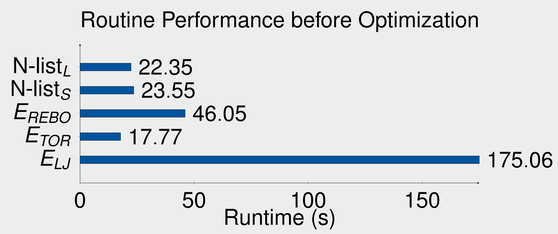


$$E_{LJ} = \sum_{i,j}^{long} (S(t_r(\mathbf{r_{ij}}))S(t_b(b_{ij}^*)) + (1 - S(t_r(\mathbf{r_{ij}})))C_{ij} V_{ij}^{LJ}(\mathbf{r_{ij}}).$$

$$C_{ij} = 1 - \max_{k,l}\{w_{ik}(\mathbf{r_{ik}})w_{kl}(\mathbf{r_{kl}})w_{lj}(\mathbf{r_{lj}})\}$$

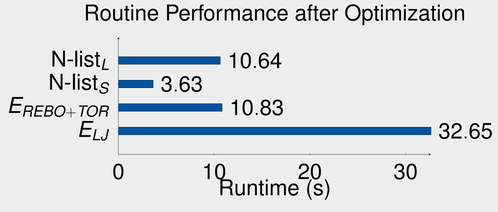
Optimization Challenges

- Need 2 neighbor lists: Short-ranged & longer-ranged.
- Due to the short-ranged nature of E_{REBO}, $E_{TORSION}$, b_{ij} and C_{ij}, the vast majority of loops are "too short" to vectorize: Need to use the outermost loop (over all atoms in the simulation).
- While most time consumed in E_{LJ}, remaining routines become significant after its optimization.

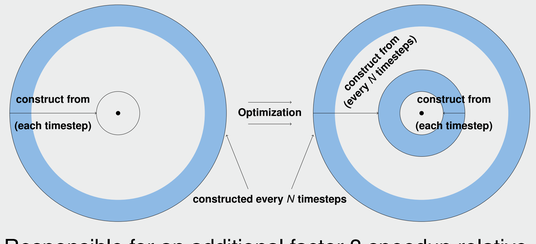


Techniques

- Integrating TORSION into REBO calculation.
- Lennard-Jones search using hashmap.
- AVX/AVX2: Optimize gather to transpose.
- Add lower precision modes.
- Automatic translation from intrinsics to library.

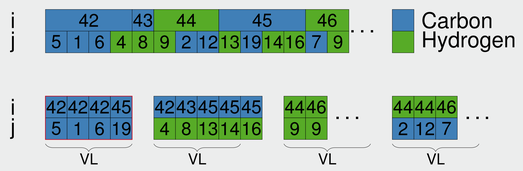


Intermediate Neighbor List



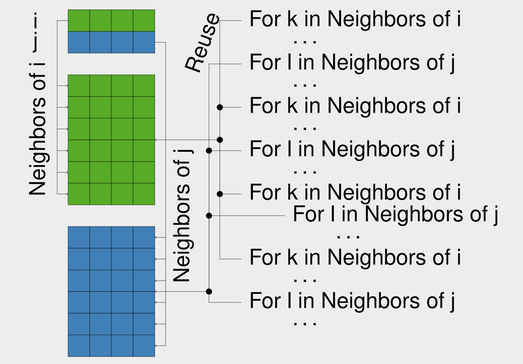
Responsible for an additional factor 3 speedup relative to just vectorization (cf. N-list$_L$ speedup of 2).

Short-Ranged Vectorization



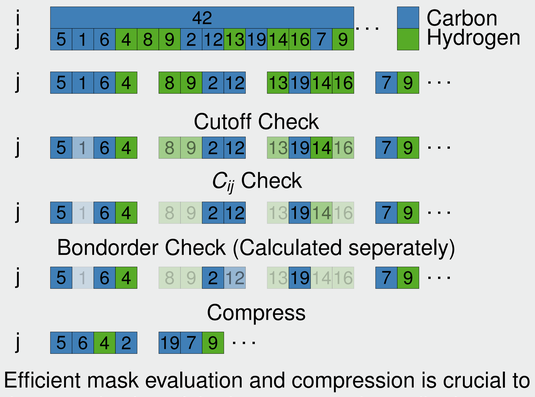
Since the neighbor list is too small to fill vectors by itself, group neighbors ("j"s) of multiple atoms ("i"s) together. For visualization purposes, assume vector length 4.

Bond-Order Vectorization



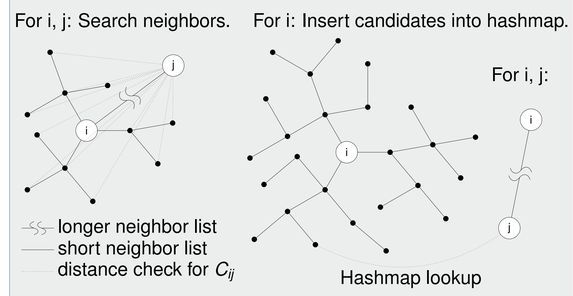
AoS/SoA transform of neighbor positions and forces is reused in all loops of the bondorder calculation.

Longer-ranged Vectorization

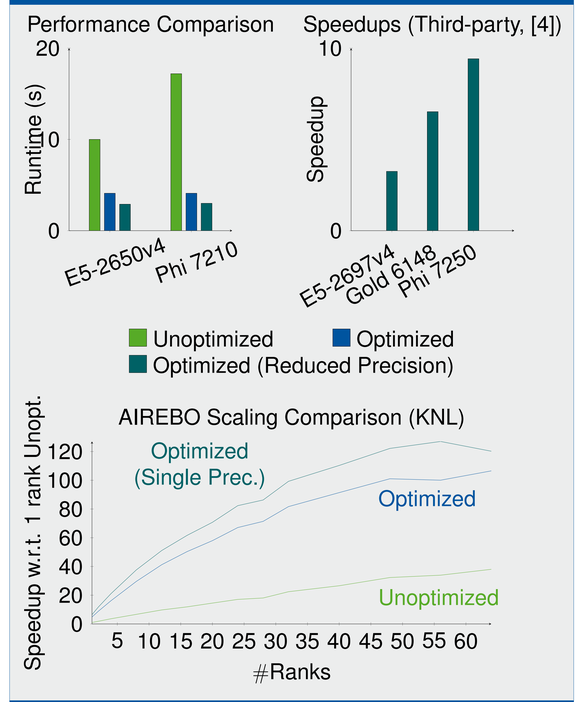


Efficient mask evaluation and compression is crucial to the vectorization of the longer-ranged contribution.

C_{ij} Vectorization



Results



References

1. Stuart, Tutein, Harrison: "A reactive potential for hydrocarbons with intermolecular interactions", J Chem Phys, 112, 6472-6486 (2000).
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