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**Algorithm 1** Computation in one time step of MD

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Receive atoms from neighboring processors

**for**  $i = 1$  to  $N_p$  **do**

**for**  $j = 1$  to  $N_i$  **do**

**if** atoms are within cutoff radius,  $r_c$  **then**

            Compute forces on pairs of atoms

**end if**

**end for**

**end for**

Update atom positions and velocities

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