The Vectorization of the Tersoff Multi-Body Potential

An Exercise in Performance Portability

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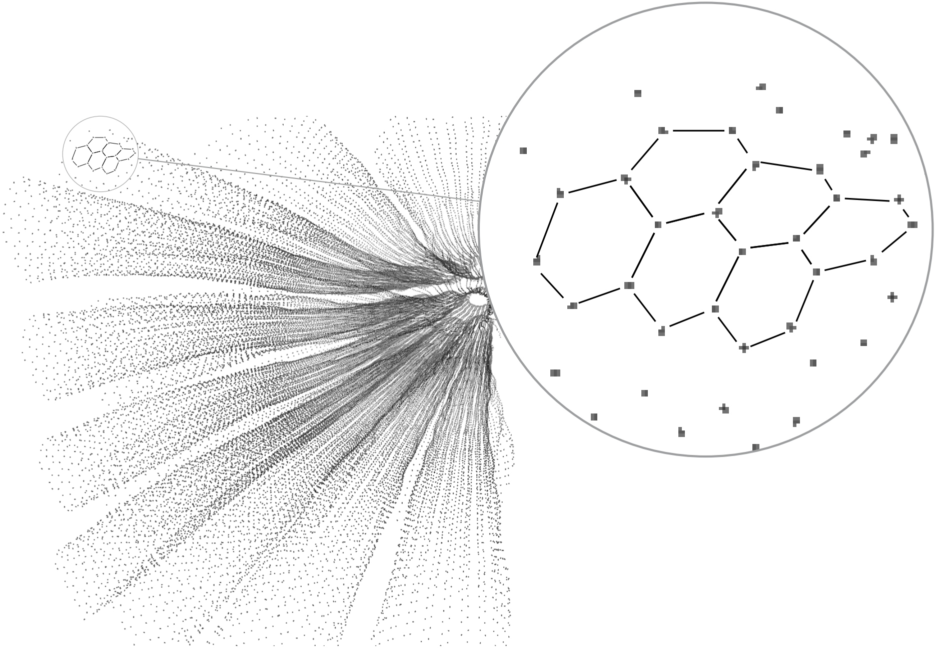
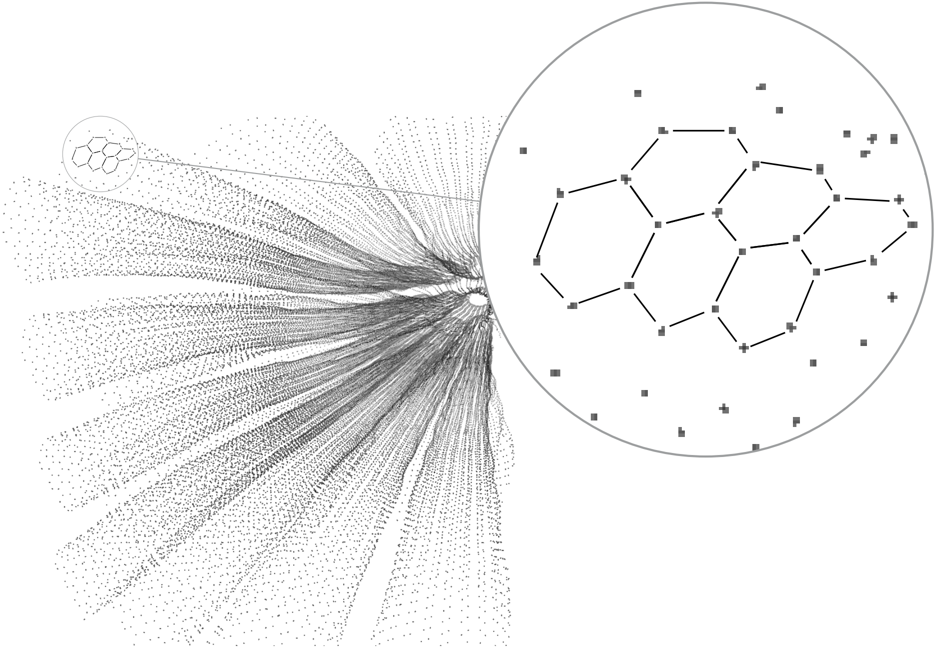
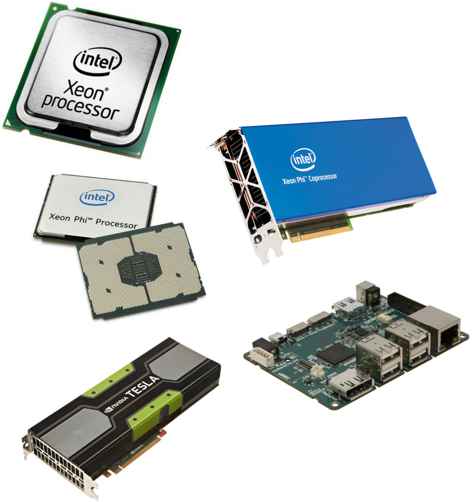
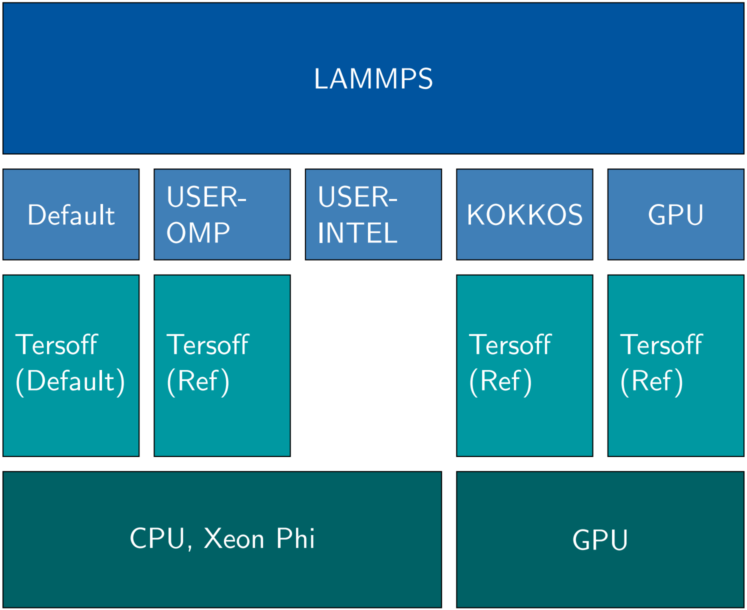
SC'16






intel
Xeon processor
intel
Xeon Phi™ Processor
intel
Xeon Phi™ Coprocessor
NVIDIA TESLA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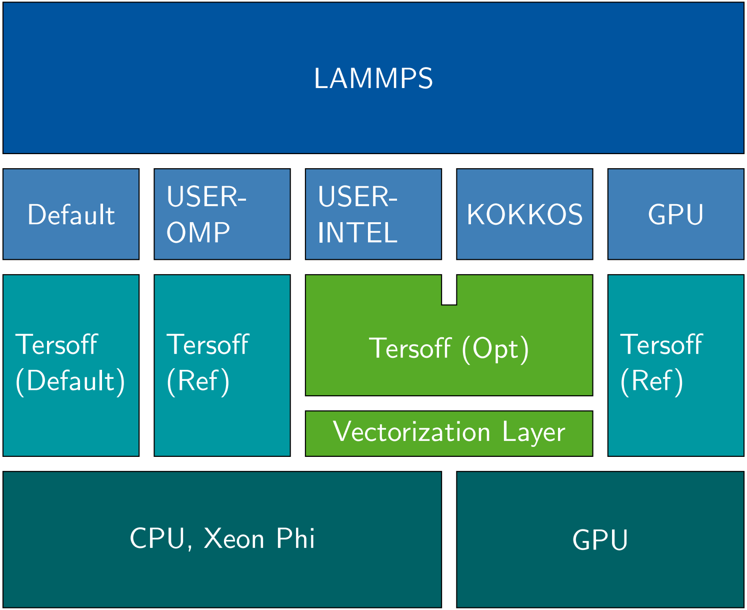
Default
USER-OMP
USER-INTEL
KOKKOS
GPU
Tersoff (Default)
Tersoff (Ref)
Tersoff (Ref)
Tersoff (Ref)
CPU, Xeon Phi
GPU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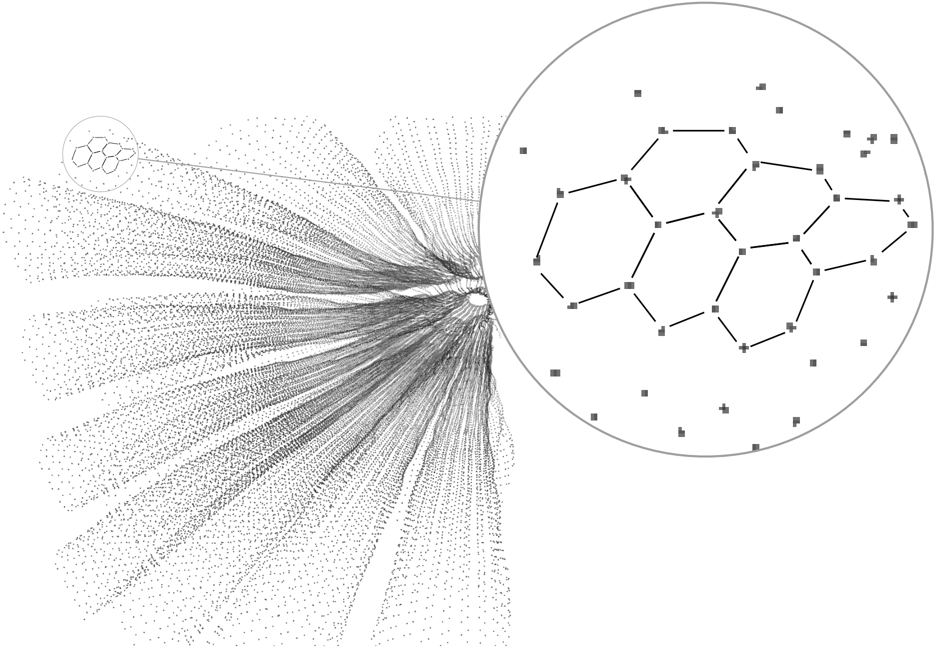
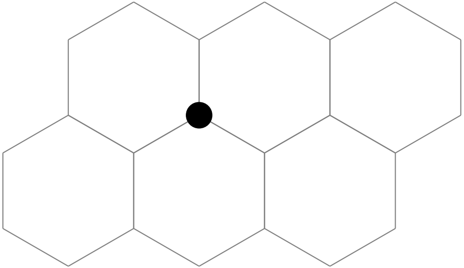
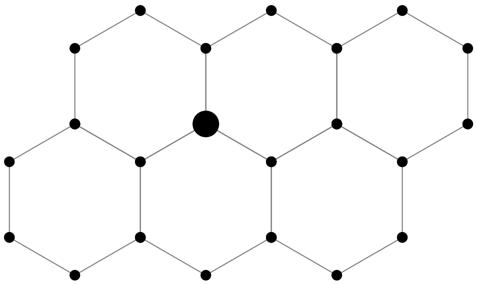
Vectorization Layer
Tersoff (Ref)
CPU, Xeon Phi
GPU

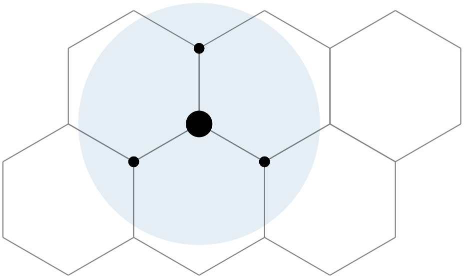




$$V = \sum_i \sum_{j:??} V(i,j)$$

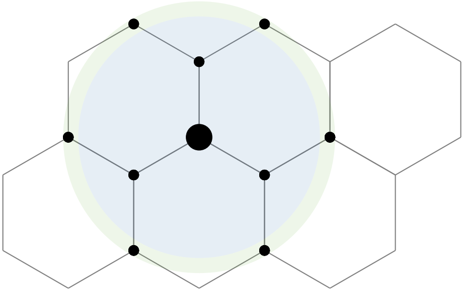


$$V = \sum_i \sum_j V(i, j)$$



$$V = \sum_i \sum_{j \in \mathcal{N}_i} V(i,j)$$

$$j \in \mathcal{N}_i \Leftrightarrow: r_{ij} < r_{ij}^{\mathrm{cutoff}}; \qquad V(i,j) = 0 \ \forall j \notin \mathcal{N}_i$$



$$V = \sum_i \sum_{j \in \mathcal{S}_i} V(i,j)$$

$$j \in \mathcal{S}_i \Leftrightarrow: r_{ij} < r_{ij}^{\mathrm{cutoff}} + r^{\mathrm{skin}}, \mathcal{N}_i \subset \mathcal{S}_i$$

$$V^{\text{two-body}} = \sum_i \sum_{j \in \mathcal{S}_i} V(i,j)$$

$$V^{\text{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_i} V(i,j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i,j,k))$$

$$V(i,j,\zeta) = f_C(r_{ij}) \left[f_R(r_{ij}) + (1 + \beta^\nu \zeta^\nu)^{-\frac{1}{2\nu}} f_A(r_{ij}) \right]$$

$$\cdots$$

$$V^{\text{two-body}} = \sum_{i} \sum_{j \in \mathcal{S}_i} V(i,j)$$

$$V^{\text{Tersoff}} = \sum_{i} \sum_{j \in \mathcal{S}_i} V(i,j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i,j,k))$$

$$V(i,j,\zeta) = f_C(r_{ij}) \left[f_R(r_{ij}) + (1 + \beta^{\nu} \zeta^{\nu})^{-\frac{1}{2\nu}} f_A(r_{ij}) \right]$$

...

$$V^{\mathrm{two-body}} = \sum_i \sum_{j \in \mathcal{S}_i} V(i,j)$$

$$V^{\mathrm{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_i} V(i,j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i,j,k))$$

$$V(i,j,\zeta) = f_C(r_{ij}) \left[f_R(r_{ij}) + (1 + \beta^\nu \zeta^\nu)^{-\frac{1}{2\nu}} f_A(r_{ij}) \right]$$

$$\cdots$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

$$V^{\mathrm{Tersoff}} = \sum_{i} \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i, j, k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do**
  for $j \in \mathcal{S}_i$ **do**
    $\zeta_{ij} \leftarrow 0$;
    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i, j, k)$;
    $V \leftarrow V + V(i, j, \zeta_{ij})$;
    $F_i \leftarrow F_i - \partial_{x_i} V(i, j, \zeta_{ij})$;
    $F_j \leftarrow F_j - \partial_{x_j} V(i, j, \zeta_{ij})$;
    $\delta\zeta \leftarrow \partial_{\zeta} V(i, j, \zeta_{ij})$;
    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
      $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i, j, k)$;
      $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i, j, k)$;
      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i, j, k)$;

$$V^{\text{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i, j, k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do** | Loop over all atoms

  for $j \in \mathcal{S}_i$ **do**

    $\zeta_{ij} \leftarrow 0$;

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i, j, k)$;

    $V \leftarrow V + V(i, j, \zeta_{ij})$;

    $F_i \leftarrow F_i - \partial_{x_i} V(i, j, \zeta_{ij})$;

    $F_j \leftarrow F_j - \partial_{x_j} V(i, j, \zeta_{ij})$;

    $\delta\zeta \leftarrow \partial_\zeta V(i, j, \zeta_{ij})$;

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i, j, k)$;

      $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i, j, k)$;

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i, j, k)$;

$$V^{\text{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i, j, k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do** | Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** | Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i, j, k);$

    $V \leftarrow V + V(i, j, \zeta_{ij});$

    $F_i \leftarrow F_i - \partial_{x_i} V(i, j, \zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i, j, \zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i, j, \zeta_{ij});$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i, j, k);$

      $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i, j, k);$

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i, j, k);$

$$V^{\text{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i,j,k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do**
    for $j \in \mathcal{S}_i$ **do**
        $\zeta_{ij} \leftarrow 0$;
        for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
            $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k)$;
        $V \leftarrow V + V(i,j,\zeta_{ij})$;
        $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij})$;
        $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij})$;
        $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij})$;
        for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
            $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i}\zeta(i,j,k)$;
            $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j}\zeta(i,j,k)$;
            $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k}\zeta(i,j,k)$;

Loop over all atoms

Loop over atoms "closeby" to i

Compute ζ

$$V^{\text{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i, j, k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0$; — Compute ζ

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i, j, k)$;

    $V \leftarrow V + V(i, j, \zeta_{ij})$; — Compute potential

    $F_i \leftarrow F_i - \partial_{x_i} V(i, j, \zeta_{ij})$;

    $F_j \leftarrow F_j - \partial_{x_j} V(i, j, \zeta_{ij})$;

    $\delta\zeta \leftarrow \partial_\zeta V(i, j, \zeta_{ij})$;

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i, j, k)$;

      $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i, j, k)$;

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i, j, k)$;

$$V^{\text{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i,j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i,j,k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do** | Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** | Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0$; | Compute ζ

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k)$;

    $V \leftarrow V + V(i,j,\zeta_{ij})$; | Compute potential

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij})$;

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij})$;

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij})$;

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i,j,k)$;

      $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i,j,k)$;

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i,j,k)$;

$$V^{\mathrm{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i, j, k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

for i **do** — Loop over all atoms
  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i
    $\zeta_{ij} \leftarrow 0$; — Compute ζ
    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i, j, k)$;
    $V \leftarrow V + V(i, j, \zeta_{ij})$; — Compute potential
    $F_i \leftarrow F_i - \partial_{x_i} V(i, j, \zeta_{ij})$; — Forces directly due to V
    $F_j \leftarrow F_j - \partial_{x_j} V(i, j, \zeta_{ij})$;
    $\delta\zeta \leftarrow \partial_\zeta V(i, j, \zeta_{ij})$;
    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
      $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i, j, k)$;
      $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i, j, k)$;
      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i, j, k)$;

$$V^{\mathrm{Tersoff}} = \sum_i \sum_{j \in \mathcal{S}_j} V(i, j, \sum_{k \in \mathcal{S}_i \setminus \{j\}} \zeta(i, j, k))$$

$$\mathbf{F}_i = -\nabla_{\mathbf{x}_i} V$$

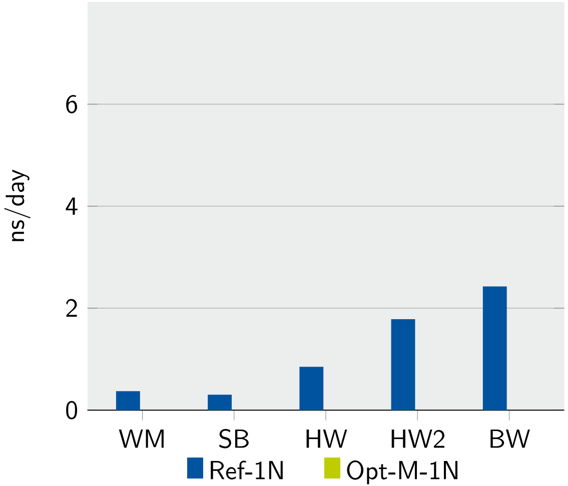
for i **do**	Loop over all atoms
for $j \in \mathcal{S}_i$ **do**	Loop over atoms "closeby" to i

$\zeta_{ij} \leftarrow 0$;
     for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
       $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i, j, k)$;
	Compute ζ

$V \leftarrow V + V(i, j, \zeta_{ij})$;	Compute potential
$F_i \leftarrow F_i - \partial_{x_i} V(i, j, \zeta_{ij})$; $F_j \leftarrow F_j - \partial_{x_j} V(i, j, \zeta_{ij})$;	Forces directly due to V

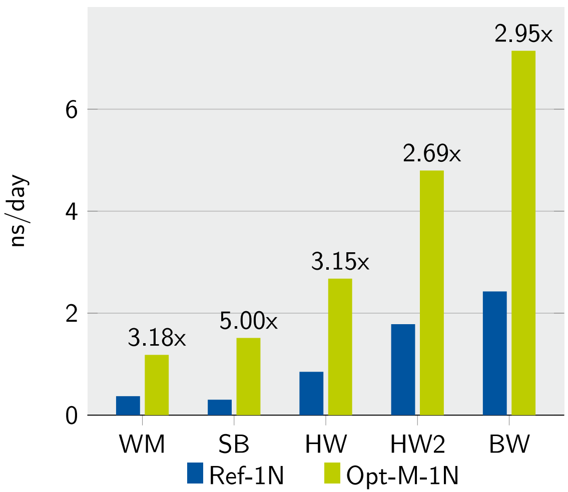
$\delta\zeta \leftarrow \partial_\zeta V(i, j, \zeta_{ij})$;
     for $k \in \mathcal{S}_i \setminus \{j\}$ **do**
       $F_i \leftarrow F_i - \delta\zeta \cdot \partial_{x_i} \zeta(i, j, k)$;
       $F_j \leftarrow F_j - \delta\zeta \cdot \partial_{x_j} \zeta(i, j, k)$;
       $F_k \leftarrow F_k - \delta\zeta \cdot \partial_{x_k} \zeta(i, j, k)$;
	Chain Rule for ζ

CPU: Single Node Execution (512 000 atoms)



Name	Processor	Cores	Vector ISA
WM	Intel Xeon X5675	2 × 6	SSE4.2
SB	Intel Xeon E5-2450	2 × 8	AVX
HW	Intel Xeon E5-2680v3	2 × 12	AVX2
HW2	Intel Xeon E5-2697v3	2 × 14	AVX2
BW	Intel Xeon E5-2697v4	2 × 18	AVX2

CPU: Single Node Execution (512 000 atoms)



Name	Processor	Cores	Vector ISA
WM	Intel Xeon X5675	2 × 6	SSE4.2
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HW2	Intel Xeon E5-2697v3	2 × 14	AVX2
BW	Intel Xeon E5-2697v4	2 × 18	AVX2

for i **do**

  for $j \in \mathcal{S}_i$ **do**

    $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$

    $\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

      $\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$

      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$

      $\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** | Loop over all atoms

- **for** $j \in \mathcal{S}_i$ **do**
  - $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$
  - $\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$
  - **for** $k \in \mathcal{S}_i \setminus \{j\}$ **do**
    - $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$
    - $\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$
    - $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$
    - $\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$
  - $V \leftarrow V + V(i,j,\zeta_{ij});$
  - $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$
  - $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$
  - $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$
  - $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$
  - $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$
  - **for** $k \in \mathcal{S}_i \setminus \{j\}$ **do**
    - $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** | Loop over all atoms

for $j \in \mathcal{S}_i$ **do** | Loop over atoms "closeby" to i

$\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$

$\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$

for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

$\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

$\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$

$\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$

$\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$

$V \leftarrow V + V(i,j,\zeta_{ij});$

$F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

$F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

$\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

$F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

$F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

$F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$ — Compute ζ

    $\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

      $\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$

      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$

      $\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$ — Compute ζ

    $\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

      $\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$

      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$ — And derivates of ζ

      $\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$ — Compute ζ

    $\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

      $\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$

      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$ — And derivates of ζ

      $\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$ — Compute potential

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

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      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$ — And derivates of ζ

      $\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$ — Compute potential

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$ — Forces directly due to V

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

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    $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$ — Compute ζ

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      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$ — And derivates of ζ

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    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$ — Chain Rule for ζ

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

    $\zeta_{ij} \leftarrow 0; \quad \partial_k\zeta \leftarrow 0 \quad \forall k;$ — Compute ζ

    $\partial_i\zeta \leftarrow 0; \quad \partial_j\zeta \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

      $\partial_i\zeta \leftarrow \partial_i\zeta + \partial_{x_i}\zeta(i,j,k);$

      $\partial_j\zeta \leftarrow \partial_j\zeta + \partial_{x_j}\zeta(i,j,k);$ — And derivates of ζ

      $\partial_k\zeta \leftarrow \partial_{x_k}\zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$ — Compute potential

    $F_i \leftarrow F_i - \partial_{x_i}V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j}V(i,j,\zeta_{ij});$ — Forces directly due to V

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$ — Chain Rule for ζ

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i\zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j\zeta;$ — Updates for F_i and F_j

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k\zeta;$

for i **do** — Loop over all atoms

  for $j \in \mathcal{S}_i$ **do** — Loop over atoms "closeby" to i

$$\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$$

Compute ζ

$$\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

$$\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$$
$$\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$$
$$\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$$
$$\partial_k \zeta \leftarrow \partial_{x_k} \zeta(i,j,k);$$

And derivates of ζ

$$V \leftarrow V + V(i,j,\zeta_{ij});$$

Compute potential

$$F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$$
$$F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$$

Forces directly due to V

$$\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$$

Chain Rule for ζ

$$F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$$
$$F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$$

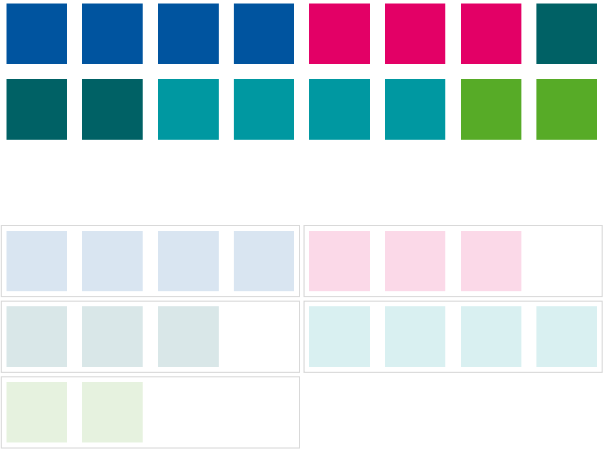
Updates for F_i and F_j

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

$$F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$$

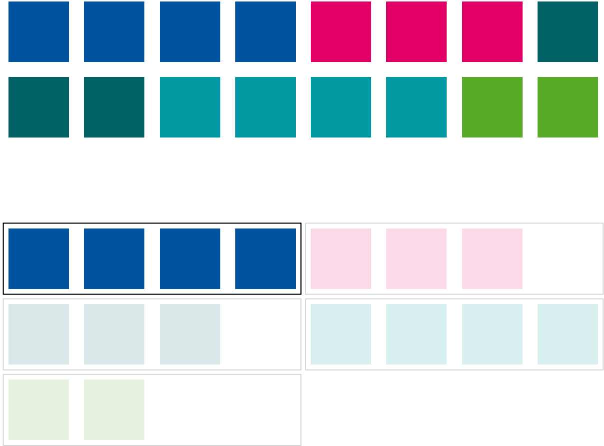
Updates for F_k

```
for i do                                          | Loop over all atoms
  for j ∈ S_i do                                  | Loop over atoms "closeby" to i
    ζ_ij ← 0;   ∂_k ζ ← 0   ∀k;                   | Compute ζ
    ∂_i ζ ← 0;   ∂_j ζ ← 0;
    for k ∈ S_i \ {j} do
      ζ_ij ← ζ_ij + ζ(i, j, k);
      ∂_i ζ ← ∂_i ζ + ∂_{x_i} ζ(i, j, k);
      ∂_j ζ ← ∂_j ζ + ∂_{x_j} ζ(i, j, k);         | And derivates of ζ
      ∂_k ζ ← ∂_{x_k} ζ(i, j, k);
    V ← V + V(i, j, ζ_ij);                        | Compute potential
    F_i ← F_i − ∂_{x_i} V(i, j, ζ_ij);            | Forces directly due to V
    F_j ← F_j − ∂_{x_j} V(i, j, ζ_ij);
    δζ ← ∂_ζ V(i, j, ζ_ij);                       | Chain Rule for ζ
    F_i ← F_i − δζ · ∂_i ζ;                       | Updates for F_i and F_j
    F_j ← F_j − δζ · ∂_j ζ;
    for k ∈ S_i \ {j} do                          | Updates for F_k
      F_k ← F_k − δζ · ∂_k ζ;
```



Option A

```
#pragma omp parallel for
for (int i = ...
  #pragma omp simd
  for (int j = ...
    ...
```



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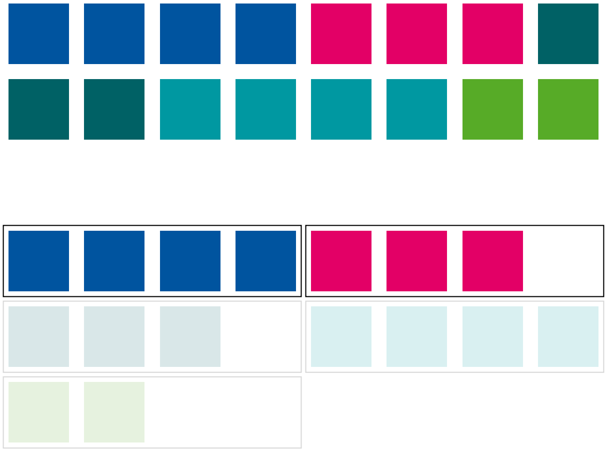
```
#pragma omp parallel for
for (int i = ...
  #pragma omp simd
  for (int j = ...
    ...
```



Option A

```
#pragma omp parallel for
for (int i = ...
  #pragma omp simd
  for (int j = ...
    ...
```

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```
#pragma omp parallel for
for (int i = ...
  #pragma omp simd
  for (int j = ...
    ...
```

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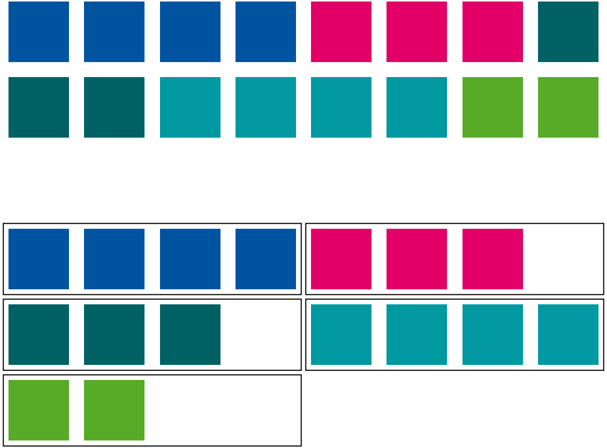
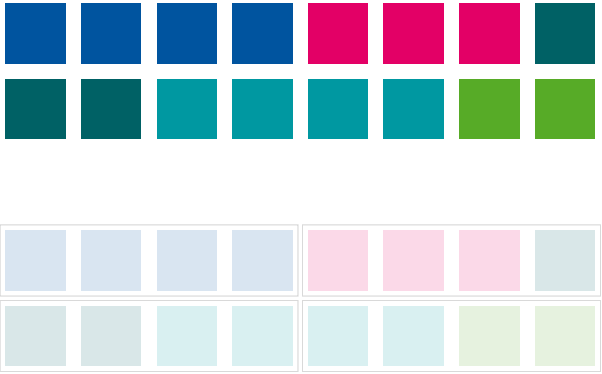
```
#pragma omp parallel for
for (int i = ...
  #pragma omp simd
  for (int j = ...
    ...
```



Option A

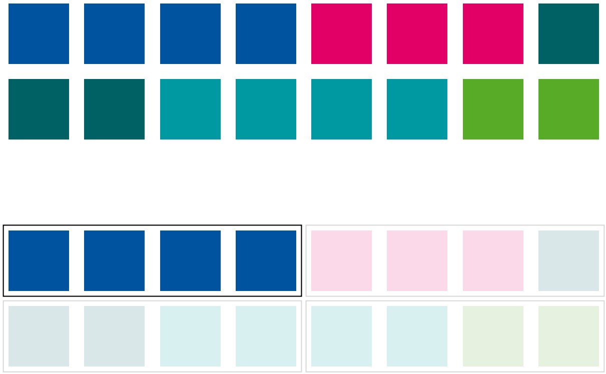
```
#pragma omp parallel for
for (int i = ...
  #pragma omp simd
  for (int j = ...
    ...
```



Option B

```
#pragma omp parallel for simd collapse(2)
for (int i = ...

  for (int j = ...
    ...
```



Option B

```
#pragma omp parallel for simd collapse(2)
for (int i = ...

  for (int j = ...
    ...
```

Option B

```
#pragma omp parallel for simd collapse(2)
for (int i = ...

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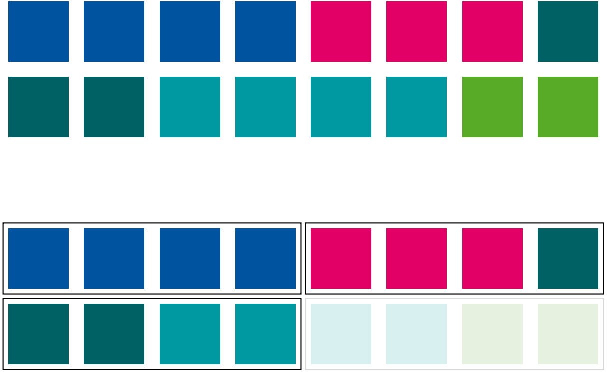
    ...
```



Option B

```
#pragma omp parallel for simd collapse(2)
for (int i = ...

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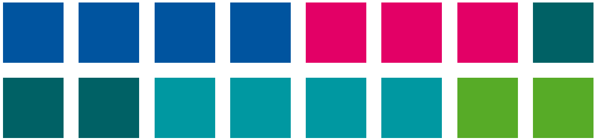
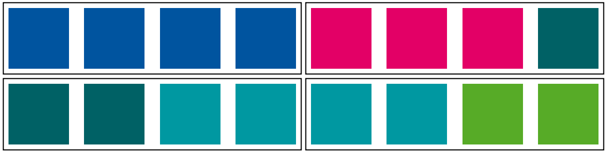
    ...
```





Option B

```
#pragma omp parallel for simd collapse(2)
for (int i = ...

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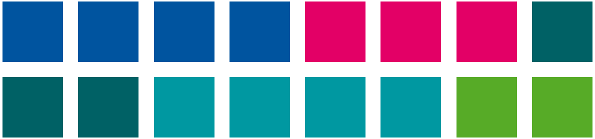
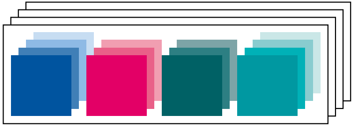
    ...
```





Option C

```
#pragma omp parallel for simd
for (int i = ...

  for (int j = ...
    ...
```

for i **do**

  for $j \in \mathcal{S}_i$ **do**

    $\zeta_{ij} \leftarrow 0; \quad \partial_k \zeta \leftarrow 0 \quad \forall k;$

    $\partial_i \zeta \leftarrow 0; \quad \partial_j \zeta \leftarrow 0;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $\zeta_{ij} \leftarrow \zeta_{ij} + \zeta(i,j,k);$

      $\partial_i \zeta \leftarrow \partial_i \zeta + \partial_{x_i} \zeta(i,j,k);$

      $\partial_j \zeta \leftarrow \partial_j \zeta + \partial_{x_j} \zeta(i,j,k);$

      $\partial_k \zeta \leftarrow \partial_k \zeta + \partial_{x_k} \zeta(i,j,k);$

    $V \leftarrow V + V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \partial_{x_i} V(i,j,\zeta_{ij});$

    $F_j \leftarrow F_j - \partial_{x_j} V(i,j,\zeta_{ij});$

    $\delta\zeta \leftarrow \partial_\zeta V(i,j,\zeta_{ij});$

    $F_i \leftarrow F_i - \delta\zeta \cdot \partial_i \zeta;$

    $F_j \leftarrow F_j - \delta\zeta \cdot \partial_j \zeta;$

    for $k \in \mathcal{S}_i \setminus \{j\}$ **do**

      $F_k \leftarrow F_k - \delta\zeta \cdot \partial_k \zeta;$

for i **do**

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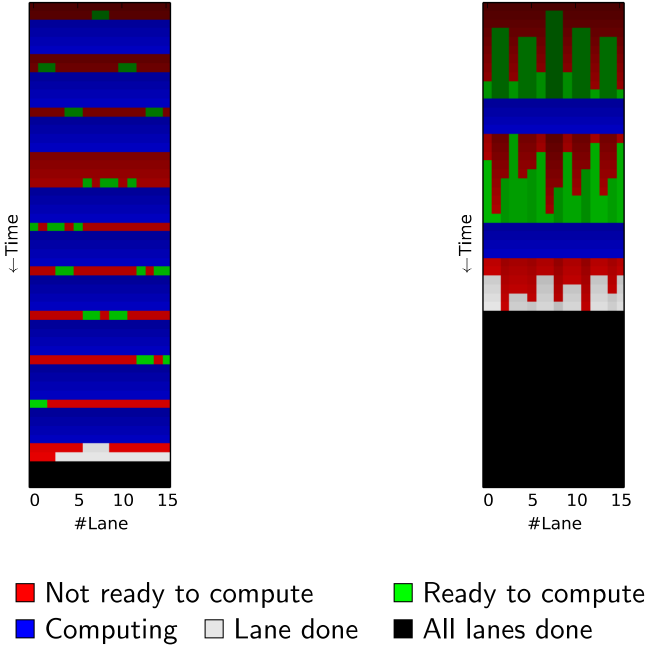
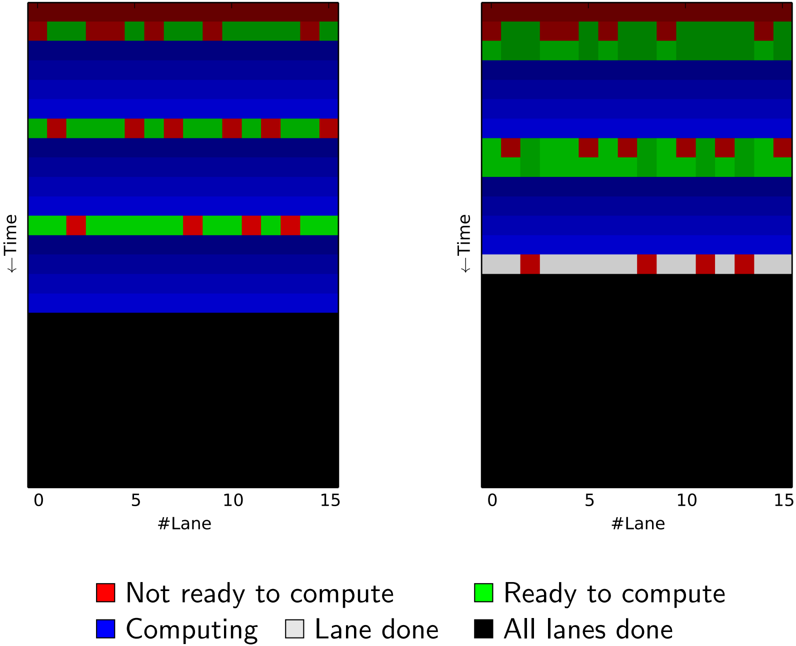

←Time
0 5 10 15
#Lane
←Time
0 5 10 15
#Lane
Not ready to compute
Ready to compute
Computing
Lane done
All lanes done



←Time
0
5
10
15
#Lane
←Time
0
5
10
15
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Not ready to compute
Ready to compute
Computing
Lane done
All lanes done

Implementation

- **Vector-Wide conditionals**: Do all elements in a vector satisfy a condition?

```
int o = 1;
for (int i = 0; i < VL; i++) if (! a[i]) o = 0;
```

- **Reductions**: Sum up all elements in a vector.

```
double o = 0;
for (int i = 0; i < VL; i++) o += a[i];
```

- **Conflict write handling**: Accumulate values from vector into memory with indices from vector. `for (int i = 0; i < VL; i++) mem[b[i]] += a[i];`

- **Adjacent gather optimizations**: Write data from indices $i_1, i_2, \ldots$ into vector a, and data from $i_1 + 1, i_2 + 1, \ldots$ into b.

```
for (i = 0; i < VL; i++) { j = idx[i];
  a[i] = mem[j]; b[i] = mem[j+1]; }
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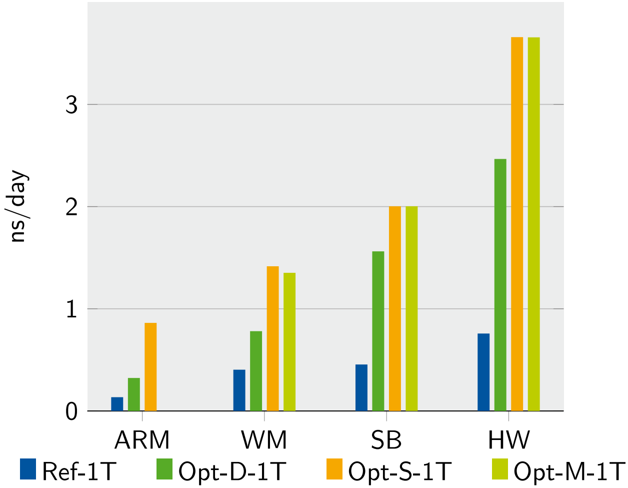
```
for (i = 0; i < VL; i++) { j = idx[i];
  a[i] = mem[j]; b[i] = mem[j+1]; }
```

```
for (; kk < numneigh_i; kk++) {
  int k = firstneigh[kk + cnumneigh_i] & NEIGHMASK;
  fvec vx_k(x[k].x);
  fvec vy_k(x[k].y);
  fvec vz_k(x[k].z);
  int w_k = x[k].w;

  fvec vdx_ik = vx_k - vx_i;
  fvec vdy_ik = vy_k - vy_i;
  fvec vdz_ik = vz_k - vz_i;
  fvec vrsq = vdx_ik * vdx_ik + vdy_ik * vdy_ik
                              + vdz_ik * vdz_ik;
  ...
  if (! v::mask_testz(veff_mask)) {
    fvec vzeta_contrib = ...;
    vzeta = v::acc_mask_add(vzeta, veff_mask,
                            vzeta, vzeta_contrib);
  }
}
```

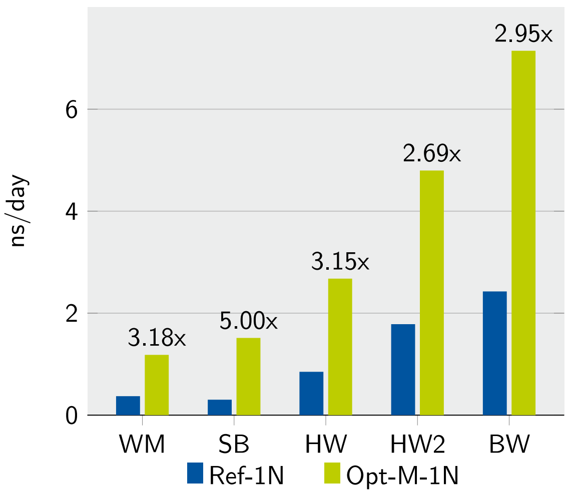
Results

CPU: Single-Threaded Execution (32 000 atoms)

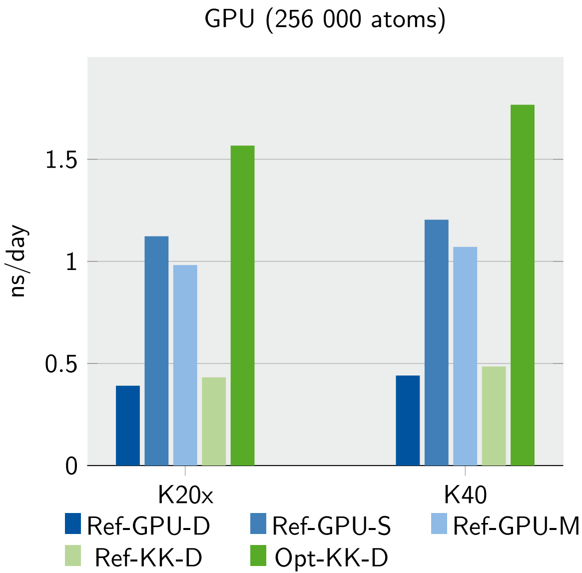


Name	Processor	Cores	Vector ISA
ARM	ARM Cortex-A15	2 × 4[1]	NEON
WM	Intel Xeon X5675	2 × 6	SSE4.2
SB	Intel Xeon E5-2450	2 × 8	AVX
HW	Intel Xeon E5-2680v3	2 × 12	AVX2

CPU: Single Node Execution (512 000 atoms)

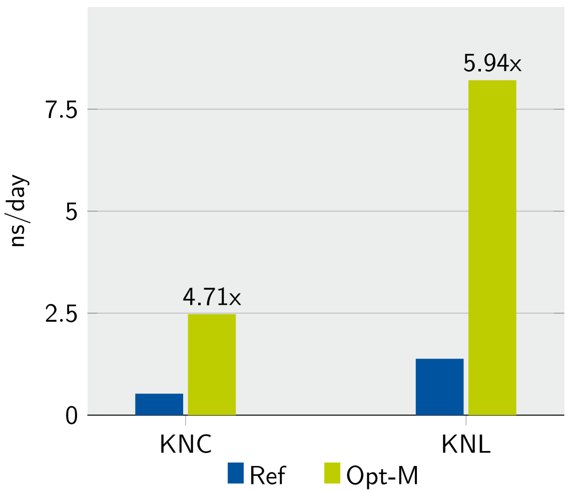


Name	Processor	Cores	Vector ISA
WM	Intel Xeon X5675	2 × 6	SSE4.2
SB	Intel Xeon E5-2450	2 × 8	AVX
HW	Intel Xeon E5-2680v3	2 × 12	AVX2
HW2	Intel Xeon E5-2697v3	2 × 14	AVX2
BW	Intel Xeon E5-2697v4	2 × 18	AVX2



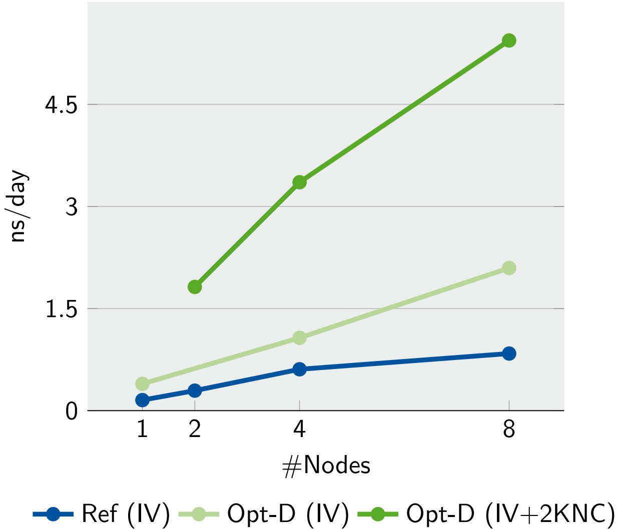
Name	CPU	Cores	ISA	Accelerator
K20X	Intel Xeon E5-2650	2×8	AVX	Nvidia Tesla K20x
K40	Intel Xeon E5-2650	2×8	AVX	Nvidia Tesla K40

Native Execution on Xeon Phi Systems (512 000 atoms)



Name	CPU	Cores	ISA	Accelerator	Cores	ISA
IV+2KNC	Intel Xeon E5-2650v2	2 × 8	AVX	Intel Xeon Phi 5110P	2 × 60	IMCI
KNL	–	–	–	Intel Xeon Phi 7250	68	AVX-512

SuperMIC: Strong Scalability (2 million atoms)



Name	CPU	Cores	ISA	Accelerator	Cores	ISA
IV+2KNC	Intel Xeon E5-2650v2	2 × 8	AVX	Intel Xeon Phi 5110P	2 × 60	IMCI

Conclusion

- Optimized Tersoff on a range of architectures
- Handling short loops (neighbor list)
- Identified necessary primitives
- Implemented using C++ abstraction
- Experimented on many architectures
- Achieved performance
- Next up: REBO/AIREBO

Done. Time for your questions...

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http://github.com/hpac/lammps-tersoff-vector