High-Performance & Automatic Computing

Fast & portable code for complex molecular dynamics simulations

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ICES, University of Texas at Austin

Deutsche Forschungsgemeinschaft DFG

HPAC High Performance and Automatic Computing

RWTH AACHEN UNIVERSITY

The world of scientific computing

The world of scientific computing

$$\boxed{\boldsymbol{y} = X\boldsymbol{\beta} + Z\boldsymbol{u} + \boldsymbol{\epsilon}}$$

$$\boxed{\min_x \|A\mathbf{x} - \mathbf{b}\|^2 + \|\Gamma\mathbf{x}\|^2}$$

Linear mixed models

$$\boxed{V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]}$$

Lennard-Jones potential

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-2\hbar}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)}$$

Schrödinger eqn.

$$\vdots$$

The world of scientific computing

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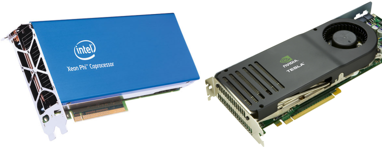

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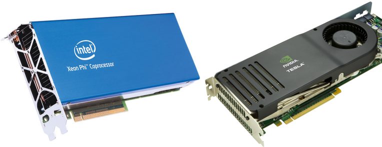

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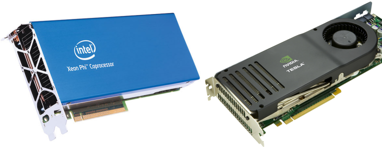


1) Linear Algebra, Applications

2) Tensor Operations

3) Molecular Dynamics

Linear Algebra

Generalized Least Squares	$b := (X^T M^{-1} X)^{-1} X^T M^{-1} y$	$n > m$; $M \in \mathbb{R}^{n \times n}$, SPD; $X \in \mathbb{R}^{n \times m}$; $y \in \mathbb{R}^{n \times 1}$
Signal Processing	$x := \left(A^{-T} B^T B A^{-1} + R^T L R\right)^{-1} A^{-T} B^T B A^{-1} y$	
Kalman Filter	$K_k := P_k^b H^T (H P_k^b H^T + R)^{-1};\; x_k^a := x_k^b + K_k(z_k - H x_k^b);\; P_k^a := (I - K_K H)\, P_k^b$	
Ensemble Kalman Filter	$X^a := X^b + \left(B^{-1} + H^T R^{-1} H\right)^{-1} \left(Y - H X^b\right)$	
Image Restoration	$x_k := (H^T H + \lambda \sigma^2 I_n)^{-1} (H^T y + \lambda \sigma^2 (v_{k-1} - u_{k-1}))$	
Rand. Matrix Inversion	$X_{k+1} := S(S^T A S)^{-1} S^T + (I_n - S(S^T A S)^{-1} S^T A) X_k (I_n - A S (S^T A S)^{-1} S^T)$	
Stochastic Newton	$B_k := \frac{k}{k-1} B_{k-1}(I_n - A^T W_k((k-1) I_l + W_k^T A B_{k-1} A^T W_k)^{-1} W_k^T A B_{k-1})$	
Optimization	$x_f := W A^T (A W A^T)^{-1} (b - Ax);\quad x_o := W(A^T (A W A^T)^{-1} A x - c)$	
Tikhonov Regularization	$x := (A^T A + \Gamma^T \Gamma)^{-1} A^T b$	$A \in \mathbb{R}^{n \times m}$; $\Gamma \in \mathbb{R}^{m \times m}$; $b \in \mathbb{R}^{n \times 1}$
Gen. Tikhonov Reg.	$x := (A^T P A + Q)^{-1} (A^T P b + Q x_0)$	$P \in \mathbb{R}^{n \times n}$, SSPD; $Q \in \mathbb{R}^{m \times m}$, SSPD; $x_0 \in \mathbb{R}^{m \times 1}$
LMMSE estimator	$K_{t+1} := C_t A^T (A C_t A^T + C_z)^{-1};\; x_{t+1} := x_t + K_{t+1}(y - A x_t);\; C_{t+1} := (I - K_{t+1} A) C_t$	

$$x := A(B^TB + A^TR^T\Lambda RA)^{-1}B^TBA^{-1}y$$

$$\begin{cases} C_\dagger := PCP^T + Q \\ K := C_\dagger H^T(HC_\dagger H^T)^{-1} \end{cases}$$

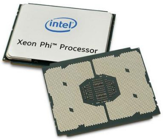
$$E := Q^{-1}U(I + U^TQ^{-1}U)^{-1}U^T$$

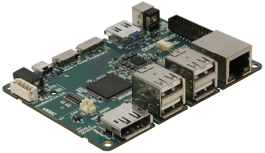
. . .

$$x := A(B^T B + A^T R^T \Lambda R A)^{-1} B^T B A^{-1} y$$

$$\begin{cases} C_\dagger := P C P^T + Q \\ K := C_\dagger H^T (H C_\dagger H^T)^{-1} \end{cases}$$

$$E := Q^{-1} U (I + U^T Q^{-1} U)^{-1} U^T \qquad \ldots$$





MUL ADD MOV

MOVAPD

VFMADDPD ...

$$x := A(B^TB + A^TR^T\Lambda RA)^{-1}B^TBA^{-1}y$$

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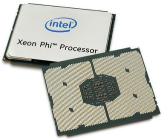
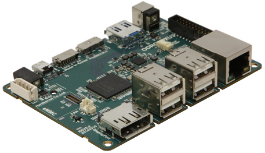
↓ ?





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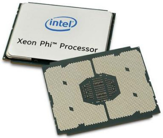
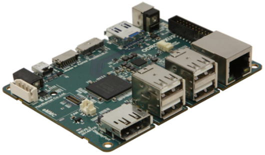
...

$\boxed{y := \alpha x + y}$ $\boxed{LU = A}$ $\cdots$ $\boxed{C := \alpha AB + \beta C}$

$\boxed{X := A^{-1}B}$ $\boxed{C := AB^T + BA^T + C}$ $\boxed{X := L^{-1}ML^{-T}}$ $\boxed{QR = A}$

BLAS ↓ **BLIS** ↓ **LAPACK** ↓ ...





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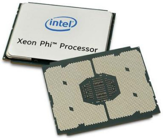
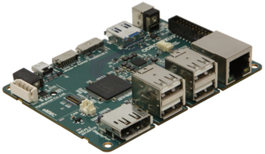
BLAS **BLIS** **LAPACK** **...**





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LINEAR ALGEBRA MAPPING PROBLEM (LAMP)

$y := \alpha x + y$

$:= \alpha AB + \beta C$

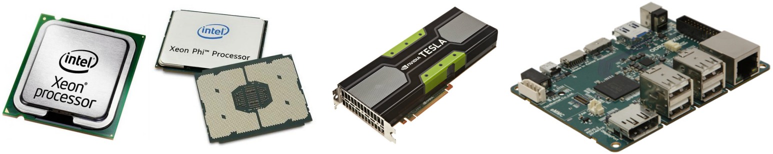
$X := A^{-1}B$

$C := A$

$^{-1}ML^{-T}$

$QR = A$

BLAS **BLIS** **LAPACK** ...



MUL ADD MOV

MOVAPD

VFMADDPD ...

Example

$$w := AB^{-1}c, \quad \text{SPD}(B)$$

H. Barthels
C. Psarras

Naive ← NEVER!!

```
w = A*inv(B)*c
```

Recommended

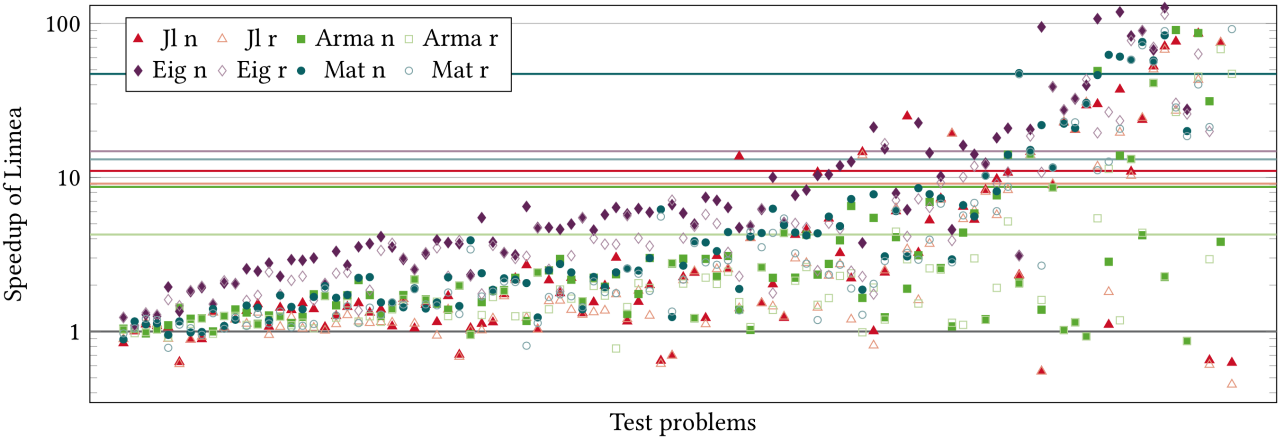
```
w = A*(B\c)
```

Expert

```
L = Chol(B)
w = A * (L'\(L\c))
```

Generated — "Linnea"

```
ml0 = A; ml1 = B; ml2 = c;
potrf!('L', ml1)
trsv!('L', 'N', 'N', ml1, ml2)
trsv!('L', 'T', 'N', ml1, ml2)
ml3 = Array{Float64}(10)
gemv!('N', 1.0, ml0, ml2, 0.0, ml3)
w = ml3
```


100
10
1
Speedup of Linnea
Test problems
▲ Jl n
△ Jl r
■ Arma n
□ Arma r
◆ Eig n
◇ Eig r
● Mat n
○ Mat r

Tensor Operations

Tensor Operations

DFT: Generation of Hamiltonian and Overlap Matrices

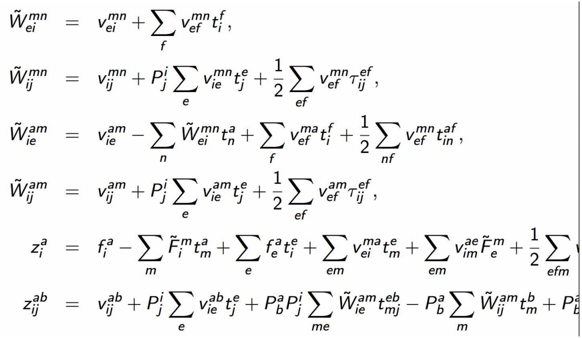
$$(S)_{G',G} = \sum_{a} \sum_{L=(l,m)} \left(A_L^{a,G'}\right)^* A_L^{a,G} + \left(B_L^{a,G'}\right)^* B_L^{a,G} \left\|\dot{u}_{l,a}\right\|^2$$

$$\begin{aligned}(H)_{G',G} = \sum_{a} \sum_{L',L} &\left(A^*_{L',a,t'}\, T^{[AA]}_{L',L;a}\, A_{L,a,t}\right) + \left(A^*_{L',a,t'}\, T^{[AB]}_{L',L;a}\, B_{L,a,t}\right) \\ &+ \left(B^*_{L',a,t'}\, T^{[BA]}_{L',L;a}\, A_{L,a,t}\right) + \left(B^*_{L',a,t'}\, T^{[BB]}_{L',L;a}\, B_{L,a,t}\right)\end{aligned}$$

Tensor Operations

Coupled-Cluster methods

$$
\begin{aligned}
\tau_{ij}^{ab} &= t_{ij}^{ab} + \frac{1}{2} P_b^a P_j^i t_i^a t_j^b, \\
\tilde{F}_e^m &= f_e^m + \sum_{fn} v_{ef}^{mn} t_n^f, \\
\tilde{F}_e^a &= (1-\delta_{ae}) f_e^a - \sum_m \tilde{F}_e^m t_m^a - \frac{1}{2} \sum_{mnf} v_{ef}^{mn} t_{mn}^{af} + \sum_{fn} v_{ef}^{an} t_n^f, \\
\tilde{F}_i^m &= (1-\delta_{mi}) f_i^m + \sum_e \tilde{F}_e^m t_i^e + \frac{1}{2} \sum_{nef} v_{ef}^{mn} t_{in}^{ef} + \sum_{fn} v_{if}^{mn} t_n^f,
\end{aligned}
$$



$$
\begin{aligned}
\tilde{W}_{ei}^{mn} &= v_{ei}^{mn} + \sum_f v_{ef}^{mn} t_i^f, \\
\tilde{W}_{ij}^{mn} &= v_{ij}^{mn} + P_j^i \sum_e v_{ie}^{mn} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{mn} \tau_{ij}^{ef}, \\
\tilde{W}_{ie}^{am} &= v_{ie}^{am} - \sum_n \tilde{W}_{ei}^{mn} t_n^a + \sum_f v_{ef}^{ma} t_i^f + \frac{1}{2} \sum_{nf} v_{ef}^{mn} t_{in}^{af}, \\
\tilde{W}_{ij}^{am} &= v_{ij}^{am} + P_j^i \sum_e v_{ie}^{am} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{am} \tau_{ij}^{ef}, \\
z_i^a &= f_i^a - \sum_m \tilde{F}_i^m t_m^a + \sum_e f_e^a t_i^e + \sum_{em} v_{ei}^{ma} t_m^e + \sum_{em} v_{im}^{ae} \tilde{F}_e^m + \frac{1}{2} \sum_{efm} \\
z_{ij}^{ab} &= v_{ij}^{ab} + P_j^i \sum_e v_{ie}^{ab} t_j^e + P_b^a P_j^i \sum_{me} \tilde{W}_{ie}^{am} t_{mj}^{eb} - P_b^a \sum_m \tilde{W}_{ij}^{am} t_m^b + P_b^a
\end{aligned}
$$

credits to D. Matthews, E. Solomonik, J. Stanton, and J. Gauss

Tensor Operations

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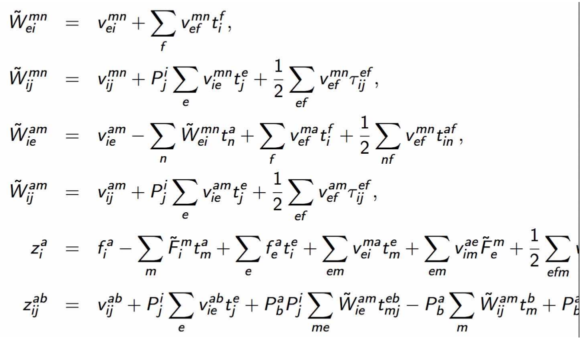

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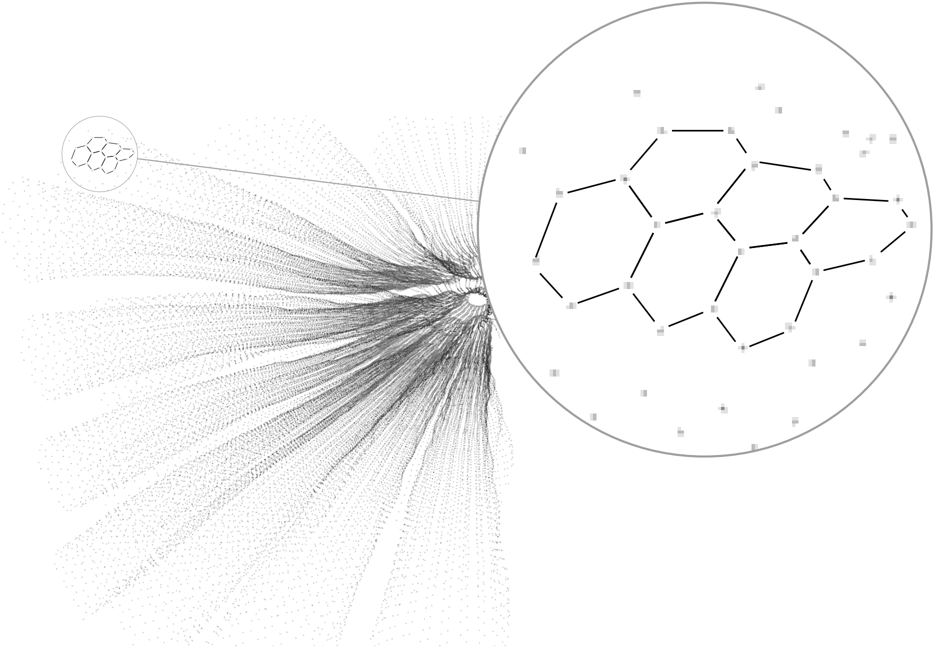
$$z_{ij}^{ab} = v_{ij}^{ab} + P_j^i \sum_e v_{ie}^{ab} t_j^e + P_b^a P_j^i \sum_{me} \tilde{W}_{ie}^{am} t_{mj}^{eb} - P_b^a \sum_m \tilde{W}_{ij}^{am} t_m^b + P_b^a$$

credits to D. Matthews, E. Solomonik, J. Stanton, and J. Gauss

P. Springer

- Tensor Transpositions Compiler TTC – github.com/HPAC/TTC
- High-Perf. Tensor Transp. Library HPTT – github.com/HPAC/HPTT
- Tensor Contraction Code Generator TCCG – github.com/HPAC/TCCG
- Tensor Contraction Library TCL – github.com/springer13/tcl
- TBLIS – by D. Matthews github.com/devinamatthews/tblis

Fast & portable code for complex molecular dynamics simulations



Molecular Dynamics Potentials

Name	**LOC-R**	**LOC-O**	**Structure**
LJ	640	+480	$\sum_i \sum_j f(i,j)$
Stillinger-Weber	600	+1250	$\sum_i \sum_j \sum_k f(i,j,k)$
EAM	840	+820	$\sum_i f(i, \sum_j g(i,j))$
Tersoff	800	+1450	$\sum_i \sum_j f(i,j, \sum_k g(i,j,k)$
MEAM	890	✗	$\sum_i f(i, \sum_j g(i,j))$
ADP	940	✗	too complex to show
BOP	5950	✗	too complex to show
(AI)REBO	4240	+4550	too complex to show
COMB3	3560	✗	too complex to show
ReaxFF	10880	✗	too complex to show

LOC-R: Lines of code of the regular code.

LOC-O: Extra LOC in the optimized/vectorized code.

Formalism: Pair vs Many-body

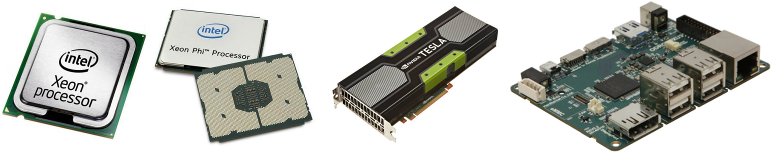
$$V = \sum_i \sum_j V(i, j)$$

$$F_i = -\nabla_{x_i} V$$

```
for i in atoms:
    for j in neighbors(i):
        V += V(i, j)
        F[i] -= dVdi(i, j)
        F[j] -= dVdj(i, j)
```

$$V = \sum_i \sum_j V(i, j, \sum_k f(i, j, k))$$

```
for i in atoms:
  for j in neighbors(i):
    tmp = 0
    for k in neighbors(i):
      tmp += f(i, j, k)
    V += V(i, j, tmp)
    F[i] -= dVdi(i, j, tmp)
    F[j] -= dVdj(i, j, tmp)
    tmp = dVdf(i, j, tmp)
    for k in neighbors(i):
      F[i] -= tmp * dfdi(i, j, k)
      F[j] -= tmp * dfdj(i, j, k)
      F[k] -= tmp * dfdk(i, j, k)
```



2013, 2014, 2015, 2016, 2017, 2018, 2019, . . .

One trend for Intel, ARM: Longer *vectors*

Need: Formulate program right, across differing HW

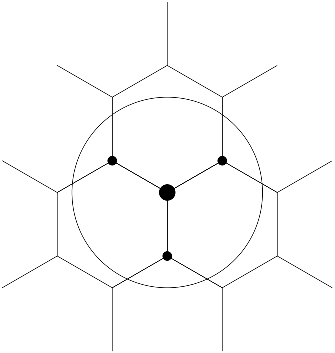
Everywhere...

x86	SSE	128 bit
	AVX(2)	256 bit
	AVX-512 (IMCI)	512 bit
ARM	NEON	128 bit
	SVE	up to 2048 bit
POWER	AltiVec/VMX/VSX	128 bit
	QPX	256 bit
SPARC	HPC-ACE	128 bit
	HPC-ACE2	256 bit

Manual Optimization: Tersoff

$\boxed{\text{Si}}\ \boxed{\text{C}}\ \boxed{\text{O}}\ \boxed{\text{Ga}}\ \boxed{\text{Ge}}\ \boxed{\text{B}}\ \boxed{\text{N}}$

$$V = \sum_i \sum_j V(i, j, \sum_k f(i, j, k))$$



Tersoff: Optimizations

Vector class library

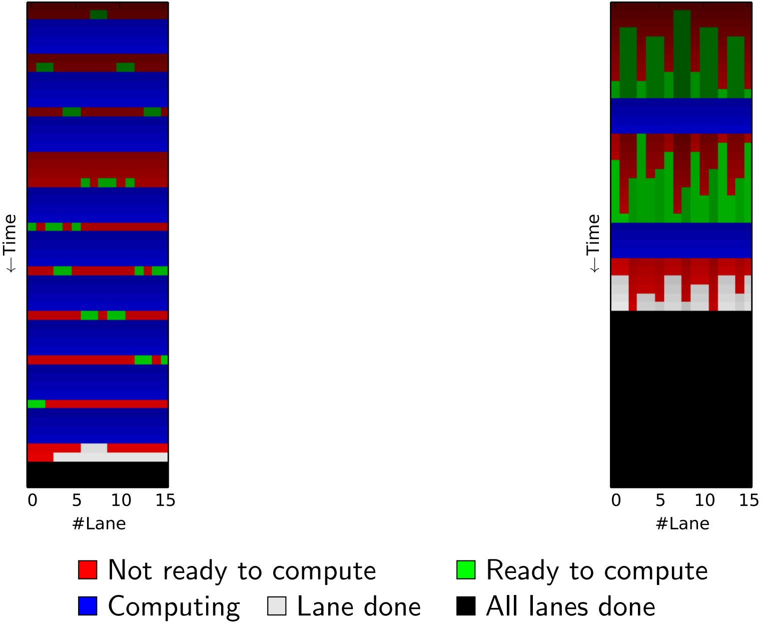
Reuse inner (k) calculation

Vectorization schemes: assign i, assign j, assign i and j

Fast forwarding

Neighbor list filtering

Tersoff: Fast forwarding



Tersoff: Neighbor list filtering

We iterate over the neighbor list multiple times.

Each time, we check whether the atom is within the cutoff

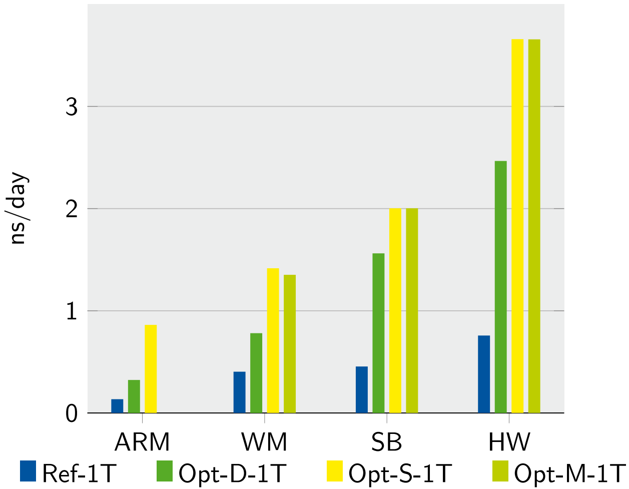
Redundant: Only do once, store the ones within cutoff

```
for (int i = ...) {
  if (foo(i)) continue;
  bar_1(i); }
bar_2();
for (int i = ...) {
  if (foo(i)) continue;
  bar_3(i); }
```

```
int n = 0, arr[MAX_N];
for (int i = ...) {
  if (foo(i)) continue;
  arr[n++] = i; }
for (int i = 0..n) {
  bar_1(arr[i]); }
bar_2();
for (int i = 0..n) {
  bar_3(arr[i]); }
```

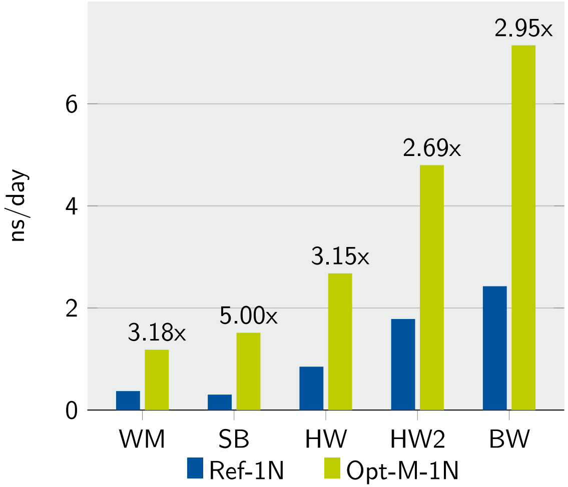
This technique has been adopted in LAMMPS

CPU: Single-Threaded Execution (32 000 atoms)



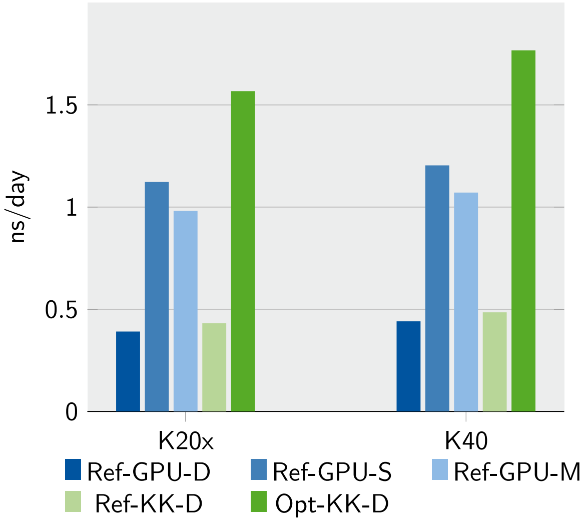
Name	Processor	Cores	Vector ISA
ARM	ARM Cortex-A15	2 × 4[1]	NEON
WM	Intel Xeon X5675	2 × 6	SSE4.2
SB	Intel Xeon E5-2450	2 × 8	AVX
HW	Intel Xeon E5-2680v3	2 × 12	AVX2

CPU: Single Node Execution (512 000 atoms)



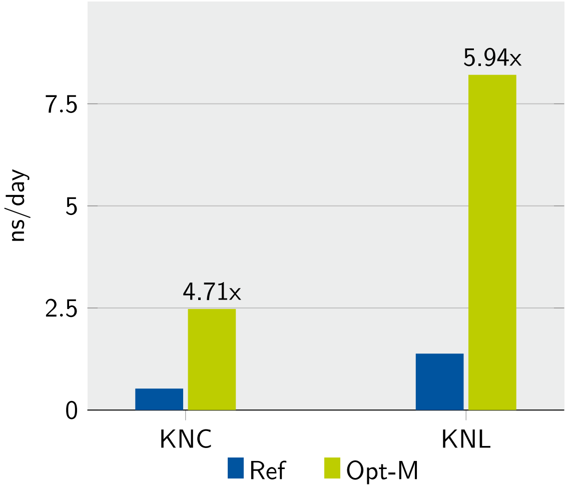
Name	Processor	Cores	Vector ISA
WM	Intel Xeon X5675	2 × 6	SSE4.2
SB	Intel Xeon E5-2450	2 × 8	AVX
HW	Intel Xeon E5-2680v3	2 × 12	AVX2
HW2	Intel Xeon E5-2697v3	2 × 14	AVX2
BW	Intel Xeon E5-2697v4	2 × 18	AVX2

GPU (256 000 atoms)



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

Manual Optimization: AIREBO

$$\boxed{\text{C}}\ \boxed{\text{H}}$$

$$V = \sum_i \sum_j^i V(i, j, \sum_k^i f(i,k), \sum_l^j f(j,l), \sum_k^i \sum_l^j g(i,j,k,l))$$

$$+ \sum_i \sum_j^i \sum_k^i \sum_l^j V'(i,j,k,l)$$

$$+ \sum_i \sum_j^{i'} V''(i, j, \max g(i,j,k,l) \forall k, l, \sum_k^i f(i,k), \sum_l^j f(j,l), \sum_k^i \sum_l^j g(i,j,k,l))$$

Two neighborhoods: Small and large ($\sum^i$ vs $\sum^{i'}$)

AIREBO: Optimizations

Intermediate neighbor list

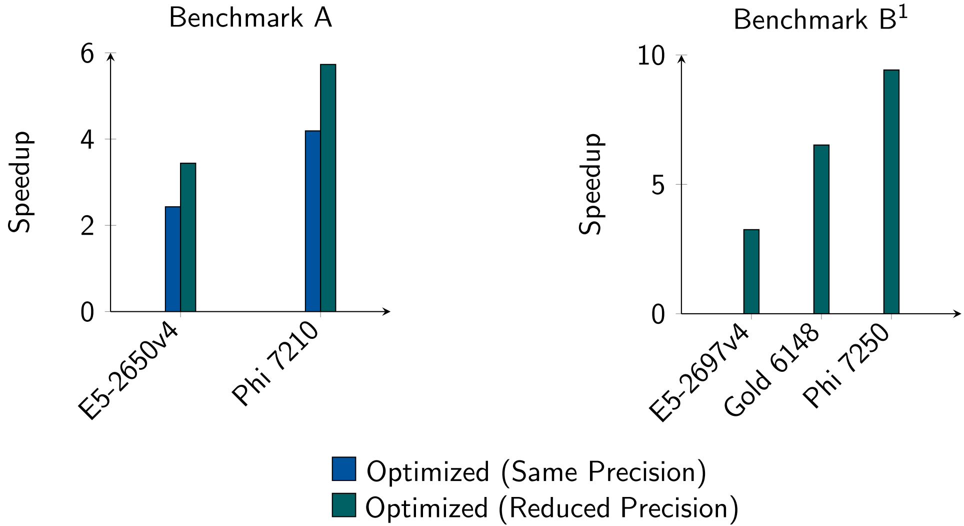
Compression

Batching by atom species

Reuse of intermediate values

Global search and lookup (hash-map) instead of local search

AIREBO: Results



[1] M. Brown (Intel): Speedups from http://lammps.sandia.gov/doc/accelerate_intel.html, Oct. 2017.

What's wrong with manual optimization?

N optimization techniques (we saw about 5 of them)

M hardware platforms (we saw more than 5 of them)

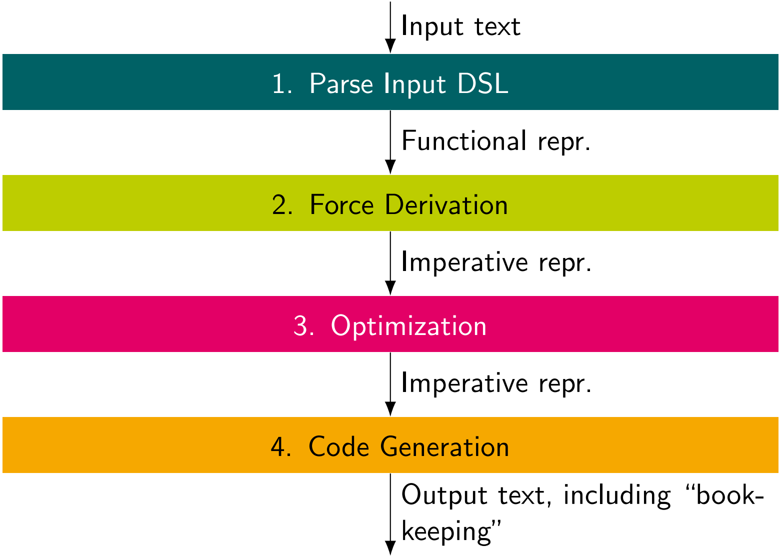
K potentials (we saw 10, but there are many more)

Without platform abstraction: $N \times M \times K$ implementations

With platform abstraction: $N \times K$ implementations

But: Technique may depend on HW platform...

Our approach: PotC, A domain-specific language and a compiler



Input text

1. Parse Input DSL

Functional repr.

2. Force Derivation

Imperative repr.

3. Optimization

Imperative repr.

4. Code Generation

Output text, including “book-keeping”

More advantages

Not *best* performane, but *good* performance

Portability

Ease of implementation

Coverage

Prototyping

Testing

Mechanical exploration (Profiling/Precision)

Other symbolic manipulations

DSL: Overview

```
parameter A(i: atom_type; j: atom_type) = file(1);
function V(i: atom; j: atom) = ...;
energy sum(i: all_atoms)
         sum(j: neighbors(A(i, j), i)) V(i, j);
```

DSL: Sums

```
sum(<index>:  all_atoms) ...

sum(<index>:  neighbors(<cutoff>, <center_atom>[,
exclusions]) ...

sum(<index>:  neighbors_half(...)  ...

sum(i: all_atoms) sum(j: neighbors(r_C(i, j), i)) V(i, j)
```

DSL: Parameters

```
parameter <name>({<name>:  atom_type;}*) = file(<n>);
```

```
parameter <name>({<name_i>:  real;}*)=
spline(<name>, <degree>, {<dimension_i>}*[,
<derivative_spec>]);
```

DSL: Functions

```
function <name>({<param>: <type>;}*) = <expr>;
```

```
function abs(x: real) = sqrt(x*x);
```

DSL: Other features

```
piecewise({<cond>: <val>;}*)

function abs(x: real) = piecewise(x < 0: -x; x >= 0: x);

let(<name>: <val>)

function abs(x: real) = let(a: x*x) sqrt(a);
```

DSL: Putting it all together

```
energy 1 / 2 * sum(i : all_atoms)
  sum(j : neighbors(i, R(i, j, j) + D(i, j, j))) V(i, j);
function V(i : atom; j : atom) =  f_C(i, j, r(i, j)) *
 (f_R(i, j, r(i, j)) + b(i, j) * f_A(i, j, r(i, j)));
function f_C(i : atom_type; j : atom_type; k : atom_type; r : distance) =
 implicit(i : i; j : j; k : k) piecewise(r <= R - D : 1;
 R - D < r < R + D: 1 / 2 - 1 / 2 * sin(pi / 2 * (r - R) / D); r >= R + D : 0);
# ...
function b(i : atom; j : atom) = (1 + beta(i, j) ^ n(i, j) *
  zeta(i, j) ^ n(i, j)) ^ (-1 / (2 * n(i, j)));
function zeta(i : atom; j : atom) =
 sum(k : neighbors(i, R(i, j, k) + D(i, j, k), j))
 implicit(i : i; j : j; k : k) f_C(r(i, k)) * g(theta(j, i, k)) *
   exp(lambda_3 ^ m * (r(i, j) - r(i, k)) ^ m);
parameter A(i : atom_type; j : atom_type) = file(1);
# ...
parameter gamma(i : atom_type; j : atom_type; k : atom_type) = file(5);
# Total: ~ 30 LOC, while LAMMPS impl > 500 LOC
```

Optimization: Overview

The initial code is far from optimal since it recomputes a lot of values.

No tape due to memory constraints.

Inlining

Loop/Conditional Fusion

Dead Code Elimination

Common Subexpression Elimination

Arithmetic Improvements (e.g Constant Folding)

Loop Invariant Code Motion

Vectorization

Check for 0

Caching

Batching

Optimization: CSE and LICM

Two techniques commonly used by any compiler.

Common Subexpression Elimination

Loop Invariant Code Motion

Compilers often are not sophisticated enough to move loop invariant control flow out

```
double a = foo(x);             double a = foo(x);
double b = foo(x) * bar(y);    double b = a * bar(y);

for (int i = ...) {            double a = foo(x);
  double a = foo(x);           for (int i = ...) {
  ...                            ...
}                              }
```

Optimization: Neighbor list filtering

We used this for both Tersoff and AIREBO

One of the crucial techniques that compilers are unlikely to ever perform

Applied as soon as a neighbor list is traversed more than once

```
for (int i = ...) {
  if (foo(i)) continue;
  bar_1(i); }
bar_2();
for (int i = ...) {
  if (foo(i)) continue;
  bar_3(i); }
```

```
int n = 0, arr[MAX_N];
for (int i = ...) {
  if (foo(i)) continue;
  arr[n++] = i; }
for (int i = 0..n) {
  bar_1(arr[i]); }
bar_2();
for (int i = 0..n) {
  bar_3(arr[i]); }
```

Optimization: Vectorization

Force the compiler: We know it will work

Apply the fast-forwarding logic we used for both AIREBO and Tersoff

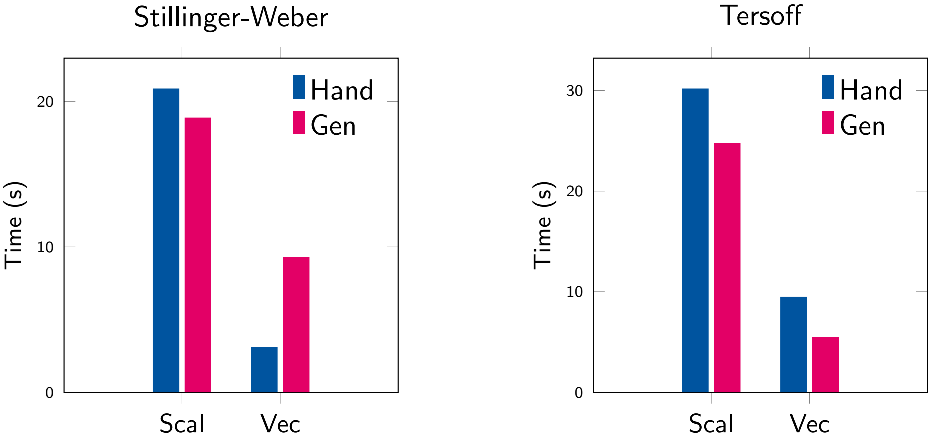
Assumption: The check is much cheaper than the calculation

Can perform idioms compilers do not yet support without intrinsics

```
for_VEC (int i=...) {
  for (int j=...) {
    if (foo(i, j)) continue;
    bar(i, j);
  }
}
```

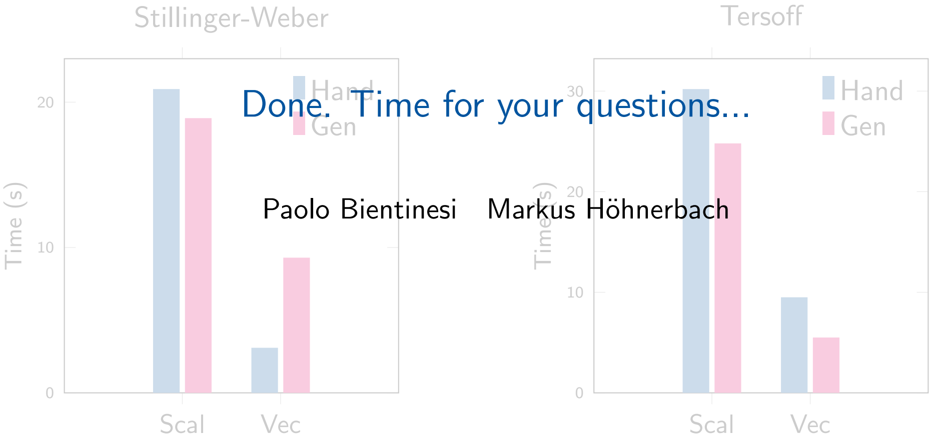
```
for_VEC (int i=...) {
  for (int j=...) {
    if (ANY(foo(i, j))) {
      if (foo(i, j)) {
        j += 1; }
      continue; }
    bar(i, j);
  }
```

Results



KNL, double precision, single core.

Results



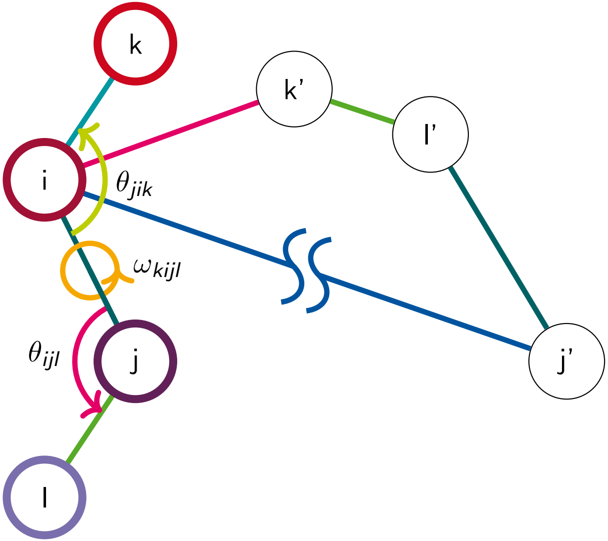
Done. Time for your questions...

Paolo Bientinesi   Markus Höhnerbach

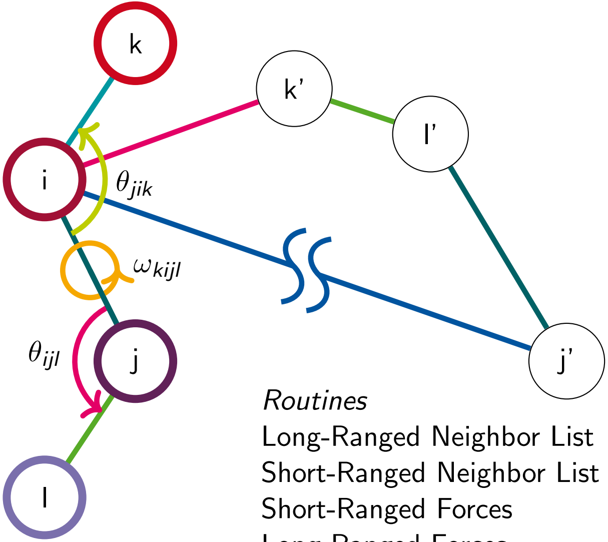
KNL, double precision, single core.

Backup

AIREBO



AIREBO



Routines

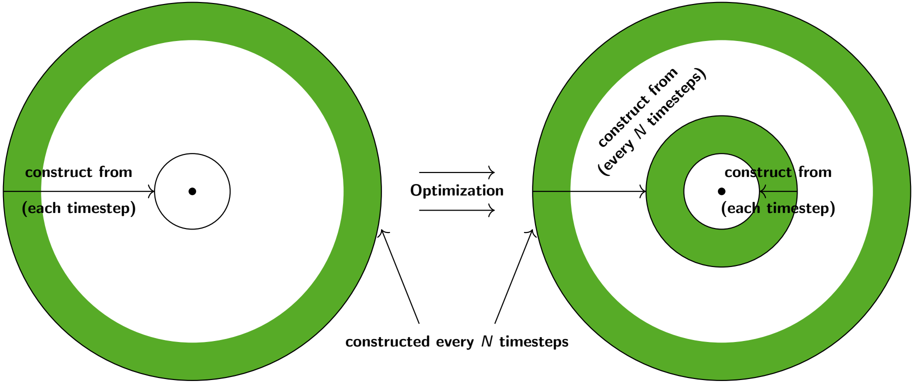
Long-Ranged Neighbor List

Short-Ranged Neighbor List

Short-Ranged Forces

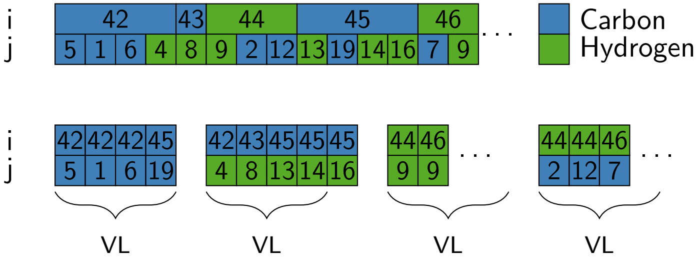
Long-Ranged Forces

Short-Ranged Neighbor List



Consider fewer atoms for short neighbor list each timestep.

Short-Ranged Contributions: Sorting



i	42				43	44			45				46		. . .
j	5	1	6	4	8	9	2	12	13	19	14	16	7	9	

🟦 Carbon

🟩 Hydrogen

i	42	42	42	45
j	5	1	6	19

VL

i	42	43	45	45	45
j	4	8	13	14	16

VL

i	44	46
j	9	9

. . .

VL

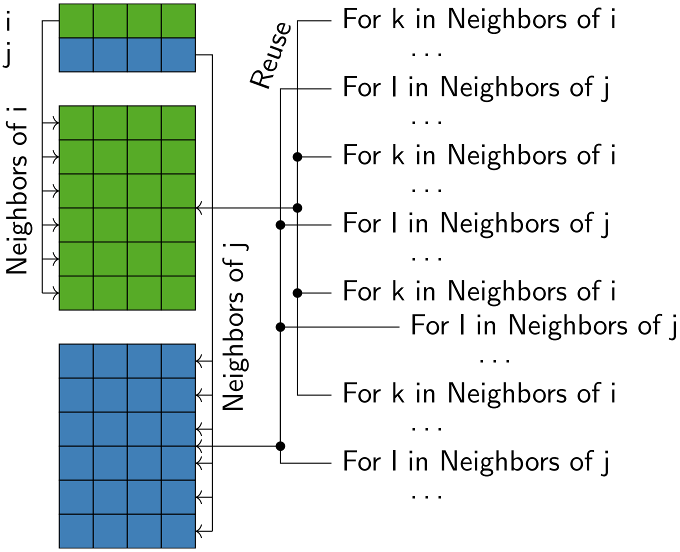
i	44	44	46
j	2	12	7

. . .

VL

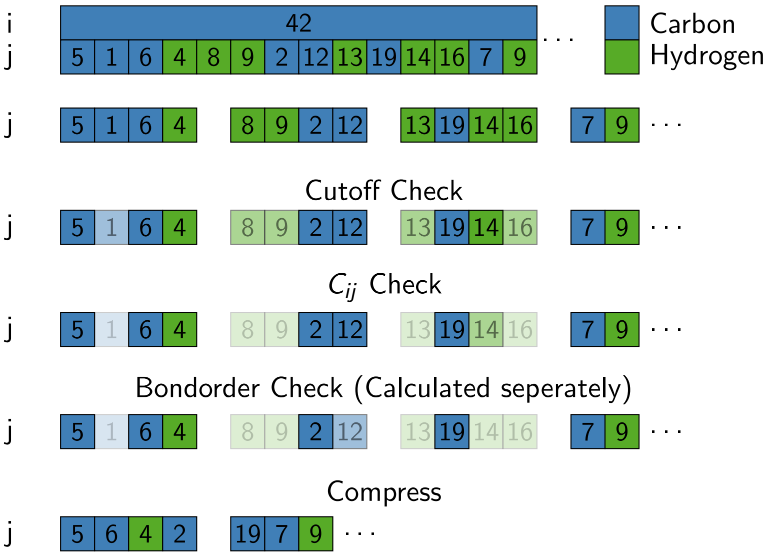
Vectorize over interactions and bin by species.

Short-Ranged Contributions: Reuse



```
For k in Neighbors of i
    . . .
For l in Neighbors of j
    . . .
For k in Neighbors of i
    . . .
For l in Neighbors of j
    . . .
For k in Neighbors of i
    For l in Neighbors of j
        . . .
For k in Neighbors of i
    . . .
For l in Neighbors of j
    . . .
```

Long-Ranged Contributions: Compression



i 42 · · ·

j 5 1 6 4 8 9 2 12 13 19 14 16 7 9

🟦 Carbon

🟩 Hydrogen

j 5 1 6 4 | 8 9 2 12 | 13 19 14 16 | 7 9 · · ·

Cutoff Check

j 5 1 6 4 | 8 9 2 12 | 13 19 14 16 | 7 9 · · ·

C_{ij} Check

j 5 1 6 4 | 8 9 2 12 | 13 19 14 16 | 7 9 · · ·

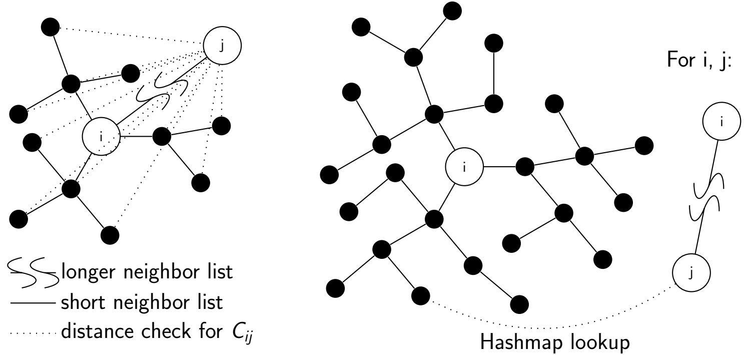
Bondorder Check (Calculated seperately)

j 5 1 6 4 | 8 9 2 12 | 13 19 14 16 | 7 9 · · ·

Compress

j 5 6 4 2 | 19 7 9 · · ·

Long-Ranged Contributions: Hashmap



For i, j: Search neighbors.

For i: Insert candidates into hashmap.

For i, j:

longer neighbor list

short neighbor list

distance check for C_{ij}

Hashmap lookup

Precompute hashmap to replace search with lookups.