Particle-Particle Particle-Mesh (P3M) on Knights Landing Processors

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Intermolecular Forces

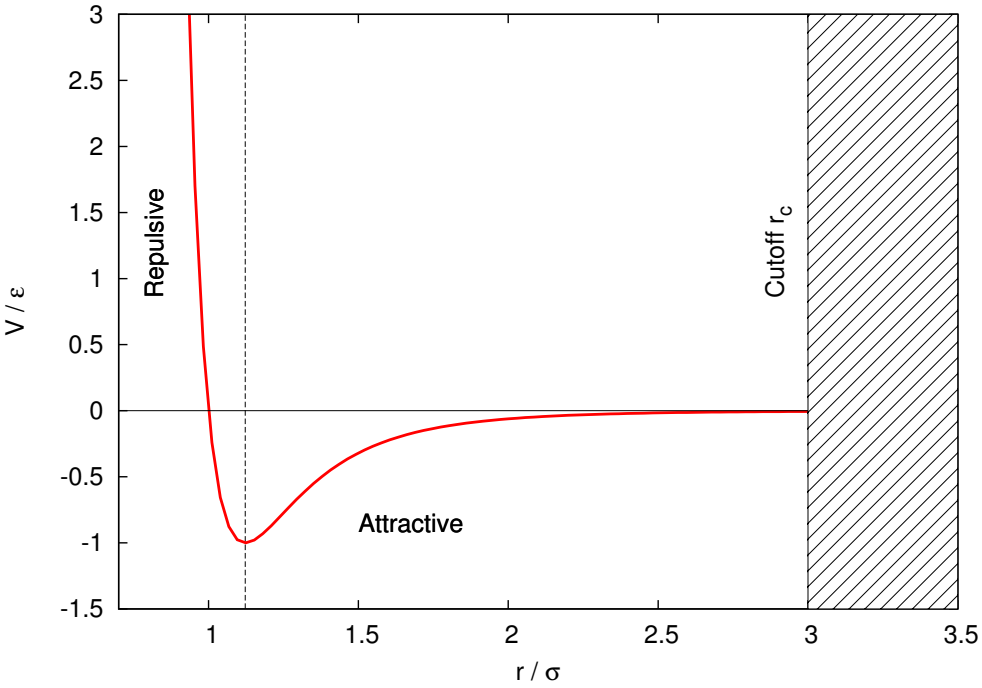
The forces on atoms are commonly taken to be the result of independent pair-wise interactions.

Lennard-Jones potential:

$$\Phi_{LJ} = \sum_{r_{ij}<r_c} 4\,\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

Where the force on an atom is given by:

$$\vec{F} = -\nabla \Phi$$



But long-range forces can be important!

The electrical potential only decreases as 1/r and doesn't perfectly cancel for polar molecules.

Interfaces can also create asymmetries that inhibit cancellation.

Particle-Particle Particle-Mesh

- PPPM[1] approximates long-range forces without requiring pair-wise calculations.

Four Steps:

1. Determine the charge distribution ρ by mapping particle charges to a grid.

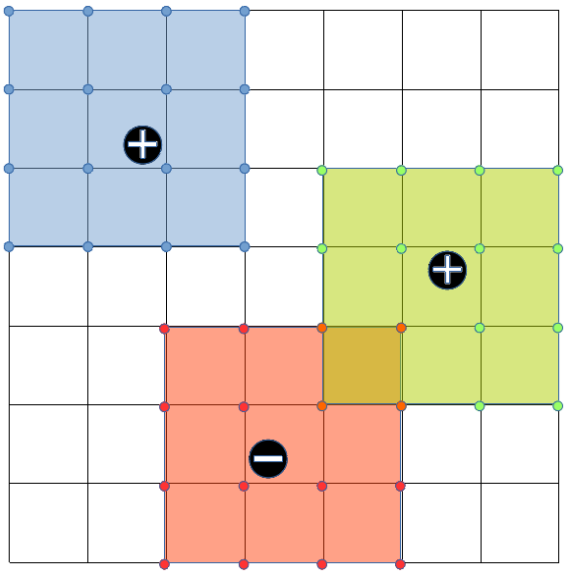
2. Take the Fourier transform of the charge distribution to find the potential:

$$\nabla^2 \Phi = -\frac{\rho}{\epsilon_0}$$

3. Obtain forces due to *all* interactions as the gradient of Φ by inverse Fourier transform:

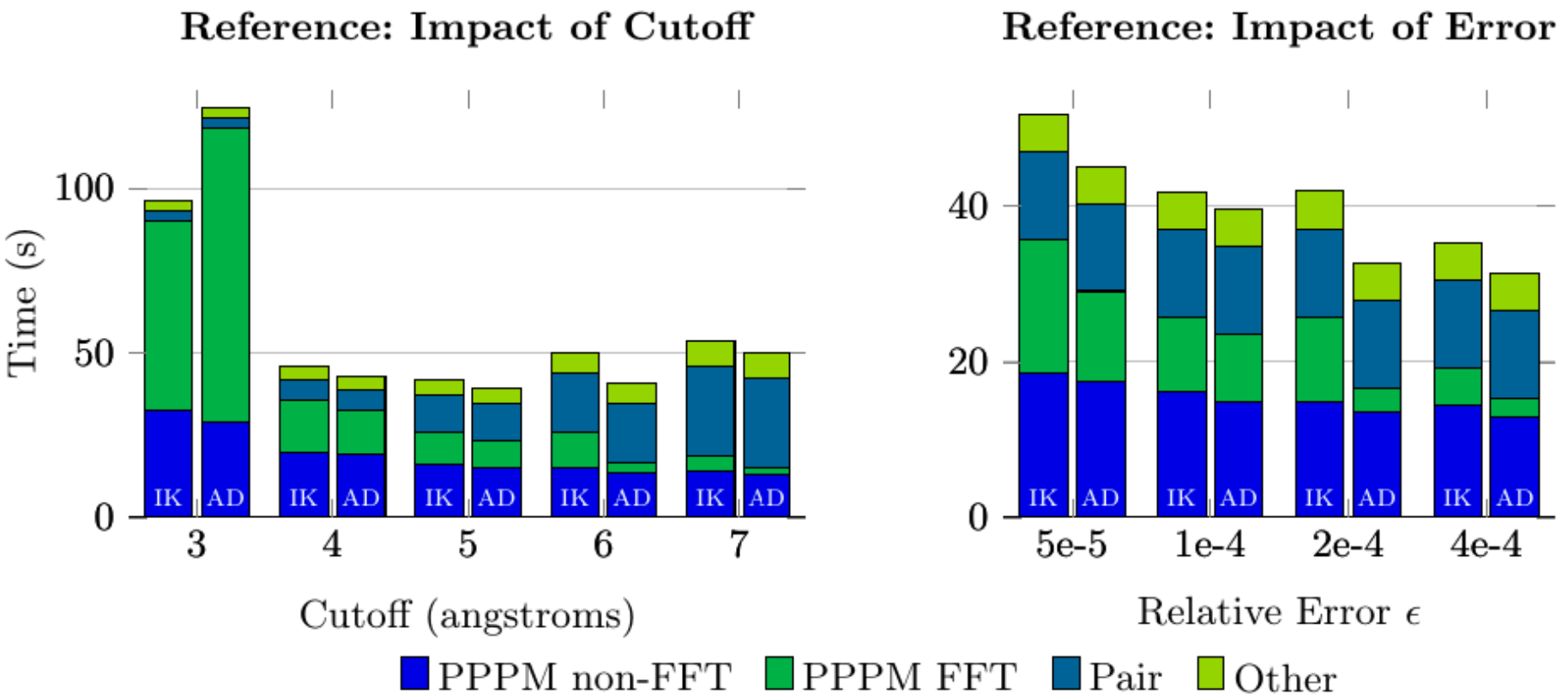
$$\vec{F} = -\nabla \Phi$$

4. Map forces back to the particles.



1. Hockney and Eastwood, 1988

Profiling LAMMPS



We use the USER-OMP implementation of LAMMPS as a baseline.
Typically: r_c is 6 angstroms, relative error is 0.0001, and stencil size is 5.

The work in FFTs increases rapidly at low cutoffs.
The non-FFT work in PPPM is insensitive to grid size.
Sometimes the FFTs take surprisingly long.

Water benchmark:
40.5k atoms
884k FFT grid points

Charge Mapping

```
for (int i = 0; i < nlocal; i++) {

  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  if( (nz+nlower-nzlo_out)*niy*nix >= jto || (nz-nzlo_out + nupper + 1)*niy*nix <= jfrom )
    continue;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1,r2,r3;
    r1 = r2 = r3 = ZEROF;

    for (int l = order-1; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR z0 = fdelvolinv * q[i];

  for (int n = nlower; n <= nupper; n++) {
    int mz = (n + nz - nzlo_out)*nix*niy;
    FFT_SCALAR y0 = z0*rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++) {
      int mzy = mz + (m + ny - nylo_out)*nix;
      FFT_SCALAR x0 = y0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l++) {
        int mzyx = mzy + l + nx - nxlo_out;
        if (mzyx >= jto) break;
        if (mzyx < jfrom) continue;
        densityThr[mzyx] += x0*rho[0][l-nlower];
      }
    }
  }
}
}
```

Loop over atoms in MPI rank

Stencil coefficients are polynomials of order stencil size. 3x[stencil size] of them are computed.

Loop over cubic stencil and contribute to grid points

USER-OMP Implementation

Charge Mapping

```
for (int i = 0; i < nlocal; i++) {

  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  if( (nz+nlower-nzlo_out)*niy*nix >= jto || (nz-nzlo_out + nupper + 1)*niy*nix <= jfrom )
    continue;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1,r2,r3;
    r1 = r2 = r3 = ZEROF;

    for (int l = order-1; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR z0 = fdelvolinv * q[i];

  for (int n = nlower; n <= nupper; n++) {
    int mz = (n + nz - nzlo_out)*nix*niy;
    FFT_SCALAR y0 = z0*rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++) {
      int mzy = mz + (m + ny - nylo_out)*nix;
      FFT_SCALAR x0 = y0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l++) {
        int mzyx = mzy + l + nx - nxlo_out;
        if (mzyx >= jto) break;
        if (mzyx < jfrom) continue;
        densityThr[mzyx] += x0*rho[0][l-nlower];
      }
    }
  }
}
}
```

```
for (int i = 0; i < nlocal; i++) {
```

Loop over atoms in MPI rank

USER-OMP Implementation

Charge Mapping

```
for (int i = 0; i < nlocal; i++) {

  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  if( (nz+nlower-nzlo_out)*niy*nix >= jto || (nz-nzlo_
    continue;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1,r2,r3;
    r1 = r2 = r3 = ZEROF;

    for (int l = order-1; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR z0 = fdelvolinv * q[i];

  for (int n = nlower; n <= nupper; n++) {
    int mz = (n + nz - nzlo_out)*nix*niy;
    FFT_SCALAR y0 = z0*rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++) {
      int mzy = mz + (m + ny - nylo_out)*nix;
      FFT_SCALAR x0 = y0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l++) {
        int mzyx = mzy + l + nx - nxlo_out;
        if (mzyx >= jto) break;
        if (mzyx < jfrom) continue;
        densityThr[mzyx] += x0*rho[0][l-nlower];
      }
    }
  }
}
}
```

USER-OMP Implementation

Stencil coefficients are polynomials of order stencil size. 3x[stencil size] are computed.

```
for (int k = nlower; k <= nupper; k++) {
  FFT_SCALAR r1,r2,r3;
  r1 = r2 = r3 = ZEROF;

  for (int l = order-1; l >= 0; l--) {
    r1 = rho_coeff[l][k] + r1*dx;
    r2 = rho_coeff[l][k] + r2*dy;
    r3 = rho_coeff[l][k] + r3*dz;
  }
  rho[0][k-nlower] = r1;
  rho[1][k-nlower] = r2;
  rho[2][k-nlower] = r3;
}
```

Charge Mapping

```
for (int i = 0; i < nlocal; i++) {

  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  if( (nz+nlower-nzlo_out)*niy*nix >= jto || (nz-nzlo_out + nupper + 1)*niy*nix <= jfrom )
    continue;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1,r2,r3;
    r1 = r2 = r3 = ZEROF;

    for (int l = order-1; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR z0 = fdelvolinv * q[i];

  for (int n = nlower; n <= nupper; n++) {
    int mz = (n + nz - nzlo_out)*nix*niy;
    FFT_SCALAR y0 = z0*rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++)
      int mzy = mz + (m + ny - nylo_out)*n
      FFT_SCALAR x0 = y0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l+
        int mzyx = mzy + l + nx - nxlo_out
        if (mzyx >= jto) break;
        if (mzyx < jfrom) continue;
        densityThr[mzyx] += x0*rho[0][l-nl
      }
    }
  }
}
```

Loop over cubic stencil and contribute to grid points

```
for (int n = nlower; n <= nupper; n++) {
  int mz = (n + nz - nzlo_out)*nix*niy;
  FFT_SCALAR y0 = z0*rho[2][n-nlower];
  for (int m = nlower; m <= nupper; m++) {
    int mzy = mz + (m + ny - nylo_out)*nix;
    FFT_SCALAR x0 = y0*rho[1][m-nlower];
    for (int l = nlower; l <= nupper; l++) {
      int mzyx = mzy + l + nx - nxlo_out;
      if (mzyx >= jto) break;
      if (mzyx < jfrom) continue;
      densityThr[mzyx] += x0*rho[0][l-nlower];
    }
  }
}
```

USER-OMP Implementation

Charge Mapping

```
for (int i = 0; i < nlocal; i++) {

  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  if( (nz+nlower-nzlo_out)*niy*nix >= jto || (nz-nzlo_out
    continue;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1,r2,r3;
    r1 = r2 = r3 = ZEROF;

    for (int l = order-1; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR z0 = fdelvolinv * q[i];

  for (int n = nlower; n <= nupper; n++) {
    int mz = (n + nz - nzlo_out)*nix*niy;
    FFT_SCALAR y0 = z0*rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++) {
      int mzy = mz + (m + ny - nylo_out)*nix;
      FFT_SCALAR x0 = y0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l++) {
        int mzyx = mzy + l + nx - nxlo_out;
        if (mzyx >= jto) break;
        if (mzyx < jfrom) continue;
        densityThr[mzyx] += x0*rho[0][l-nlower];
      }
    }
  }
}
}
```

USER-OMP Implementation

```
  for (int i = jfrom; i < jto; i++) {

    int nx = part2grid[i][0];
    int ny = part2grid[i][1];
    int nz = part2grid[i][2];

    int nysum = nlower + ny - nylo_out;
    int nxsum = nlower + nx - nxlo_out + ngrid*tid;
    int nzsum = (nlower + nz - nzlo_out)*nix*niy + nysum*nix + nxsum;

    FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
    FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
    FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

#pragma simd
    for (int k = nlower; k <= nupper; k++) {
      FFT_SCALAR r1,r2,r3;
      r1 = r2 = r3 = ZEROF;

      for (int l = order-1; l >= 0; l--) {
        r1 = rho_coeff[l][k] + r1*dx;
        r2 = rho_coeff[l][k] + r2*dy;
        r3 = rho_coeff[l][k] + r3*dz;
      }
      rho[0][k-nlower] = r1;
      rho[1][k-nlower] = r2;
      rho[2][k-nlower] = r3;
    }

    FFT_SCALAR z0 = fdelvolinv * q[i];

#pragma loop_count=7
    for (int n = 0; n < tripcount; n++) {
      int mz = n*nix*niy + nzsum;
      FFT_SCALAR y0 = z0*rho[2][n];

#pragma loop_count=7
      for (int m = 0; m < tripcount; m++) {
        int mzy = mz + m*nix;
        FFT_SCALAR x0 = y0*rho[1][m];
#pragma simd
        for (int l = 0; l < 8; l++) {
          int mzyx = mzy + l;
          localDensity[mzyx] += x0*rho[0][l];
        }
      }
    }

  }
}
```

Our Implementation

Thread over atoms

#pragma simd
for coefficients

Charge Mapping

Innermost loop vectorized with bigger stencil.
Private grids prevent race conditions.

```
#pragma loop_count=7
    for (int n = 0; n < tripcount; n++) {
      int mz = n*nix*niy + nzsum;
      FFT_SCALAR y0 = z0*rho[2][n];

#pragma loop_count=7
      for (int m = 0; m < tripcount; m++) {
        int mzy = mz + m*nix;
        FFT_SCALAR x0 = y0*rho[1][m];
#pragma simd
        for (int l = 0; l < 8; l++) {
          int mzyx = mzy + l;
          localDensity[mzyx] += x0*rho[0][l];
        }
      }
    }
```

Our Implementation

Distributing Forces **ik**

Very similar to charge mapping:
Computes stencil coefficients
Loops over stencil points.

More work and accesses more memory

Water benchmark:
40.5k atoms
884k FFT grid points

```
#if defined(LMP_SIMD_COMPILER)
#pragma vector aligned nontemporal
#pragma simd
#endif
for (int i = iifrom; i < iito; i++) {
  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1 = rho_coeff[order-1][k];
    FFT_SCALAR r2 = rho_coeff[order-1][k];
    FFT_SCALAR r3 = rho_coeff[order-1][k];
    for (int l = order-2; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR ekx, eky, ekz;
  ekx = eky = ekz = ZEROF;
  for (int n = nlower; n <= nupper; n++) {
    int mz = n+nz;
    FFT_SCALAR z0 = rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++) {
      int my = m+ny;
      FFT_SCALAR y0 = z0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l++) {
        int mx = l+nx;
        FFT_SCALAR x0 = y0*rho[0][l-nlower];
        ekx -= x0*vdx_brick[mz][my][mx];
        eky -= x0*vdy_brick[mz][my][mx];
        ekz -= x0*vdz_brick[mz][my][mx];
      }
    }
  }
```

#pragma simd around atom loop

Update 3 force components

Distributing Forces **ik**

Update 3 force components

```
FFT_SCALAR ekx, eky, ekz;
ekx = eky = ekz = ZEROF;
for (int n = nlower; n <= nupper; n++) {
  int mz = n+nz;
  FFT_SCALAR z0 = rho[2][n-nlower];
  for (int m = nlower; m <= nupper; m++) {
    int my = m+ny;
    FFT_SCALAR y0 = z0*rho[1][m-nlower];
    for (int l = nlower; l <= nupper; l++) {
      int mx = l+nx;
      FFT_SCALAR x0 = y0*rho[0][l-nlower];
      ekx -= x0*vdx_brick[mz][my][mx];
      eky -= x0*vdy_brick[mz][my][mx];
      ekz -= x0*vdz_brick[mz][my][mx];
    }
  }
}
```

```
#if defined(LMP_SIMD_COMPILER)
#pragma vector aligned nontemporal
#pragma simd
#endif
for (int i = iifrom; i < iito; i++) {
  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];
  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  flt_t rho[3][INTEL_P3M_MAXORDER];

  for (int k = nlower; k <= nupper; k++) {
    FFT_SCALAR r1 = rho_coeff[order-1][k];
    FFT_SCALAR r2 = rho_coeff[order-1][k];
    FFT_SCALAR r3 = rho_coeff[order-1][k];
    for (int l = order-2; l >= 0; l--) {
      r1 = rho_coeff[l][k] + r1*dx;
      r2 = rho_coeff[l][k] + r2*dy;
      r3 = rho_coeff[l][k] + r3*dz;
    }
    rho[0][k-nlower] = r1;
    rho[1][k-nlower] = r2;
    rho[2][k-nlower] = r3;
  }

  FFT_SCALAR ekx, eky, ekz;
  ekx = eky = ekz = ZEROF;
  for (int n = nlower; n <= nupper; n++) {
    int mz = n+nz;
    FFT_SCALAR z0 = rho[2][n-nlower];
    for (int m = nlower; m <= nupper; m++) {
      int my = m+ny;
      FFT_SCALAR y0 = z0*rho[1][m-nlower];
      for (int l = nlower; l <= nupper; l++) {
        int mx = l+nx;
        FFT_SCALAR x0 = y0*rho[0][l-nlower];
        ekx -= x0*vdx_brick[mz][my][mx];
        eky -= x0*vdy_brick[mz][my][mx];
        ekz -= x0*vdz_brick[mz][my][mx];
      }
    }
  }
```

Distributing Forces **ik**

Inner SIMD

```
  for (int i = iifrom; i < iito; i++) {
    int nx = part2grid[i][0];
    int ny = part2grid[i][1];
    int nz = part2grid[i][2];

    int nxsum = nx + nlower;
    int nysum = ny + nlower;
    int nzsum = nz + nlower;

    FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
    FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
    FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

    #pragma simd
    for (int k = nlower; k <= nupper; k++) {
      FFT_SCALAR r1, r2, r3;
      r1 = r2 = r3 = ZEROF;
      for (int l = order-1; l >= 0; l--) {
        r1 = rho_coeff[l][k] + r1*dx;
        r2 = rho_coeff[l][k] + r2*dy;
        r3 = rho_coeff[l][k] + r3*dz;
      }
      rho[0][k-nlower] = r1;
      rho[1][k-nlower] = r2;
      rho[2][k-nlower] = r3;
    }

    FFT_SCALAR ekx[8]={ZEROF}, eky[8]={ZEROF}, ekz[8]={ZEROF};
    FFT_SCALAR ekxsum, ekysum, ekzsum;
    ekxsum = ekysum = ekzsum = ZEROF;

    for (int n = 0; n < tripcount; n++) {
      int mz = n+nzsum;
      FFT_SCALAR z0 = rho[2][n];

      for (int m = 0; m < tripcount; m++) {
        int my = m+nysum;
        FFT_SCALAR y0 = z0*rho[1][m];
#pragma simd
        for (int l = 0; l < 8; l++) {
          int mx = l+nxsum;
          FFT_SCALAR x0 = y0*rho[0][l];
          ekx[l] -= x0*vdx_brick[mz][my][mx];
          eky[l] -= x0*vdy_brick[mz][my][mx];
          ekz[l] -= x0*vdz_brick[mz][my][mx];
        }
      }
    }

    for (int l = 0; l < tripcount; l++){
        ekxsum += ekx[l];
        ekysum += eky[l];
        ekzsum += ekz[l];
    }
```

Distributing Forces **ik**

```
for (int i = iifrom; i < iito; i++) {
  int nx = part2grid[i][0];
  int ny = part2grid[i][1];
  int nz = part2grid[i][2];

  int nxsum = nx + nlower;
  int nysum = ny + nlower;
  int nzsum = nz + nlower;

  FFT_SCALAR dx = nx+fshiftone - (x[i].x-lo0)*xi;
  FFT_SCALAR dy = ny+fshiftone - (x[i].y-lo1)*yi;
  FFT_SCALAR dz = nz+fshiftone - (x[i].z-lo2)*zi;

  for (int n = 0; n < tripcount; n++) {
    int mz = n+nzsum;
    FFT_SCALAR z0 = rho[2][n];

    for (int m = 0; m < tripcount; m++) {
      int my = m+nysum;
      FFT_SCALAR y0 = z0*rho[1][m];
#pragma simd
      for (int l = 0; l < 8; l++) {
        int mx = l+nxsum;
        FFT_SCALAR x0 = y0*rho[0][l];
        ekx[l] -= x0*vdx_brick[mz][my][mx];
        eky[l] -= x0*vdy_brick[mz][my][mx];
        ekz[l] -= x0*vdz_brick[mz][my][mx];
      }
    }
  }

  for (int l = 0; l < tripcount; l++){
    ekxsum += ekx[l];
    ekysum += eky[l];
    ekzsum += ekz[l];
  }
}
```

Inner SIMD

10% faster with tripcount instead of 7

50% faster with 8 instead of 7

Reduction of force component arrays

Distributing Forces **ik**

```
for (int iz = 0; iz < niz; iz++) {
  for (int iy = 0; iy < niy; iy++) {
    for ( int ix = 0; ix < nix; ix++) {
    int iter = 2*(iz*niy*nix + iy*nix + ix);
      vdxy_brick[iter] = vdx_brick[nzlo_out + iz][nylo_out + iy][nxlo_out + ix];
      vdxy_brick[iter+1] = vdy_brick[nzlo_out + iz][nylo_out + iy][nxlo_out + ix];
      vdz0_brick[iter] = vdz_brick[nzlo_out + iz][nylo_out + iy][nxlo_out + ix];
      vdz0_brick[iter+1] = 0.;
    }
  }
}
```

```
    for (int n = 0; n < tripcount; n++) {
      int mz = 2*n*nix*niy+nzsum;
      FFT_SCALAR z0 = rho2[n];

      for (int m = 0; m < tripcount; m++) {
        int mzy = mz + 2*m*nix;
        FFT_SCALAR y0 = z0*rho1[m];
#pragma simd
        for (int l = 0; l < 16; l++) {
          FFT_SCALAR x0 = y0*rho0[l];
          ekxy[l] -= x0*vdxy_brick[mzy+l];
          ekz0[l] -= x0*vdz0_brick[mzy+l];
        }
      }
    }

    for (int l = 0; l < 16; l=l+2){
        ekxsum += ekxy[l];
        ekysum += ekxy[l+1];
        ekzsum += ekz0[l];
    }
```

3 vector operations instead of 4: 60% faster

16-iteration loops are faster on KNL, even with extra 0s

Distributing Forces **ad**

Different “flavors” of PPPM have the same overall structure

```
for (int k = nlower; k <= nupper; k++) {
  FFT_SCALAR r1,r2,r3,dr1,dr2,dr3;
  dr1 = dr2 = dr3 = ZEROF;

  r1 = rho_coeff[order-1][k];
  r2 = rho_coeff[order-1][k];
  r3 = rho_coeff[order-1][k];
  for (int l = order-2; l >= 0; l--) {
    r1 = rho_coeff[l][k] + r1 * dx;
    r2 = rho_coeff[l][k] + r2 * dy;
    r3 = rho_coeff[l][k] + r3 * dz;
    dr1 = drho_coeff[l][k] + dr1 * dx;
    dr2 = drho_coeff[l][k] + dr2 * dy;
    dr3 = drho_coeff[l][k] + dr3 * dz;
  }
  rho[0][k-nlower] = r1;
  rho[1][k-nlower] = r2;
  rho[2][k-nlower] = r3;
  drho[0][k-nlower] = dr1;
  drho[1][k-nlower] = dr2;
  drho[2][k-nlower] = dr3;
}
```

6 coefficients are computed for each stencil point

Distributing Forces **ad**

Different “flavors” of PPPM have the same overall structure

```
for (int n = nlower; n <= nupper; n++) {
  int mz = n+nz;
  for (int m = nlower; m <= nupper; m++) {
    int my = m+ny;
    FFT_SCALAR ekx_p = rho[1][m-nlower] * rho[2][n-nlower];
    FFT_SCALAR eky_p = drho[1][m-nlower] * rho[2][n-nlower];
    FFT_SCALAR ekz_p = rho[1][m-nlower] * drho[2][n-nlower];
    for (int l = nlower; l <= nupper; l++) {
      int mx = l+nx;
      ekx += drho[0][l-nlower] * ekx_p * u_brick[mz][my][mx];
      eky += rho[0][l-nlower] * eky_p * u_brick[mz][my][mx];
      ekz += rho[0][l-nlower] * ekz_p * u_brick[mz][my][mx];
    }
  }
}
```

Only one set of grid values is used to compute every component of the potential by choosing different combinations of coefficients

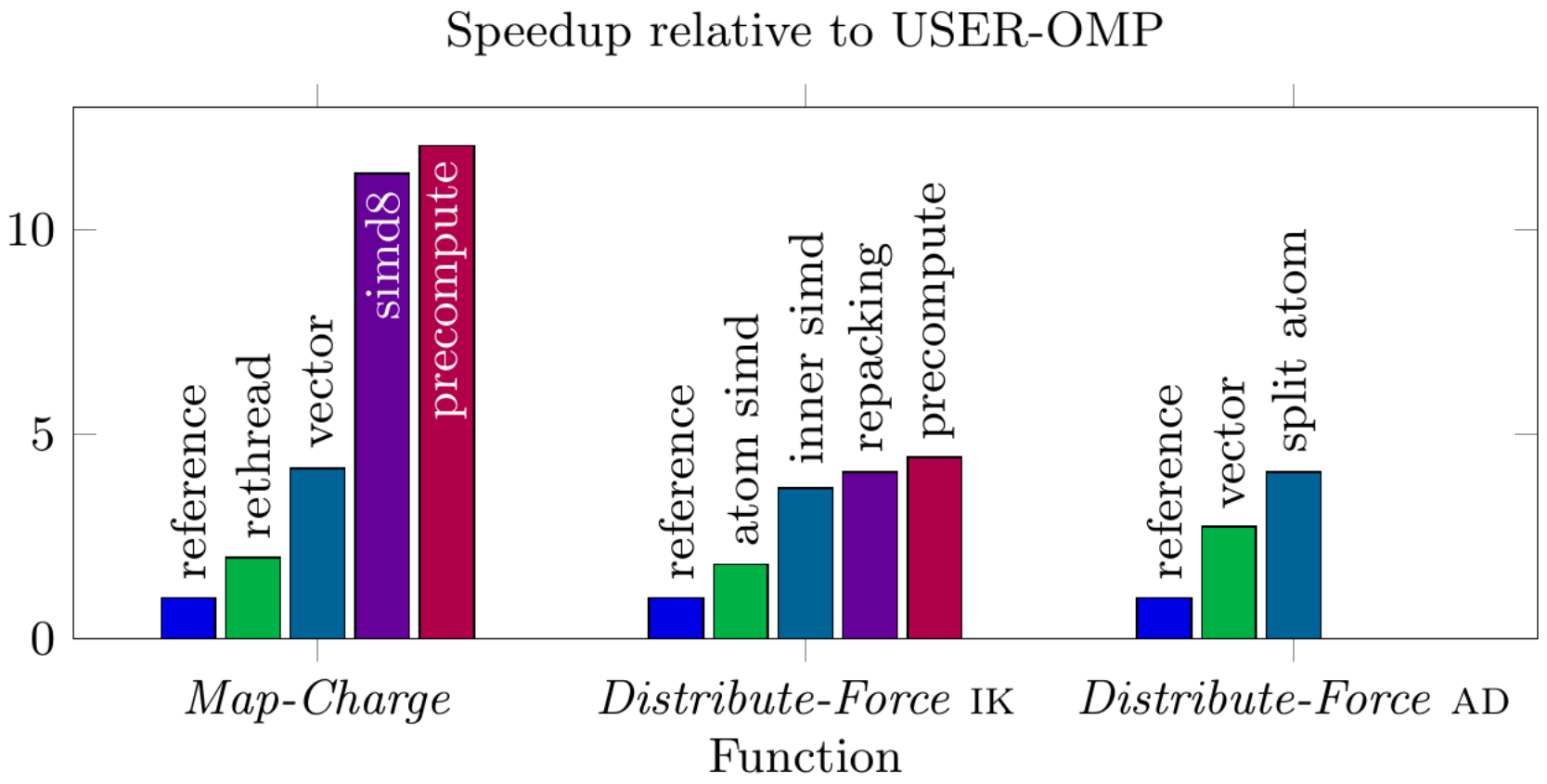
Distributing Forces **ad**

Different “flavors” of PPPM have the same overall structure

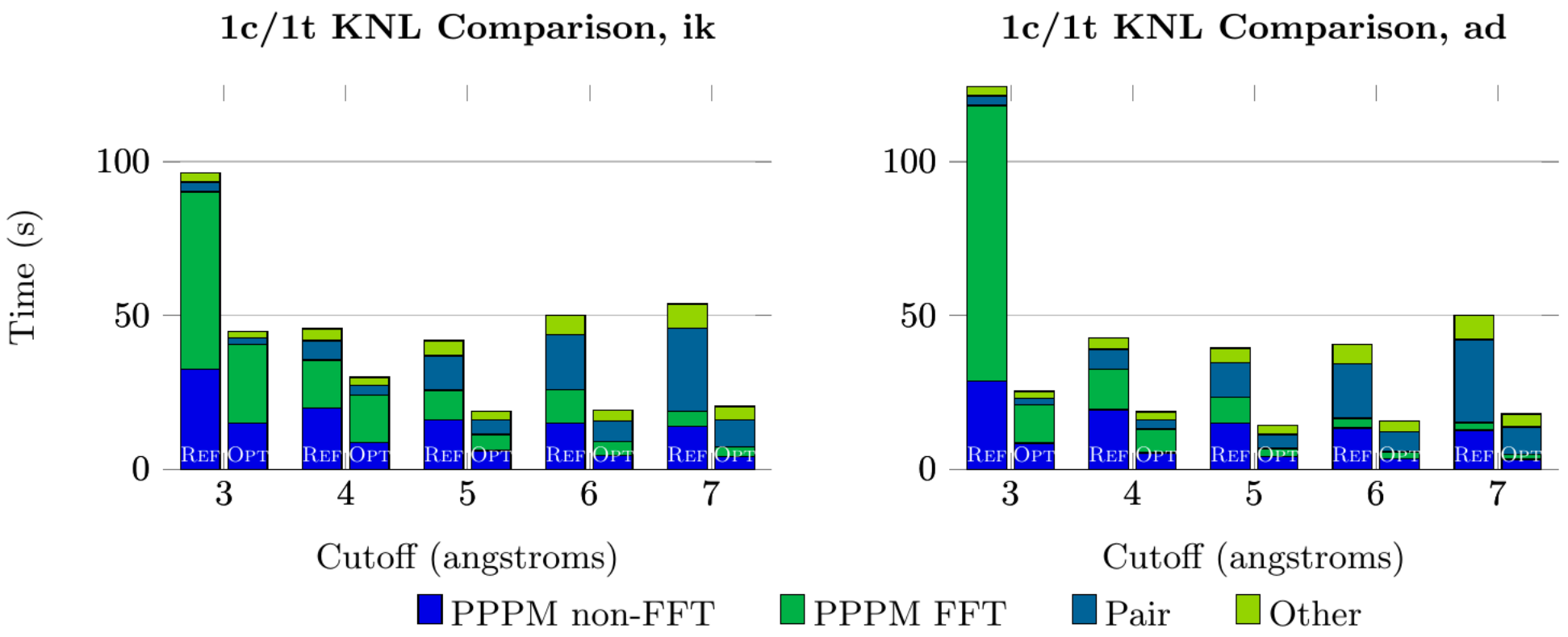
```
ekx *= hx_inv;
eky *= hy_inv;
ekz *= hz_inv;

// convert E-field to force

const flt_t qfactor = fqqrd2es * q[i];
const flt_t twoqsq = (flt_t)2.0 * q[i] * q[i];

const flt_t s1 = x[i].x * hx_inv;
const flt_t s2 = x[i].y * hy_inv;
const flt_t s3 = x[i].z * hz_inv;
flt_t sf = fsf_coeff0 * sin(ftwo_pi * s1);
sf += fsf_coeff1 * sin(ffour_pi * s1);
sf *= twoqsq;
f[i].x += qfactor * ekx - fqqrd2es * sf;

sf = fsf_coeff2 * sin(ftwo_pi * s2);
sf += fsf_coeff3 * sin(ffour_pi * s2);
sf *= twoqsq;
f[i].y += qfactor * eky - fqqrd2es * sf;

sf = fsf_coeff4 * sin(ftwo_pi * s3);
sf += fsf_coeff5 * sin(ffour_pi * s3);
sf *= twoqsq;

if (slabflag != 2) f[i].z += qfactor * ekz - fqqrd2es * sf;
```

Work is done after the stencil loop to convert potential for each atom into force

Subroutine Speedup



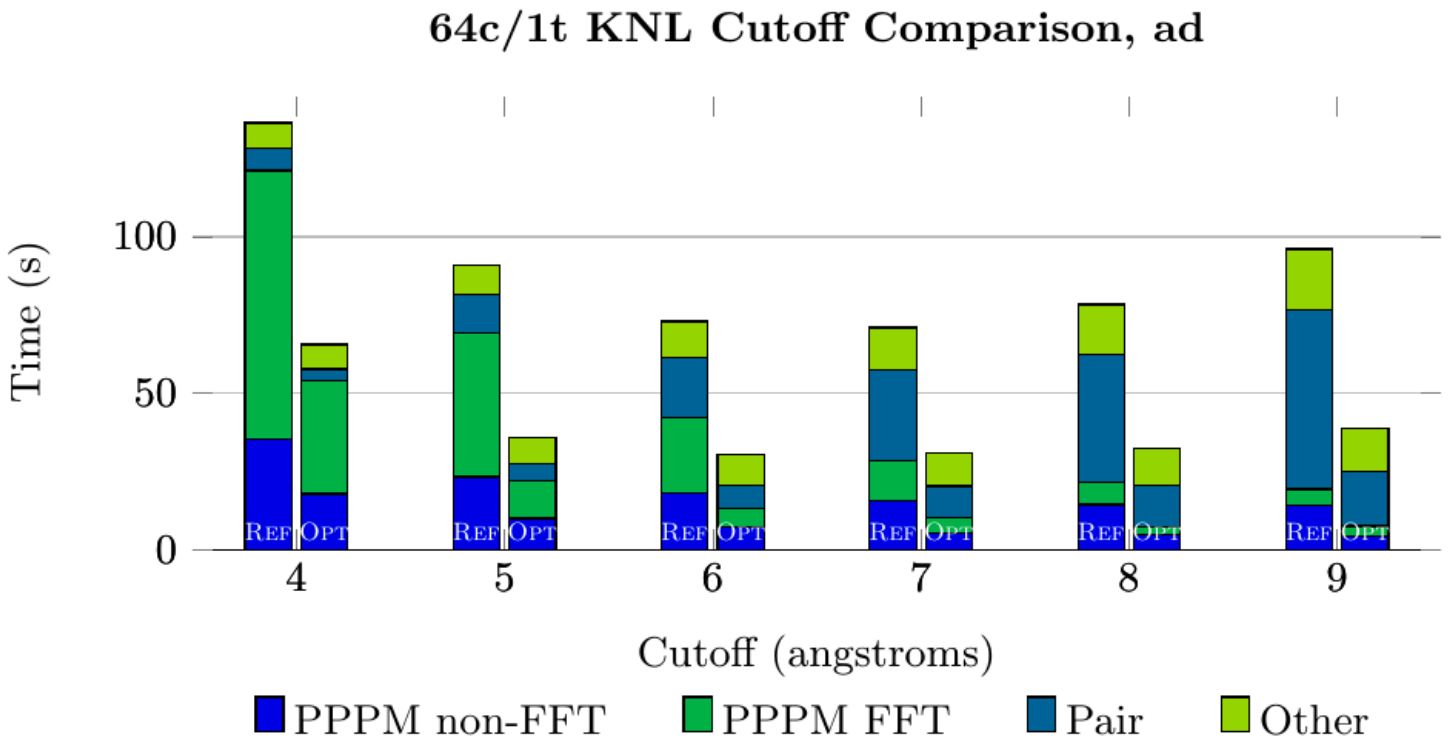
Overall Speedup (1 core / 1 thread)



Together with optimization of the pair interactions (by Mike Brown of Intel), we achieve overall speedsups of 2-3x.

PPPM speedup shifts the optimal cutoff lower, while pair interaction speedup shifts it higher.

Overall Speedup (parallel)

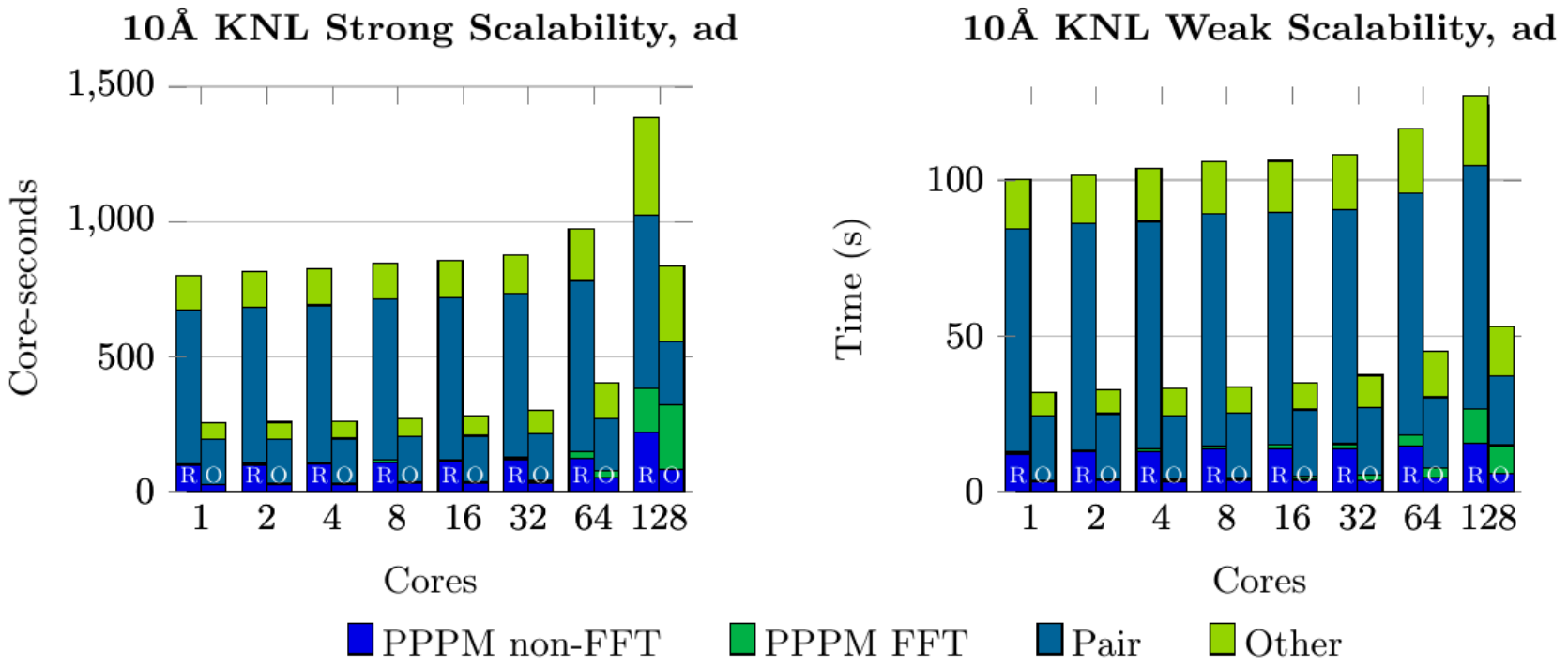


In parallel, the FFTs become more expensive – other than occasionally communicating atoms moving through the domain, this is the only communication.

The runtime-optimal cutoff rises and work should be shifted into pair interactions.

If we choose a cutoff based on few processors, scalability is very bad!

Overall Speedup (parallel)



Scalability worsens across multiple nodes (64 to 128 cores).

We end up with worse overall scaling but better real performance because everything *except* the FFTs is much faster.

You can pick cutoffs that make scalability look good but this is misleading.

A better-scaling method for solving Poisson's Equation is needed (MSM?).

Particle-Particle Particle-Mesh (P3M) on Knights Landing Processors

William McDoniel Ahmed E. Ismail Paolo Bientinesi

SIAM CSE ‘17
Atlanta

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