Erlangen Regional Computing Center

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

A HPM based Methodology for SIMD Code Analysis

High Performance Computing

Example: MiniMD proxy app

Proxy app from **MANTEVO**.

`https://mantevo.org`

- **`MiniMD`** – MPI + OpenMP
  - App. 3000 lines, C++
  - Extracted from LAMMPS (`http://lammps.sandia.gov`) Molecular dynamics application code
  - Other implementations: OpenACC, OpenCL, Kokkos
  - Supports Lennard-Jones (default) and eam force calculation
  - Uses neighbour lists

Runtime profile

% time	self seconds	calls	name
83.05	21.44	402	ForceLJ::compute(Atom&, Neighbor&, Comm&, int)
13.29	3.43	21	Neighbor::build(Atom&)
1.63	0.42	1	Integrate::run(Atom&, Force*, Neighbor&, Comm&
0.50	0.13	2280	Atom::pack_comm(int, int*, double*, int*)
0.46	0.12	2412	Atom::unpack_reverse(int, int*, double*)
0.23	0.06	41	Neighbor::binatoms(Atom&, int)
0.19	0.05	2280	Atom::unpack_comm(int, int, double*)
0.19	0.05	21	Comm::borders(Atom&)
0.15	0.04	20	Atom::sort(Neighbor&)
0.12	0.03		intel_avx_rep_memcpy*

Code review

- `ForceLJ::compute` is a proxy routine to jump to different implementations:
  - `compute_halfneigh` – Default for running with 1 thread
  - `compute_halfneigh_threaded` – Default with more than 1 thread
  - `compute_fullneigh` – Optional algorithm

- The optimal algorithm is halfneigh updating both partners for force calculations. But requires atomics for OpenMP parallelisation and only vectorizes if forced with pragma SIMD.

Code review halfneigh compute

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78

```
for(int i = 0; i < nlocal; i++) {
    neighs = &neighbor.neighbors[i * neighbor.maxneighs];
    const int numneighs = neighbor.numneigh[i];
    const MMD_float xtmp =
    const MMD_float ytmp =
    const MMD_float ztmp =
    MMD_float fix = 0.0;
    MMD_float fiy = 0.0;
    MMD_float fiz = 0.0;

    for(int k = 0; k < numneighs; k++) {
        const int j = neighs[k];
        const MMD_float delx = xtmp -
        const MMD_float dely = ytmp -
        const MMD_float delz = ztmp -
        const MMD_float rsq = delx * delx + dely * dely + delz * delz;
        // CUTOFF LOOP SEE NEXT SLIDE
    }
    f[i * PAD + 0] += fix;
    f[i * PAD + 1] += fiy;
    f[i * PAD + 2] += fiz;
}
```

Code review cutoff loop `halfneigh` vs `fullneigh`

halfneigh

```
if(rsq < cutforcesq) {
            const MMD_float sr2 = 1.0 / rsq;
            const MMD_float sr6 = sr2 * sr2 * sr2 * sigma6;
            const MMD_float force = 48.0 * sr6 * (sr6 - 0.5) * sr2 * epsilon;

            fix += delx * force;
            fiy += dely * force;
            fiz += delz * force;

            f[j * PAD + 0] -= delx * force;
            f[j * PAD + 0] -= dely * force;
            f[j * PAD + 0] -= delz * force;
}
```

Enter 54 times of 78

fullneigh

```
if(rsq < cutforcesq) {
            const MMD_float sr2 = 1.0 / rsq;
            const MMD_float sr6 = sr2 * sr2 * sr2 * sigma6;
            const MMD_float force = 48.0 * sr6 * (sr6 - 0.5) * sr2 * epsilon;

            fix += delx * force;
            fiy += dely * force;
            fiz += delz * force;
}
```

`mul`: **10**

`add`: **4**

`div`: **1 reciprocal**

Xeon Broadwell system (2 sockets, 18 cores per socket, 2.3 GHz)

Runtime [s]	scalar	sse	avx	avx2
halfneigh	9.00	8.13	6.98	8.19
fullneigh	**15.17** (+69%)	9.15 (+13%)	5.92 (-15%)	**5.68** (-19%)

Scalar vs SIMD	FullNeigh	HalfNeigh
Runtime factor	2.56	1.29
Arithmetic instr. factor	**3.04**	2.66
Total instruction factor	1.80	**0.91**
CPI factor	1.42	1.42
Overall scaling	2.55	1.29

- Halfneigh requires a factor 1.78 less **arithmetic work** which is reflected in a scalar runtime scaling of 1.69
- But because Fullneigh is easier to SIMD vectorize and with AVX it beats the better algorithm by a small margin

Likwid HPM instruction breakdown

Instruction type	Full scalar	Full AVX	Half scalar	Half AVX
CPI	0.98	**0.69**	0.78	**0.55**
Arithmetic Scalar	69.16%	4.83%	51.5%	4.84%
Arithmetic SSE	0%	0.21%	0%	0.14%
Arithmetic AVX	0%	35.82%	0%	12.6%
Arithmetic Total	**69.16%**	40.85%	51.5%	**17.58%**
Load	14.19%	17.03%	16.96%	13.65%
Store	0.23%	1.06%	4.49%	5.64%
Branch	5.27%	3.61%	4.06%	14.34%
Other	10.45%	**37.45%**	22.99%	**48.80%**

MiniMD Assembly AVX

```
const int j = neighs[k];
```

AVX: k in blocks of 4

```
const MMD_float delx = xtmp - x[j * PAD + 0];
const MMD_float dely = ytmp - x[j * PAD + 1];
const MMD_float delz = ztmp - x[j * PAD + 2];

const MMD_float rsq = delx * delx + dely * dely
+ delz * delz;
```

```
vmulpd     %ymm9, %ymm9, %ymm12
vfmadd231pd %ymm7, %ymm7, %ymm12
vfmadd231pd %ymm10, %ymm10, %ymm12
```

X[j+x]

0+0	0+1	0+2	1+0	1+1	1+2
2+0	2+1	2+2	3+0	3+1	3+2

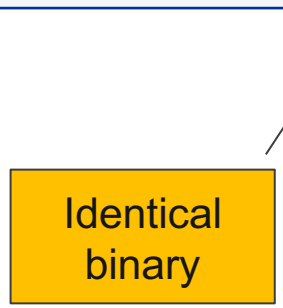
ymm[0-3]

0+0	1+0	2+0	3+0
0+1	1+1	2+1	3+1
0+2	1+2	2+2	3+2

Xeon Skylake system (2 sockets, 20 cores per socket, 2.4 GHz)

Runtime [s]	scalar	sse	avx	avx2
halfneigh	9.00	8.13	6.98	8.19
fullneigh	**15.17** (+69%)	9.15 (+13%)	5.92 (-15%)	**5.68** (-31%)

Runtime [s]	scalar	sse	avx	avx512
halfneigh	13.70	13.62	7.17	3.39
fullneigh	**24.43** (+78%)	24.20 (+78%)	5.53 (-33%)	**2.44** (-38%)



AVX512 version

```
        vpcmpgtd  %ymm23, %ymm22, %k3
        vmovdqu32 (%r13,%r14,4), %ymm14{%k3}{z}
        kmovw     %k3, %r8d
        vpaddd    %ymm14, %ymm14, %ymm15
        vpaddd    %ymm15, %ymm14, %ymm18
..B12.39:
        kmovw     %k3, %k1
        kmovw     %k3, %k2
        vpxord    %zmm19, %zmm19, %zmm19
        vpxord    %zmm16, %zmm16, %zmm16
        vpxord    %zmm14, %zmm14, %zmm14
        vgatherdpd 16(%rdx,%ymm18,8), %zmm19{%k1}
        vgatherdpd 8(%rdx,%ymm18,8), %zmm16{%k2}
        vgatherdpd (%rdx,%ymm18,8), %zmm14{%k3}
..B12.40:
        vsubpd    %zmm19, %zmm24, %zmm19
        vsubpd    %zmm16, %zmm20, %zmm17
        vsubpd    %zmm14, %zmm21, %zmm15
        vpaddd    %ymm18, %ymm9, %ymm14
        vpaddd    %ymm18, %ymm8, %ymm16
        vmulpd    %zmm17, %zmm17, %zmm26
        vfmadd231pd %zmm15, %zmm15, %zmm26
        vfmadd231pd %zmm19, %zmm19, %zmm26
```