INTRODUCTION TO PERFORMANCE AND VECTORIZATION

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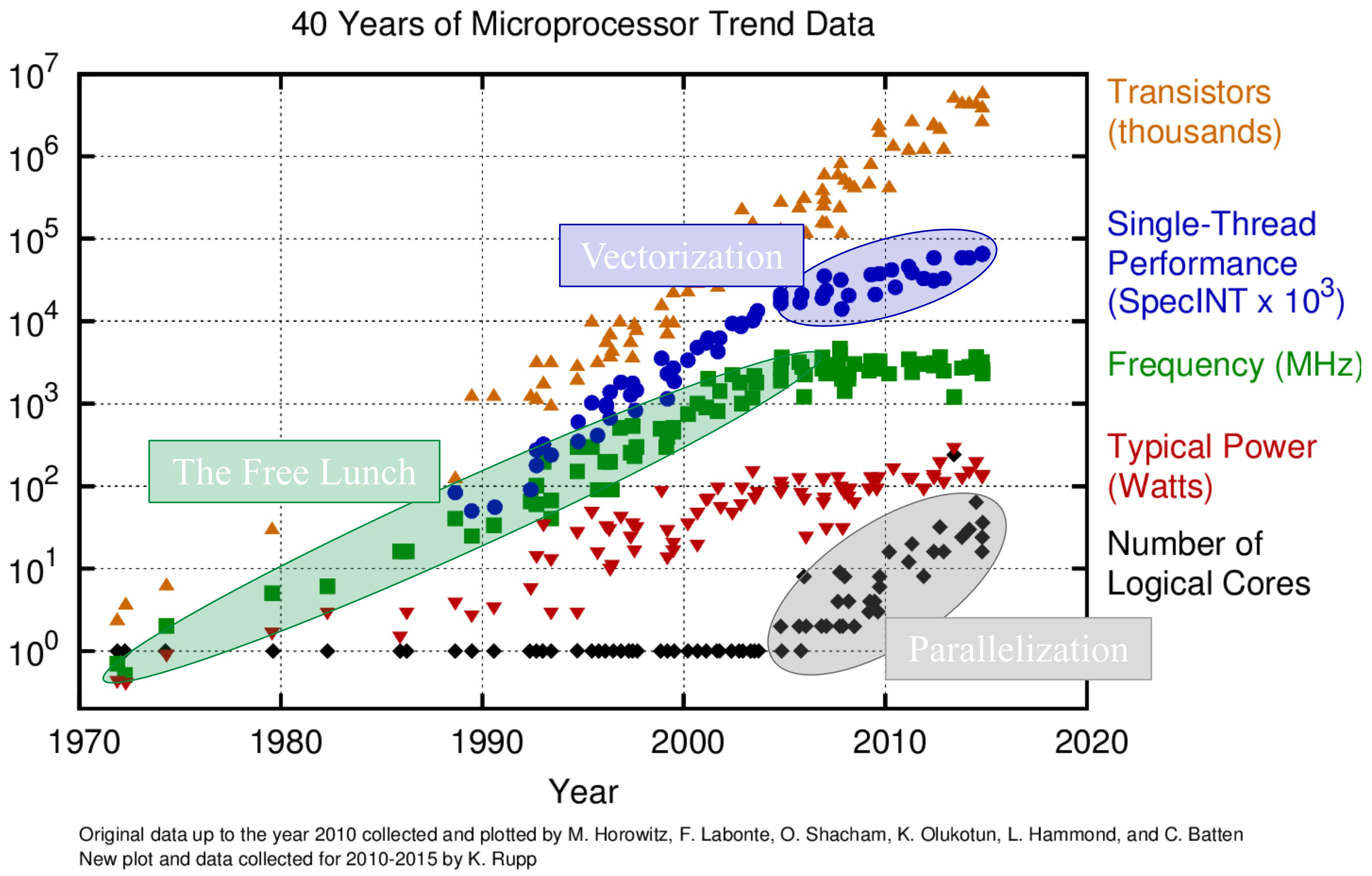
Fall 2020 Virtual Workshop
Nov 02, 2020

Outline

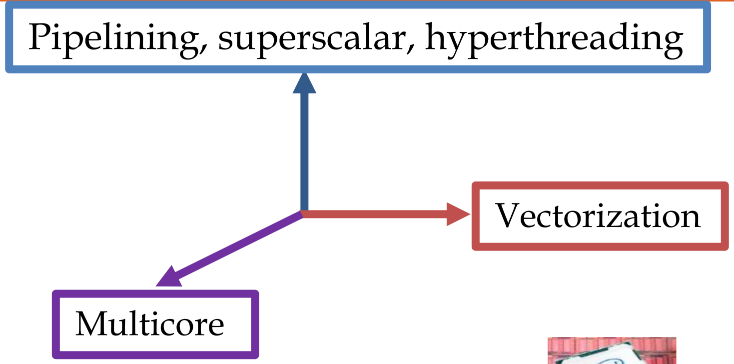
- A **practical guidance** to performance optimization and tuning using **vectorization**
    - Hardware evolution
    - Auto-vectorization
    - Explicit vectorization with OpenMP SIMD
    - Vectorization efficiency
    - Intel Advisor
- Focused primarily on the **HPC recourses at Princeton**
    - Hardware: Intel Broadwell and Skylake processor
    - Compiler: Intel compiler
    - Software: Written in C/C++ and Fortran language
    - Most principles apply universally

“Free Lunch is Over”

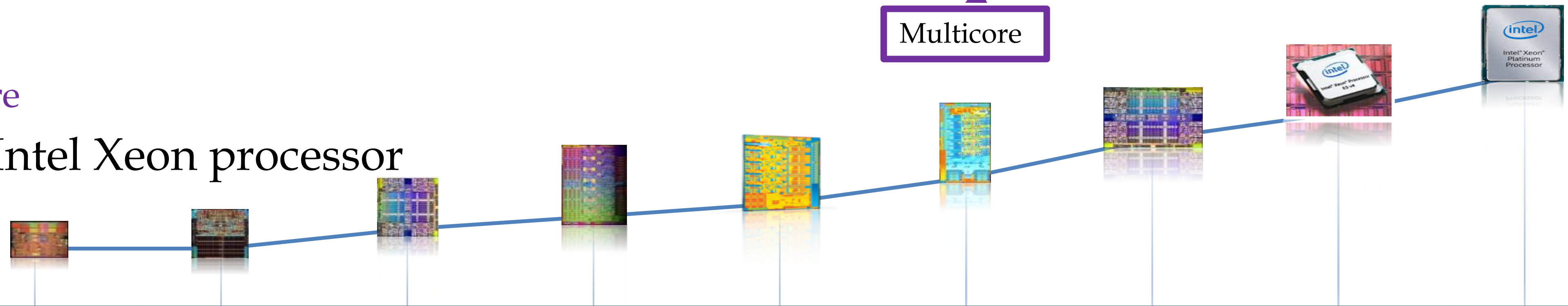


https://www.karlrupp.net/2015/06/40-years-of-microprocessor-trend-data/

Trend of Processor Evolution



- From high frequency to massive parallelism
  - Core
    - Pipelining, superscalar and hyperthreading
    - Vectorization
  - Processor
    - Multicore
- Example: Intel Xeon processor



Intel® Xeon® Processor	64-bit	5100 series	5500 series	5600 series	E5-2600	E5-2600 V2	E5-2600 V3	E5-2600 V4	Platinum 8180
Cores	1	2	4	6	8	12	18	22	28
Threads	2	2	8	12	16	24	36	44	56
SIMD Width	128	128	128	128	256	256	256	256	512
	2005	2007	2009	2010	2012	2013	2014	2016	2017

- Application developers need to write software to take advantage of the computing power

Peak FLOPS

- Peak FLOPS: How many floating point operations the system can theoretically execute in a second

$$sockets \text{ x } \frac{cores}{socket} \text{ x } \frac{cycles}{second} \text{ (frequency)x } FLOPs/cycle/core$$

- *FLOPs/cycle/core* depends on the chip micro-architecture:
  - $\frac{instructions}{cycle} \; x \; \frac{operations}{instruction} \; x \; \frac{FLOPs}{operation}$
  - Haswell/Broadwell(AVX2, 256-bit)
    16 double precision (DP) FLOPs/cycle: 2 VPUs/core, 4 (4-wide)x2 (FMA) flops/VPU
    32 single precision (SP) FLOPs/cycle: 2 VPUs/core, 8 (8-wide)x2 (FMA) flops/VPU
  - Skylake (AVX512, 512-bit)
    32 DP FLOPs/cycle: 2 VPUs/core, 8 (8-wide)x 2 (FMA) flops/VPU
    64 SP FLOPs/cycle: 2 VPUs/core, 16 (16-wide) 2 (FMA) flops/VPU

FLOSs = Floating-point Operations
FLOPS = Floating-point Operations Per Second
VPUs = Vector Processing Units
FMA = Fused Multiply-Add

Exercise 1: Find the Peak FLOPS of Intel Skylake Processor on Adroit

- Log in Adroit: ssh -l usersname adroit.princeton.edu
- Find the CPU information: lscpu
  - How many sockets?
  - How many cores per socket?
  - What's the processor frequency?
- The Skylake processor has 2 VPUs (each can execute a FMA operation) and 512-bits vector register per core
- What is the peak FLOPS?
  - DP FLOPS = 2(sockets)x16(cores)x2.6x10^9(freq)x2(VPUs)x2(FMA)x8(512 bits) = 2,662 GFLOPS
  - SP FLOPS = 2(sockets)x16(cores)x2.6x10^9(freq)x2(VPUs)x2(FMA)x16(512 bits) = 5,324 GFLOPS

Takeaway Message #1:
Vectorization is important for archiving peak performance

Vectorization 101

- Simple example:

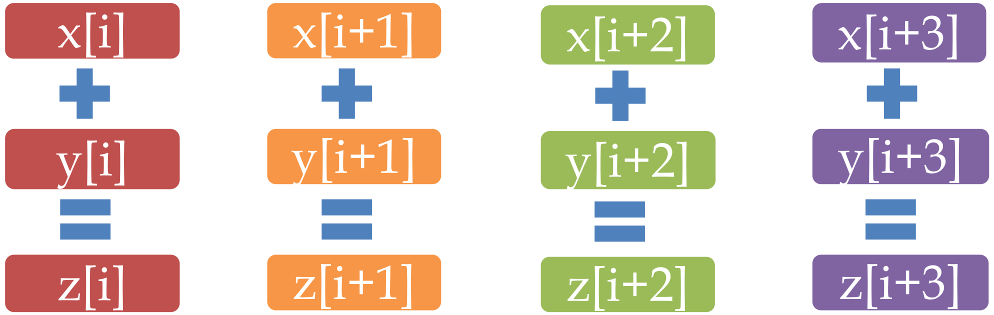
```
for (int i=0; i<N; i++)
    z[i] = x[i] + y[i];
```

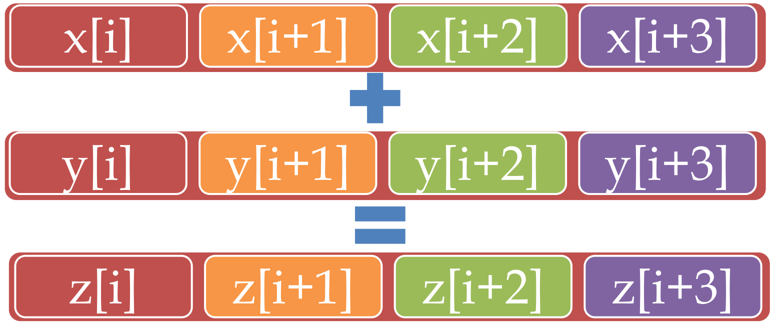
Scalar machine code (Loop N Times)

```
ld r1, addr1
ld r2, addr2
add r3, r1, r2
st addr3, r3
```

Vector machine code (Loop N/4 Times)

```
vld vr1, addr1
vld vr2, addr2
vadd vr3, vr1, vr2
vst addr3, vr3
```





Three Aspects of Vectorization

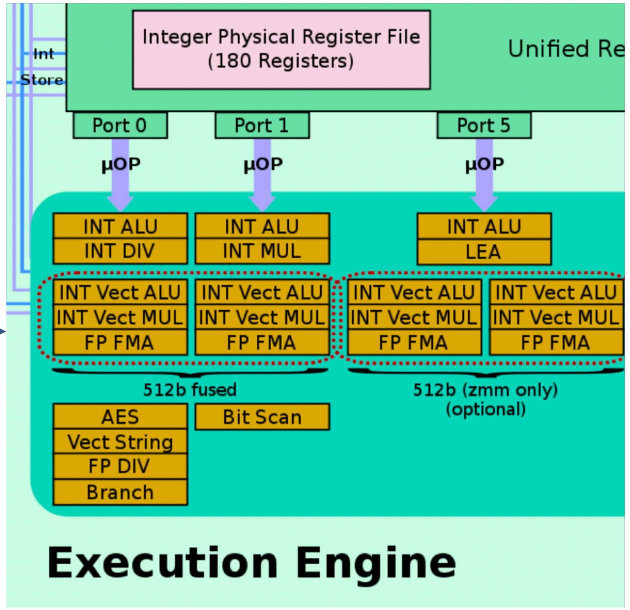
1. **Hardware**
   - Special registers and vector processing units
   - Vector instructions sets (e.g., SSE, AVX…)
2. **Software**
   a) Compiler-based vectorization (portable)
   - **Auto-Vectorization** (no change of code)
   - **Semi-Auto-Vectorization**: auto-vectorization enhanced by compiler directives (e.g., #pragma vector…)
   - **Explicit Vector Programming**: auto-vectorization with explicitly control using OpenMP (e.g., #pragma omp simd)

   b) Manually by explicit syntax (not portable)
   - Vector intrinsics
   - Assembly language

   c) Vendor-supplied optimized libraries (e.g, Intel Math Kernel Library)
3. **User's**
   - Determine how to write a code such that the

Easy Use

Programmer Control



Auto-Vectorization by Compiler

To be vectorizable by the compiler (auto-vectorization), loops must meet the following criteria:

1. Countable: the number of iterations should be known at entry of the loop at runtime. Exit of the loop must not be data dependent.
   - No conditional termination (e.g., break, while loops, …)
2. Straight-line code: no jump or branch such as “switch” statements, but masked assignments are allowed
   - Compiler can convert “if-then-else” statements to masked assignments
3. Must be the innermost loop if nested, unless the compiler is able to
   - Fully unroll the inner loop
   - Interchange the inner and outer loops
4. No function or subroutine calls, unless these are
   - Math library functions such as sin, cos, pow, sqrt, etc
   - Inlined
5. No loop-carried dependency
   - E.g., for (int i=1; i<N; i++) a[i] = a[i-1] + 1;

https://software.intel.com/en-us/articles/requirements-for-vectorizable-loops

Compiler Options for Vectorization I

- Intel compilers start vectorizing at optimization level **-O2**
  - Default is SSE2 instructions, 128-bit vector width
  - To tune vectors to the host machine: **-xHost**
  - To optimize across objects (e.g., to inline functions): **-ipo**
  - To disable vectorization: **-no-vec**
- GCC compilers start vectorizing at optimization level **-O3**
  - Default for x86_64 is SSE (see output from gcc -v, no other flags)
  - To tune vectors to the host machine: **-march=native**
  - To optimize across objects (e.g., to inline): **-fwhole-program**
  - To disable vectorization: **-fno-tree-vectorize** (after **-O3**)
- Why disable or downsize vectors? To gauge their benefit!

https://cvw.cac.cornell.edu/vector/compilers_enabling

Compiler Options for Vectorization II

- Intel compilers for specific instruction sets: -x<feature>
  - Use **-xCORE-AVX2** to compile for AVX2, 256-bit vector register
  - For SKL-SP: **-xCORE-AVX512 -qopt-zmm-usage=high**
    - Intel® Compiler is conservative in its use of ZMM (512bit) registers so to enable their use with Skylake the additional flag **-qopt-zmm-usage=high** must be set.
  - For KNL (MIC architecture): **-xMIC-AVX512**
- GCC compilers for specific instruction sets: -m<feature>
  - Use **-mavx2** to compile for AVX2
  - GCC 4.9+ has separate options for each AVX-512 extension
  - GCC 5.3+ has **-march=skylake-avx512 -mprefer-vector-width=512**
    - When using -march=skylake-avx512 by default it is using -mprefer-vector-width=256. We need to set -mprefer-vector-width=512 explicitly to use ZMM registers.
  - GCC 6.1+ has **-march=knl**

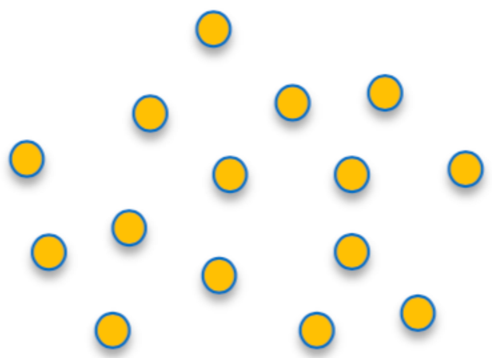
Vectorization Report

- Intel compiler options:
  - -qopt-report[=n]: tells the compiler to generate an optimization report in an *.optrpt file (https://software.intel.com/en-us/cpp-compiler-developer-guide-and-reference-qopt-report-qopt-report#62679876-5691-40B3-BC90-E2D32643960D)
    - The –n controls the amount of detail of the *.optrpt report
  - -qopt-report-phase[=list]: specify one and more optimizer phases for which optimization reports are generated (https://software.intel.com/en-us/cpp-compiler-developer-guide-and-reference-qopt-report-phase-qopt-report-phase#2058006C-1E74-4ECB-AA1A-E4F0E018E839)
    - vec: the phase for vectorization
    - all: all optimizer phases (default)
  - -qopt-report-filter[=string]: specified the indicated parts of your code and generate optimization reports for those parts only
- GCC compiler option:
  - -ftree-vectorizer-verbose[=n] (deprecated in version 6.3.0)
  - -fopt-info-vec
  - -fopt-info-vec-missed

Note: for the rest of the lecture, we will focus on Intel compilers

N-Body Problem

```
struct Particle {
  float x, y, z;
  float vx, vy, vz;
};

for (int i = 0; i < nParticles; i++) {
  // Components of the gravity force on particle i
  float Fx = 0, Fy = 0, Fz = 0;

  const float xi = particle[i].x;
  const float yi = particle[i].y;
  const float zi = particle[i].z;

  for (int j = 0; j < nParticles; j++) {
    // Newton's law of universal gravity
    const float dx = particle[j].x - xi;
    const float dy = particle[j].y - yi;
    const float dz = particle[j].z - zi;

    const float drPower32  = pow(drSquared, 3.0/2.0);

    const float drPower32Inv = 1.0f / drPower32;
    // Calculate the net force
    Fx += dx * G * drPower32Inv;
    Fy += dy * G * drPower32Inv;
    Fz += dz * G * drPower32Inv;
  }

  // Accelerate particles in response to the gravitational force
  particle[i].vx += dt*Fx;
  particle[i].vy += dt*Fy;
  particle[i].vz += dt*Fz;
}
```



$$\vec{F}_{ij} = \frac{G m_i m_j}{|\vec{r}_j - \vec{r}_i|^3}(\vec{r}_j - \vec{r}_i)$$

$$\vec{F} = m\vec{a} = m\frac{d\vec{v}}{dt} = m\frac{d^2\vec{x}}{dt^2}$$

The example code assumes m=1 for all particles

Exercise 2: Check Performance with Different Compiler Vectorization Flags

- Log into Adroit:
  - ssh –l usersname adroit.princeton.edu
- Clone the repo:
  - git clone https://github.com/beiwang2003/Intro_to_Perf_Vectorization.git
- Load the intel compiler:
  - module load intel
- Compile and run the code with different compiling flags
  1. Edit “ICXXFLAGS” in Makefile, e.g., ICXXFLAGS=-O0
  2. Compile the code with ”make app-ICC”
  3. Check the vectorization report (look at the “nbody.oicc.optrpt” file)
  4. Run the code with “./app-ICC”
  5. Record the performance number
  6. Repeat the above steps for
     - ICXXFLAGS=-O2
     - ICXXFLAGS=-O2 –xCORE-AVX2
     - ICXXFLAGS=-O2 –xCORE-AVX512 –qopt-zmm-usage=high

Note: do “make app-ICC clean” before each make

Follow-up Questions

- Observe how the performance change with different compiling flags (The performance test is compiled with intel/19.0/64/19.0.3.199 compiler and ran on Adroit login node)

Compiler flags	Register width (bits)	Performance GFLOPS
-O0	scalar	0.6
-O2	128	9.0
-O2 –xCORE-AVX2	256	14.7
-O2 –xCORE-AVX512 –qopt-zmm-usage=high	512	13.5

- Does the code have any performance issue?
- What is the maximum performance we can expect?

The Vectorization Report

```
Compiler options: -c -O2 -xCORE-AVX512 -qopt-zmm-usage=high -qopenmp -g -qopt-report=5 -qopt-report-phase=vec -inline-level=0 -qopt-report-filter=nbody.cc,56-111
-qopt-report-file=nbody.oicc.optrpt -o nbody.oicc

Begin optimization report for: MoveParticles(int, Particle *, float)

    Report from: Vector optimizations [vec]


LOOP BEGIN at nbody.cc(56,3)
   remark #15542: loop was not vectorized: inner loop was already vectorized

   LOOP BEGIN at nbody.cc(77,5)
      remark #15415: vectorization support: non-unit strided load was generated for the variable <particle->x[j]>, stride is 6   [ nbody.cc(84,24) ]
      remark #15415: vectorization support: non-unit strided load was generated for the variable <particle->y[j]>, stride is 6   [ nbody.cc(85,24) ]
      remark #15415: vectorization support: non-unit strided load was generated for the variable <particle->z[j]>, stride is 6   [ nbody.cc(86,24) ]
      remark #15305: vectorization support: vector length 16
      remark #15309: vectorization support: normalized vectorization overhead 0.482
      remark #15417: vectorization support: number of FP up converts: single precision to double precision 2   [ nbody.cc(94,32) ]
      remark #15418: vectorization support: number of FP down converts: double precision to single precision 1   [ nbody.cc(94,32) ]
      remark #15300: LOOP WAS VECTORIZED
      remark #15452: unmasked strided loads: 3
      remark #15475: --- begin vector cost summary ---
      remark #15476: scalar cost: 127
      remark #15477: vector cost: 14.250
      remark #15478: estimated potential speedup: 8.150
      remark #15486: divides: 1
      remark #15487: type converts: 3
      remark #15488: --- end vector cost summary ---
   LOOP END

   LOOP BEGIN at nbody.cc(77,5)
   <Remainder loop for vectorization>
      remark #15305: vectorization support: vector length 16
      remark #15309: vectorization support: normalized vectorization overhead 0.099
      remark #15417: vectorization support: number of FP up converts: single precision to double precision 2   [ nbody.cc(94,32) ]
      remark #15418: vectorization support: number of FP down converts: double precision to single precision 1   [ nbody.cc(94,32) ]
      remark #15301: REMAINDER LOOP WAS VECTORIZED
      remark #15452: unmasked strided loads: 3
      remark #15475: --- begin vector cost summary ---
      remark #15476: scalar cost: 127
      remark #15477: vector cost: 14.250
      remark #15478: estimated potential speedup: 8.150
      remark #15486: divides: 1
      remark #15487: type converts: 3
      remark #15488: --- end vector cost summary ---
   LOOP END
LOOP END
```

Performance seems impeded by non-unit strided memory access and type conversion

Exercise 3: Removing FP Conversion

- Edit “ICXXFLAGS” in Makefile:
  - ICXXFLAGS=-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv”
- Compile the code: make app-ICC
- Check the vectorization report

```
pow(drSquared, 3.0/2.0);
```

```
powf(drSquared, 3.0f/2.0f);
```

```
LOOP BEGIN at nbody.cc(77,5)
   remark #15415: vectorization support: non-unit strided load was generated for the variable <particle->x[j]>, stride is 6   [ nbody.cc(84,24) ]
   remark #15415: vectorization support: non-unit strided load was generated for the variable <particle->y[j]>, stride is 6   [ nbody.cc(85,24) ]
   remark #15415: vectorization support: non-unit strided load was generated for the variable <particle->z[j]>, stride is 6   [ nbody.cc(86,24) ]
   remark #15305: vectorization support: vector length 16
   remark #15309: vectorization support: normalized vectorization overhead 0.659
   remark #15300: LOOP WAS VECTORIZED
   remark #15452: unmasked strided loads: 3
   remark #15475: --- begin vector cost summary ---
   remark #15476: scalar cost: 102
   remark #15477: vector cost: 10.620
   remark #15478: estimated potential speedup: 8.710
   remark #15488: --- end vector cost summary ---
LOOP END
```

- Run the code: ./app-ICC

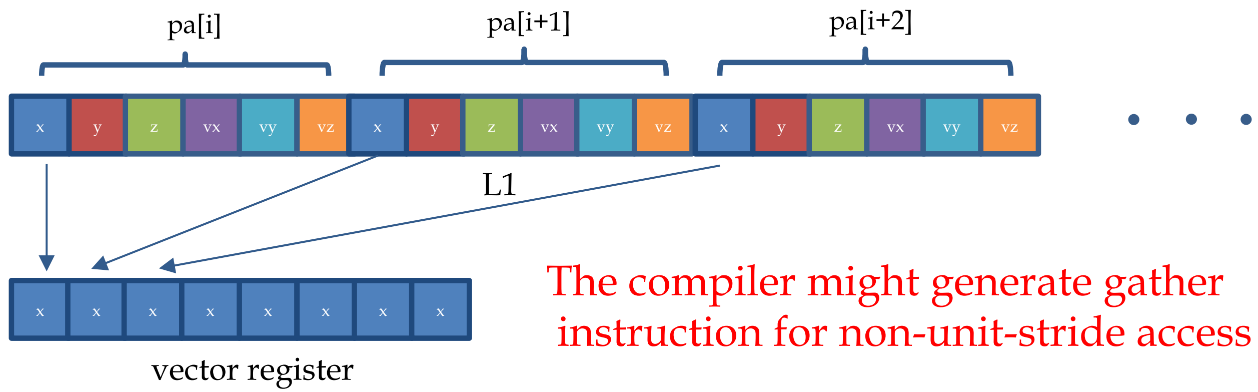
Compiler flags	Performance GFLOPS
-O2 –xCORE-AVX512 –qopt-zmm-usage=high	13.5
-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv	32.6

Data Access

- Using Structure of Array (SoA) vs. Array of Structure (AoS) data layout

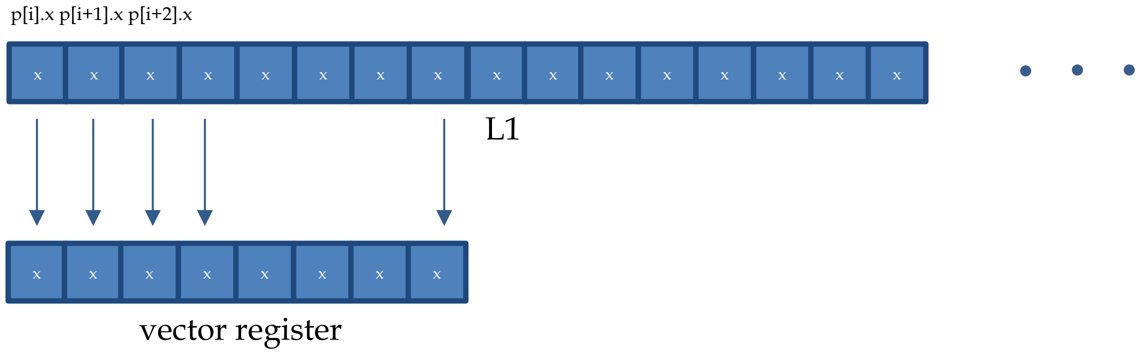
AoS

```
struct Particle {
  float x, y, z;
  float vx, vy, vz;
};

Particle* particle = new Particle[nParticles];
```



SoA

```
struct ParticleArrays {
  float *x, *y, *z;
  float *vx, *vy, *vz;
};
ParticleArrays particle;

particle.x  = new float[nParticles];
particle.y  = new float[nParticles];
particle.z  = new float[nParticles];
particle.vx = new float[nParticles];
particle.vy = new float[nParticles];
particle.vz = new float[nParticles];
```



Exercise 4: Switch to SoA Data Layout

- Edit “ICXXFLAGS” in Makefile:
  - ICXXFLAGS=-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv -DSoA”
- Compile the code: make app-ICC
- Check the vectorization report

```
LOOP BEGIN at nbody.cc(77,5)
   remark #15389: vectorization support: reference xp[j] has unaligned access   [ nbody.cc(80,24) ]
   remark #15389: vectorization support: reference yp[j] has unaligned access   [ nbody.cc(81,24) ]
   remark #15389: vectorization support: reference zp[j] has unaligned access   [ nbody.cc(82,24) ]
   remark #15381: vectorization support: unaligned access used inside loop body
   remark #15305: vectorization support: vector length 16
   remark #15309: vectorization support: normalized vectorization overhead 1.153
   remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
   remark #15450: unmasked unaligned unit stride loads: 3
   remark #15475: --- begin vector cost summary ---
   remark #15476: scalar cost: 102
   remark #15477: vector cost: 6.930
   remark #15478: estimated potential speedup: 12.440
   remark #15488: --- end vector cost summary ---
LOOP END
```

- Run the code: ./app-ICC

Compiler flags	Performance GFLOPS
-O2 –xCORE-AVX512 –qopt-zmm-usage=high	13.5
-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv	32.6
-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv -DSoA	57.9

Any Remaining Performance Issue

```
Compiler options: -c -O2 -xCORE-AVX512 -qopt-zmm-usage=high -DNo_FP_Conv -DSoA -DOMP_SIMD -qopenmp -g -qopt-report=5 -qopt-report-phase=vec -inline-level=0
-qopt-report-filter=nbody.cc,56-111 -qopt-report-file=nbody.oicc.optrpt -o nbody.oicc

Begin optimization report for: MoveParticles(int, ParticleArrays &, float)

    Report from: Vector optimizations [vec]


LOOP BEGIN at nbody.cc(56,3)
   remark #15542: loop was not vectorized: inner loop was already vectorized

   LOOP BEGIN at nbody.cc(77,5)
   <Peeled loop for vectorization>
      remark #15389: vectorization support: reference xp[j] has unaligned access   [ nbody.cc(80,24) ]
      remark #15389: vectorization support: reference yp[j] has unaligned access   [ nbody.cc(81,24) ]
      remark #15389: vectorization support: reference zp[j] has unaligned access   [ nbody.cc(82,24) ]
      remark #15381: vectorization support: unaligned access used inside loop body
      remark #15305: vectorization support: vector length 16
      remark #15309: vectorization support: normalized vectorization overhead 0.293
      remark #15301: PEEL LOOP WAS VECTORIZED
      remark #15450: unmasked unaligned unit stride loads: 3
      remark #15475: --- begin vector cost summary ---
      remark #15476: scalar cost: 102
      remark #15477: vector cost: 6.930
      remark #15478: estimated potential speedup: 12.440
      remark #15488: --- end vector cost summary ---
   LOOP END

   LOOP BEGIN at nbody.cc(77,5)
      remark #15389: vectorization support: reference xp[j] has unaligned access   [ nbody.cc(80,24) ]
      remark #15389: vectorization support: reference yp[j] has unaligned access   [ nbody.cc(81,24) ]
      remark #15389: vectorization support: reference zp[j] has unaligned access   [ nbody.cc(82,24) ]
      remark #15381: vectorization support: unaligned access used inside loop body
      remark #15305: vectorization support: vector length 16
      remark #15309: vectorization support: normalized vectorization overhead 1.153
      remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
      remark #15450: unmasked unaligned unit stride loads: 3
      remark #15475: --- begin vector cost summary ---
      remark #15476: scalar cost: 102
      remark #15477: vector cost: 6.930
      remark #15478: estimated potential speedup: 12.440
      remark #15488: --- end vector cost summary ---
   LOOP END

   LOOP BEGIN at nbody.cc(77,5)
   <Remainder loop for vectorization>
      remark #15389: vectorization support: reference xp[j] has unaligned access   [ nbody.cc(80,24) ]
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      remark #15476: scalar cost: 102
      remark #15477: vector cost: 6.930
      remark #15478: estimated potential speedup: 12.440
      remark #15488: --- end vector cost summary ---
   LOOP END
```
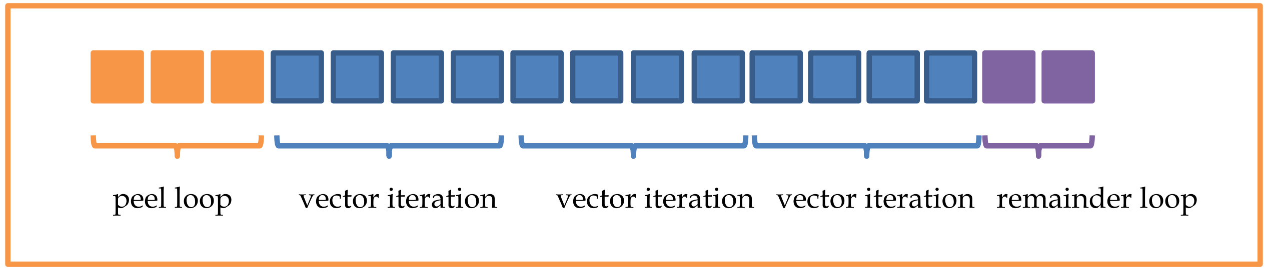

Data Alignment

- Data alignment with certain byte boundary
  - Align the base pointer where the space is allocated for the array
    - Replace malloc() and free() with alignment specified replacement, e.g., _mm_malloc() and _mm_free() (Intel), posix_memalign() and free() etc
  - Use pragmas/directives and clauses to tell the compiler that memory accesses are aligned
    - #pragma vector aligned (Intel)
    - #pragma omp simd aligned (OpenMP)

Peel and remainder loop are scalar or masked vector iterations



Exercise 5: Memory Alignment

- Edit “ICXXFLAGS” in Makefile:
  - ICXXFLAGS=-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv –DSoA –DOMP_SIMD –DAligned”
- Compile the code: make app-ICC
- Check the vectorization report

```
LOOP BEGIN at nbody.cc(77,5)
   remark #15388: vectorization support: reference xp[j] has aligned access   [ nbody.cc(80,24) ]
   remark #15388: vectorization support: reference yp[j] has aligned access   [ nbody.cc(81,24) ]
   remark #15388: vectorization support: reference zp[j] has aligned access   [ nbody.cc(82,24) ]
   remark #15305: vectorization support: vector length 16
   remark #15309: vectorization support: normalized vectorization overhead 1.047
   remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
   remark #15448: unmasked aligned unit stride loads: 3
   remark #15475: --- begin vector cost summary ---
   remark #15476: scalar cost: 102
   remark #15477: vector cost: 6.680
   remark #15478: estimated potential speedup: 13.580
   remark #15488: --- end vector cost summary ---
LOOP END
```

- Run the code: ./app-ICC

Compiler flags	Performance GFLOPS
-O2 –xCORE-AVX512 –qopt-zmm-usage=high	13.5
-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv	32.6
-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv -DSoA	57.9
-O2 –xCORE-AVX512 –qopt-zmm-usage=high –DNo_FP_Conv -DSoA –DOMP_SIMD –DAligned	66.9
Peak FLOPS	166

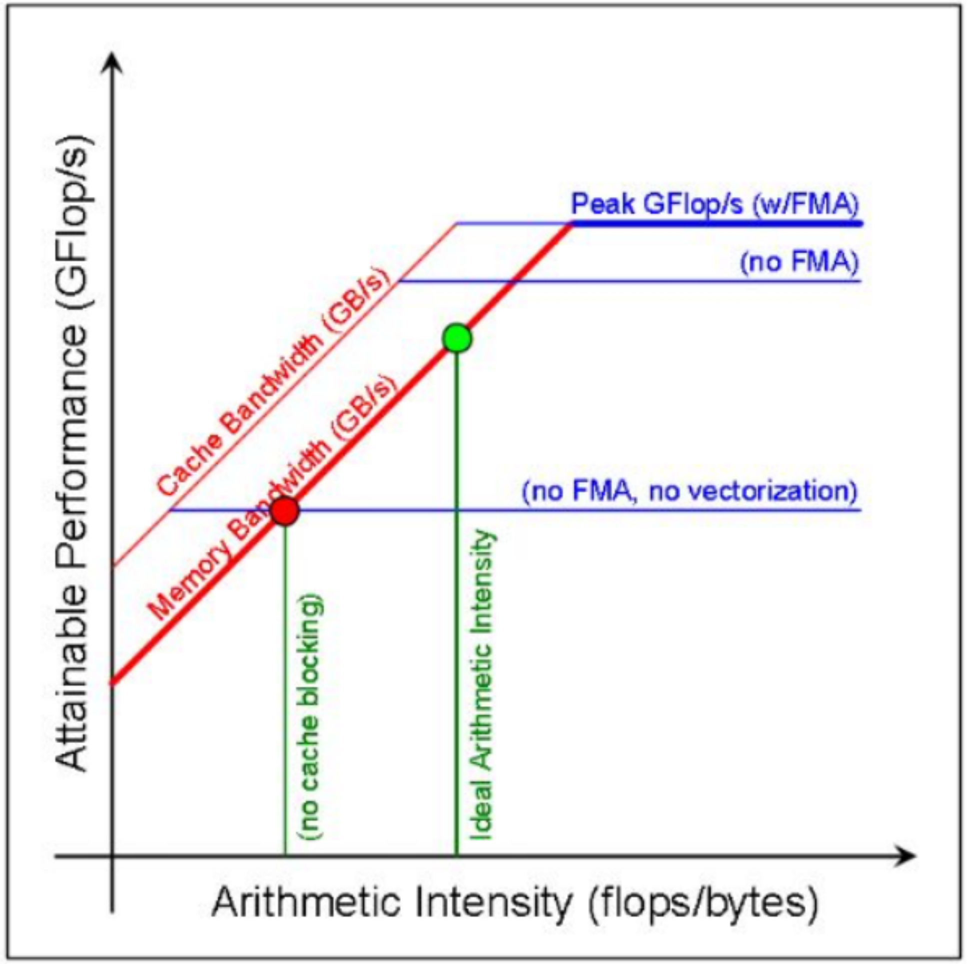
Peak FLOPS is (Almost) a Fiction

It is based on the assumptions that:

1. Arithmetic intensity (AI=flop/byte) is high
   - Otherwise VPU becomes stalled waiting for loads and stores to complete
2. Code is perfectly vectorized
   - Otherwise the scalar fraction of work limits the performance (Amdahl's Law)
3. No slow operations, e.g., division, square root
4. Clock rate is fixed
   - If all cores are active, clock is actually reduced to prevent overheating

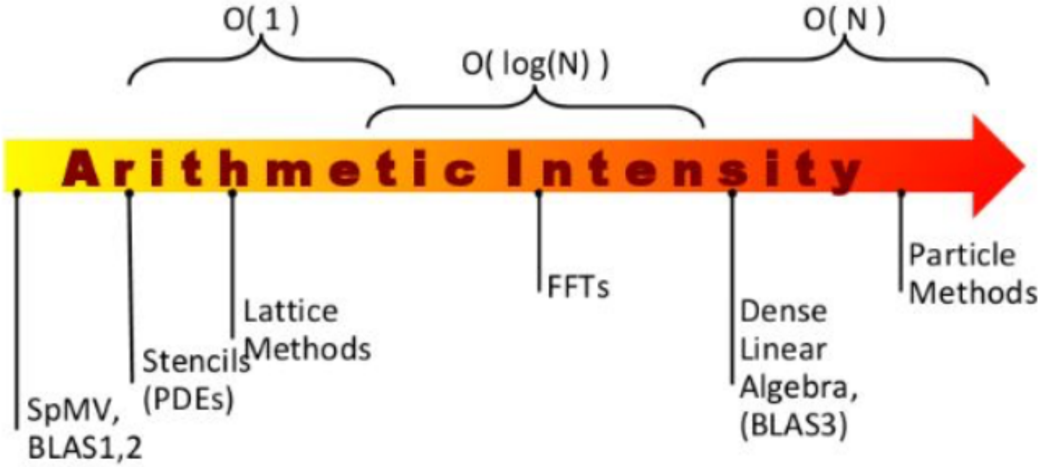
Takeaway Message #2:
In reality, it is hard to achieve the peak FLOPS

Roofline



$$\frac{\textit{Attainable}}{\textit{FLOPs / sec}} = \min\begin{cases} \textit{Peak FLOPs / sec}, \\ \textit{Peak Memory Bandwidth} \; x \; \textit{Arithmetic Intensity} \end{cases}$$

$$\textit{Arithmetic Intensity} = \frac{\textit{Total FLOPs}}{\textit{Total Bytes}}$$

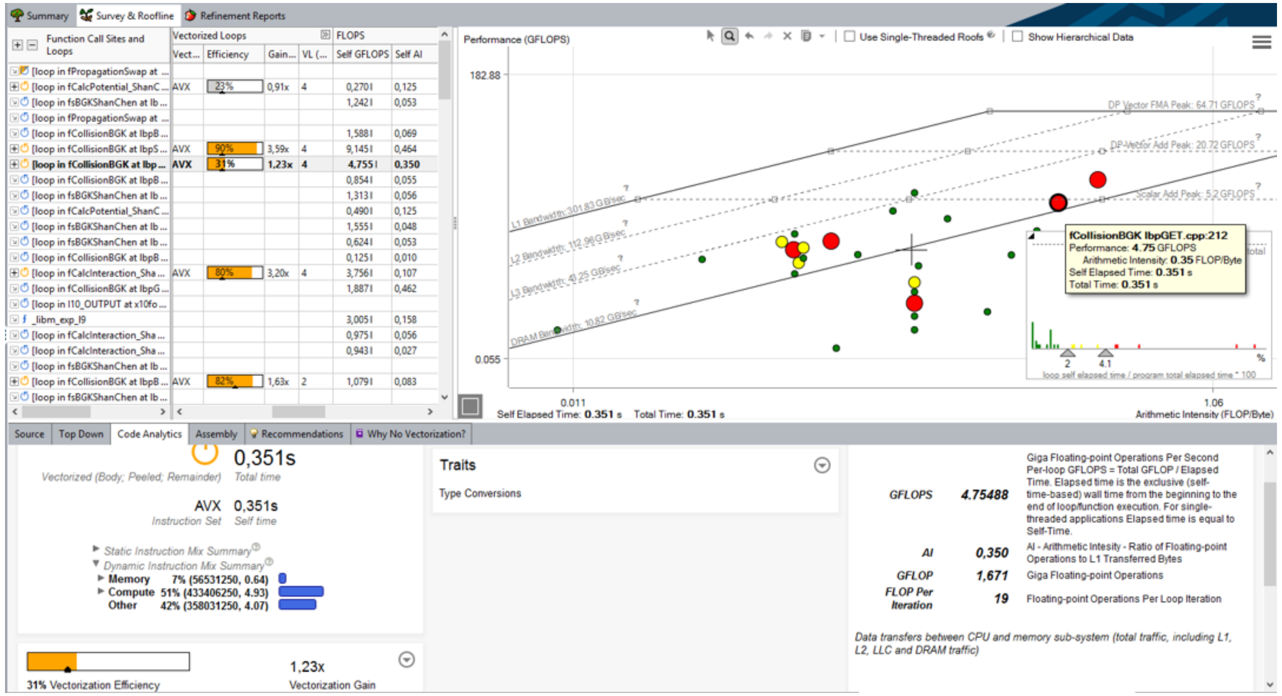


https://anl.app.box.com/v/IXPUG2016-presentation-29

INTEL ADVISOR

Vectorization Advisor & Roofline

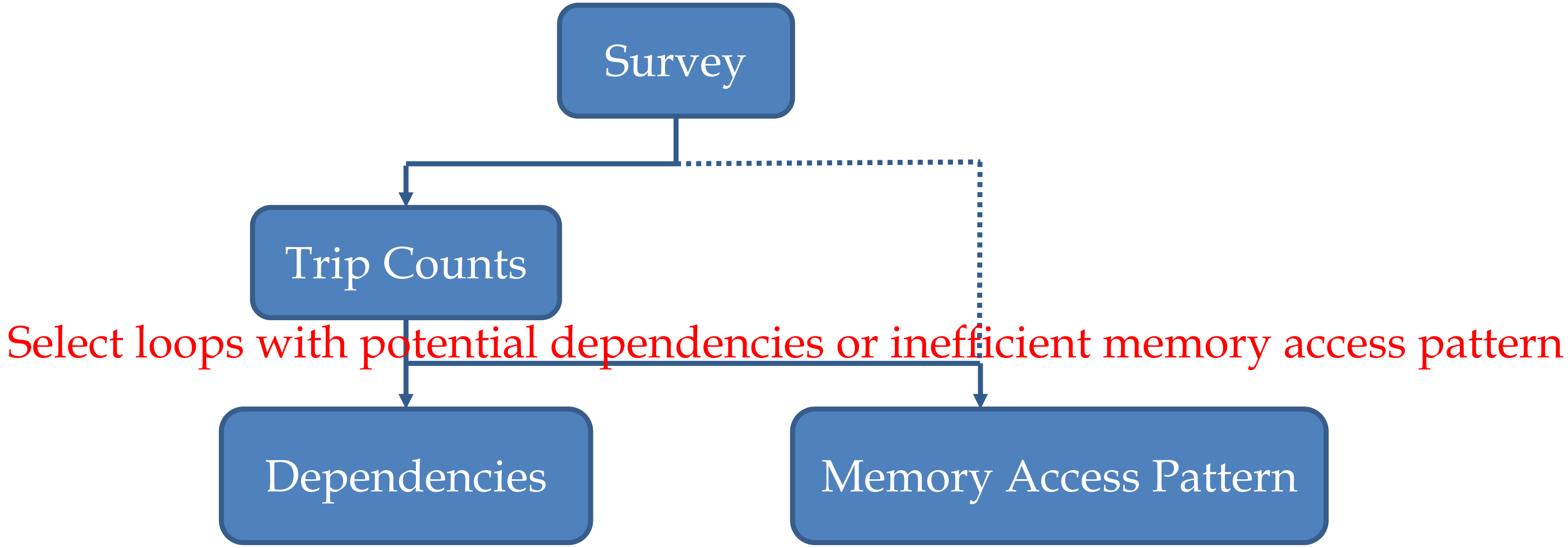
- **Vectorization advisor**
  - Provide graphical view for information from vectorization report
  - Identify the hotspots where your efforts pay off the most
  - Identify the performance and vectorization issues
  - Check memory access pattern
  - Check dependencies
  - More …
- **Roofline analysis**
  - How much performance is being left on the table
  - Where are the bottlenecks
  - Which can be improved
  - Which are worth improving



https://en.wikipedia.org/wiki/Intel_Advisorb

Workflow of Advisor Analysis

- **Survey**: find the vectorization information for loops and provide suggestions for improvement
- **Trip Counts**: generate a Roofline Chart
- **Memory Access Patterns** (MAP): see how you access the data
- **Dependencies**: determine if it is safe to force vectorization



Survey

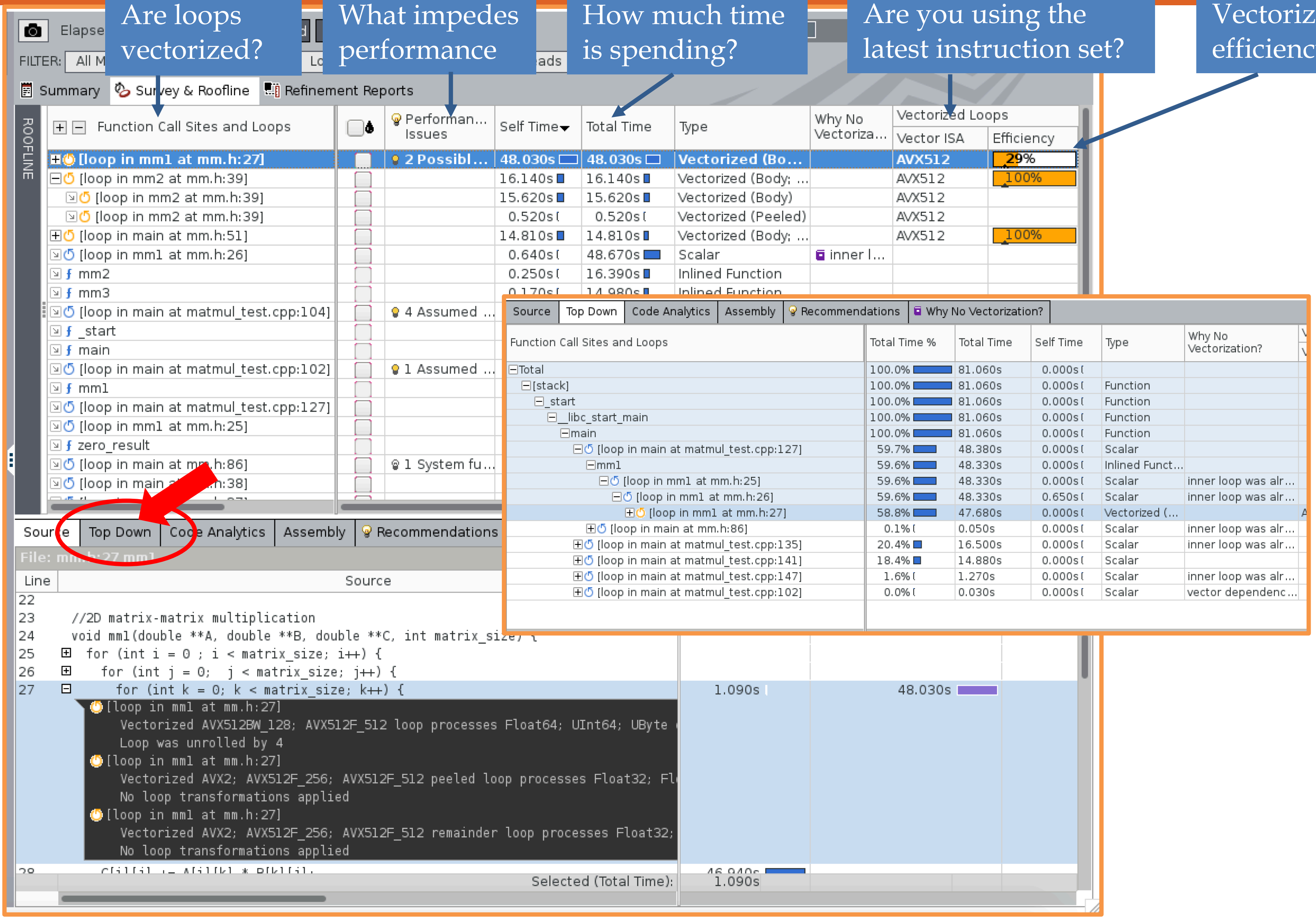
Are loops vectorized?

What impedes performance

How much time is spending?

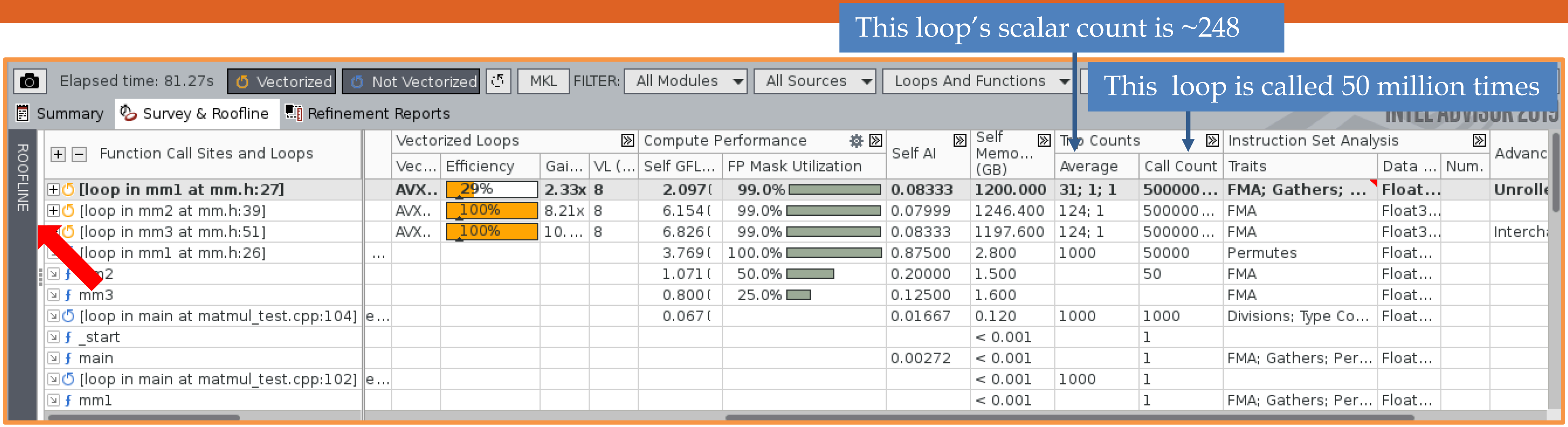
Are you using the latest instruction set?

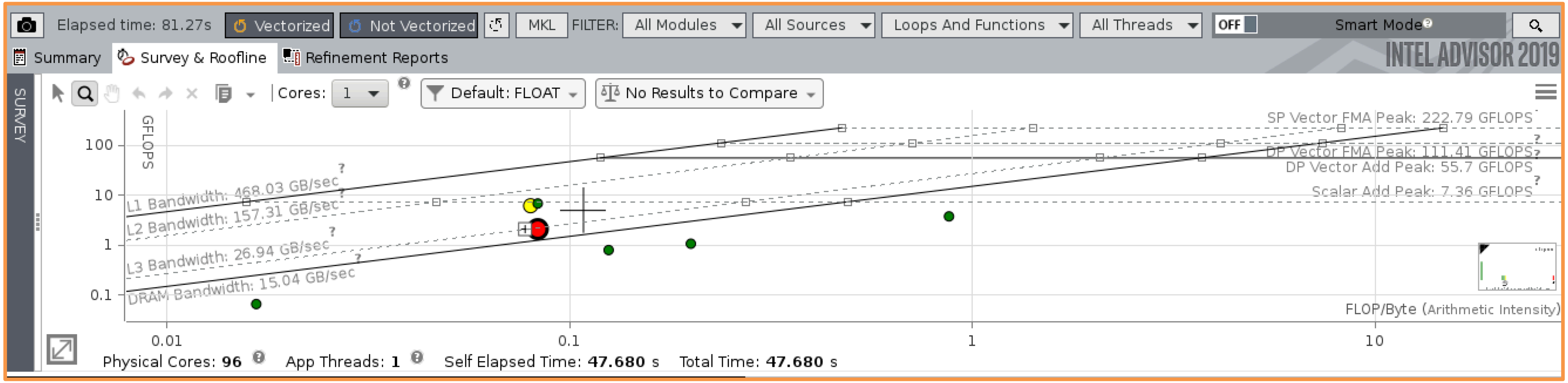
Vectorization efficiency



Run this command to collect the data (remotely): advixe-cl –c survey -project-dir $<PROJ_DIR> -no-auto-finalize -- $<EXE> $<ARGS>

Trip Counts





Run the following command to collect the data (remotely):

advixe-cl –c tripcounts -flop -project-dir $<PROJ_DIR> -no-auto-finalize -- $<EXE> $<ARGS>

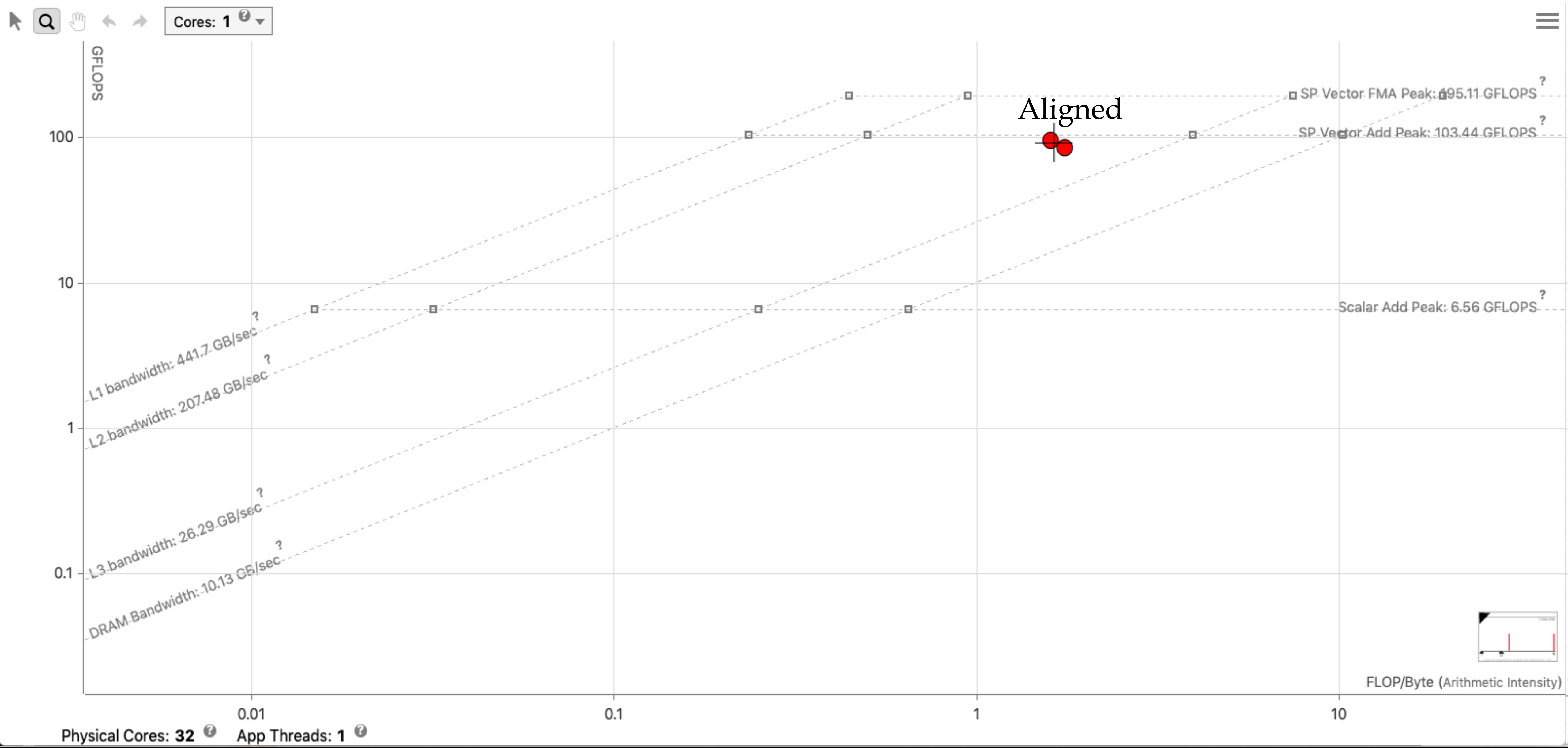
Note: it is important to use the same project directory as the survey analysis

Exercise 6: Using Advisor to Examine Nbody Problem

- Enable X11 forwarding
  - “ssh –Y -C <user>@adroit.princeton.edu
  - Will need local xserver (XQuartz for OSX, Xming for Windows)
- Load environment modules
  - module load intel intel-advisor
- Run the provided script to submit a Advisor wrapped job to the scheduler
  - bash ./submit_to_scheduler.sh
- Open the resulting directory with Intel Advisor
  - advixe-gui nbody-advisor
- Explore “Survey” report
- Run the provided script to submit a Advisor wrapped job with tripcounts analysis
  - In ./submit.slurm, change the job execution command to advisor command line with tripcounts analysis
  - bash ./submit_to_scheduler.sh
- Open the resulting directory with Intel Advisor
  - advixe-gui nbody-advisor
- Explore “Tripcounts & Roofline” report

N-Body Advisor Roofline Demo

Roofline Comparison



Help the Compiler to Vectorize (Intel)

COMPILER HINT	DESCRIPTION
#pragma ivdep	ignore potential (unproven) data dependences
#pragma vector always	override efficiency heuristics
#pragma vector [non]temporal	hint to use or not use streaming stores
#pragma vector [un]aligned	assert [un]aligned property
#pragma novector	disable vectorization for the loop
#pragma distribute point	hint to split loop at this point
#pragma loop count <int>	hint for likely trip count
restrict	Keyword to assert exclusive access through pointer; requires command line option "-restrict"
__assume_aligned(<var>, <int>)	Assert alignment property

https://software.intel.com/en-us/articles/a-guide-to-auto-vectorization-with-intel-c-compilers

Note: compiler directives are only hint to the compiler

Example: Pointer Aliasing

1. restrict restrict

```
void scale(double *a, double *b, int size)  {
                                    2. #pragma ivdep
                                    3. #pragma omp simd
                                    for (int i=0; i<size; i++)
                                        b[i] = 2.5*a[i]
}
```

- The compiler may not vectorize a loop if there is a potential dependency.
- For example, how about "if b[i] is pointed to a[i-1]"?
- If you know that this is not the case, you can help the compiler by
  1. -restrict –std=c90 compiler flags and 'restrict' keyword
  2. #pragma ivdep
  3. #pragma omp simd (more later)

Example: Indirect Addressing

```
void fun(double * restrict a, double * restrict b, double * restrict x, int * restrict index, int size){
    1. #pragma vector always
    2. #pragma omp simd
    for (int i=0; i<size; i++)
        b[i] += a[i] * x[index[i]];
}
```

- The compiler rarely vectorizes loops with non-unit stride or with indirect addressing unless the amount of computational work is large compared to the overhead from non-contiguous memory access
- You can help the compiler to vectorize the loop by
    1. #pragma vector always
    2. #pragma omp simd (more later)

Guided Auto-Vectorization by OpenMP SIMD

- Used to "enforce vectorization of loops", which includes
  - Loops with SIMD-enabled functions
  - Second innermost loops
  - Failed vectorization due to compiler decision
  - Where guidance is required (vector length, alignment, etc)
- OpenMP SIMD directives are commands to the compiler, not hints
  - E.g., #pragma omp simd
  - Compiler does no dependency and cost-benefit analysis
  - Programmer is responsible for correctness
- Available for OpenMP 4.0 and beyond (portable)
  - -qopenmp or –qopenmp-simd to enable

OpenMP SIMD Directives (5.0)

- Apply **#pragma omp simd** to a loop to indicate the loop can be transformed to a SIMD loop
  - **Available clauses:**
    - SAFELEN (max iteration which can be executed concurrently)
    - SIMDLEN (vector length)
    - LINEAR
    - ALGINED (tell compiler about the alignment information)
    - NONTEMPORAL (use streaming store)
    - PRIVATE
    - LASTPRIVATE
    - REDUCTION
    - COLLAPSE

    Similar to OpenMP for threading
- Apply **#pragma omp declare simd** to a function to enable the creation of vectorized versions of the function
- Apply **#pragma omp ordered simd** to a statement to enable serial operation of the statement

https://www.openmp.org/wp-content/uploads/OpenMP-API-Specification-5.0.pdf

Example: Histogram

```
#pragma omp simd
for (int i=0; i<N; i++) {
    double y = fun(x[i]);
    int ih = floor( (y-y0)*invbinw );
    #pragma omp ordered simd
    bin[ih] = bin[ih]+1;
}
```

```
#pragma omp declare simd
double fun(double x) {
    double twopi = 2.0*acos(1.0);
    double y = sin(x*twopi);

    return y;
}
```

- Compiler will refuse to vectorize the above loop due to
  - User defined function call
  - Data dependency
- Can be vectorized with OpenMP SIMD by:
  - Making fun() a SIMD function
  - Using OMP ORDERED SIMD pragma to address data dependency

Strip Mining

Original loop:

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

// do work

}
```

Loop with strip mining:

```
for (int i=0; i<N; i+=STRIP_SIZE) {
    for (int j=0; j<STRIP_SIZE; j++) {
        // do work
    }
}
```

- Transform a single loop into two nested loops
- The outer loop strides through “strips” of the iteration space
- The inner loop operates in iterations inside the strip (“mining” it)
- The strip size usually be chosen as a multiply of the vector length
- If the iteration count is not a multiple of the strip size, we need to implement a remainder loop

Case Study with Athena++
Particle subroutines

We would like to thank Lev Arzamasskiy and Matthew Kunz in the Princeton University Department of Astrophysical Sciences for sharing their source code

move.cpp

Interpolate from grid to particle (gather) and then update the particle properties

```
Real *x1, *x2, *x3, *v1, *v2, *v3;
__mm_malloc(&x1,…);
…
__mm_malloc(&v3,…);

….

for (long p=0; p<nparticle; p++)
  {
    a = (x1[p] - x1s) * dx1 + isg;
    ig = (int)(a);
    is = ig - 1;
    d = a - ig;
    wei1[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei1[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei1[2] = 0.5 * d * d;

    a = (x2[p] - x2s) * dx2 + jsg;
    ig = (int)(a);
    js = ig - 1;
    d = a - ig;
    wei2[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei2[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei2[2] = 0.5 * d * d;


    a = (x3[p] - x3s) * dx3 + ksg;
    ig = (int)(a);
    ks = ig - 1;
    d = a - ig;
    wei3[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei3[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei3[2] = 0.5 * d * d;


    bfld1 = 0.0; bfld2 = 0.0; bfld3 = 0.0;
    efld1 = 0.0; efld2 = 0.0; efld3 = 0.0;
    totwei=0; eb=0.0;

    // interpolate from grid to particle (gather)
    for (k0=0; k0<=2; k0++){
      for (j0=0; j0<=2; j0++){
        for (i0=0; i0<=2; i0++){
          w = wei3[k0] * wei2[j0] * wei1[i0];
          totwei += w;
          bfld1 += w * fcoup(0,ks+k0,js+j0,is+i0);
          bfld2 += w * fcoup(1,ks+k0,js+j0,is+i0);
          bfld3 += w * fcoup(2,ks+k0,js+j0,is+i0);
          efld1 += w * fcoup(3,ks+k0,js+j0,is+i0);
          efld2 += w * fcoup(4,ks+k0,js+j0,is+i0);
          efld3 += w * fcoup(5,ks+k0,js+j0,is+i0);
          eb    += w * fcoup(6,ks+k0,js+j0,is+i0);
        }
      }
    }

    bsq    = std::max(bfld1 * bfld1 + bfld2 * bfld2 +     bfld3 *
bfld3, TINY_NUMBER);
    edotb = efld1 * bfld1 + efld2 * bfld2 + efld3 * bfld3;
    diff = (eb*totwei - edotb)/bsq;
    efld1 += diff*bfld1;
    efld2 += diff*bfld2;
    efld3 += diff*bfld3;
    …

    // update particle position and velocity
    v1[p] = v1n + efld1 + vp2 * s3 - vp3 * s2;
    v2[p] = v2n + efld2 + vp3 * s1 - vp1 * s3;
    v3[p] = v3n + efld3 + vp1 * s2 - vp2 * s1;

    x1[p] = x1n + v1[p] * 0.5 * dt;
    x2[p] = x2n + v2[p] * 0.5 * dt;
    x3[p] = x3n + v3[p] * 0.5 * dt;
}
```

deposit.cpp

Interpolate from particle to grid (scatter)

```
for (long p=0; p<nparticle; p++)
  {
    a = (x1[p] - x1s) * dx1 + isg;
    ig = (int)(a);
    is = ig - 1;
    d = a - ig;
    wei1[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei1[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei1[2] = 0.5 * d * d;

    a = (x2[p] - x2s) * dx2 + jsg;
    ig = (int)(a);
    js = ig - 1;
    d = a - ig;
    wei2[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei2[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei2[2] = 0.5 * d * d;

    a = (x3[p] - x3s) * dx3 + ksg;
    ig = (int)(a);
    ks = ig - 1;
    d = a - ig;
    wei3[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei3[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei3[2] = 0.5 * d * d;

    // interpolate from particle to grid (scatter)

    for (k0=0; k0<=2; k0++){
      for (j0=0; j0<=2; j0++){
        for (i0=0; i0<=2; i0++){
          w = wei3[k0] * wei2[j0] * wei1[i0];
          mcoup(0,ks+k0,js+j0,is+i0) += w;
          mcoup(1,ks+k0,js+j0,is+i0) += w * v1[p];
          mcoup(2,ks+k0,js+j0,is+i0) += w * v2[p];
          mcoup(3,ks+k0,js+j0,is+i0) += w * v3[p];
        }
      }
    }
  }
```

Are *Move* and *Deposit* Being Vectorized?

(move.optrpt)

```
LOOP BEGIN at src/particle/move.cpp(64,3)
   remark #25096: Loop Interchange not done due to: Imperfect Loop Nest (Either at Source or due to other Compiler Transformations)
   remark #25451: Advice: Loop Interchange, if possible, might help loopnest. Suggested Permutation : ( 1 2 3 4 ) --> ( 2 3 1 4 )
   remark #15541: outer loop was not auto-vectorized: consider using SIMD directive

   LOOP BEGIN at src/particle/move.cpp(99,5)
      remark #25101: Loop Interchange not done due to: Original Order seems proper
      remark #25452: Original Order found to be proper, but by a close margin
      remark #15541: outer loop was not auto-vectorized: consider using SIMD directive
      remark #25436: completely unrolled by 3

      LOOP BEGIN at src/particle/move.cpp(100,7)
         remark #15541: outer loop was not auto-vectorized: consider using SIMD directive
         remark #25436: completely unrolled by 3

         LOOP BEGIN at src/particle/move.cpp(101,9)
            remark #15388: vectorization support: reference wei1[i0] has aligned access   [ src/particle/move.cpp(102,37) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0))] has unaligned access   [ src/particle/move.cpp(104,29) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup.nx3_))] has unaligned access   [ src/particle/move.cpp(105,29) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup.nx3_*2))] has unaligned access   [ src/particle/move.cpp(106,29) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup.nx3_*3))] has unaligned access   [ src/particle/move.cpp(107,29) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup.nx3_*4))] has unaligned access   [ src/particle/move.cpp(108,29) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup.nx3_*5))] has unaligned access   [ src/particle/move.cpp(109,29) ]
            remark #15389: vectorization support: reference fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup.nx3_*6))] has unaligned access   [ src/particle/move.cpp(110,29) ]
            remark #15381: vectorization support: unaligned access used inside loop body
            remark #15335: loop was not vectorized: vectorization possible but seems inefficient. Use vector always directive or -vec-threshold0 to override
            remark #15305: vectorization support: vector length 2
            remark #15309: vectorization support: normalized vectorization overhead 0.373
            remark #15448: unmasked aligned unit stride loads: 1
            remark #15450: unmasked unaligned unit stride loads: 7
            remark #15475: --- begin vector cost summary ---
            remark #15476: scalar cost: 74
            remark #15477: vector cost: 41.500
            remark #15478: estimated potential speedup: 1.180
            remark #15488: --- end vector cost summary ---
            remark #25436: completely unrolled by 3
         LOOP END

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END
      LOOP END

      LOOP BEGIN at src/particle/move.cpp(100,7)

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END
      LOOP END

      LOOP BEGIN at src/particle/move.cpp(100,7)

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END

         LOOP BEGIN at src/particle/move.cpp(101,9)
         LOOP END
      LOOP END
   LOOP END
LOOP END
```

The compiler failed to vectorize the inner most loop

deposit.optrpt

```
LOOP BEGIN at src/particle/deposit.cpp(57,3)
   remark #25096: Loop Interchange not done due to: Imperfect Loop Nest (Either at Source or due to other Compiler Transformations)
   remark #25452: Original Order found to be proper, but by a close margin
   remark #15541: outer loop was not auto-vectorized: consider using SIMD directive

   LOOP BEGIN at src/particle/deposit.cpp(83,5)
      remark #25101: Loop Interchange not done due to: Original Order seems proper
      remark #25452: Original Order found to be proper, but by a close margin
      remark #15541: outer loop was not auto-vectorized: consider using SIMD directive
      remark #25436: completely unrolled by 3

      LOOP BEGIN at src/particle/deposit.cpp(84,7)
         remark #15541: outer loop was not auto-vectorized: consider using SIMD directive
         remark #25436: completely unrolled by 3

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
            remark #15344: loop was not vectorized: vector dependence prevents vectorization
            remark #15346: vector dependence: assumed OUTPUT dependence between mcoup.pdata_[?-1+i0+mcoup.nx1_*(?-1+j0+mcoup.nx2_*(ig-1+k0))] (87:16) and mcoup.pdata_[?-1+i0+mcoup.nx1_*(?-1+j0+mcoup.nx2
            remark #15346: vector dependence: assumed OUTPUT dependence between mcoup.pdata_[?-1+i0+mcoup.nx1_*(?-1+j0+mcoup.nx2_*(ig-1+k0+mcoup (90:16) and mcoup.pdata_[?-1+i0+mcoup.nx1_*(?-1+j0+mcoup.
            remark #25436: completely unrolled by 3
         LOOP END

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END
      LOOP END

      LOOP BEGIN at src/particle/deposit.cpp(84,7)

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END
      LOOP END

      LOOP BEGIN at src/particle/deposit.cpp(84,7)

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END

         LOOP BEGIN at src/particle/deposit.cpp(85,9)
         LOOP END
      LOOP END
   LOOP END
LOOP END
```

The compiler failed to vectorize the inner most loop because of vector dependence in scatter operation

First Attempt:

- Using **#pragma omp simd** in the outer most loop

move.cpp

Use simd directives

```
#pragma omp simd private(…)
for (long p=0; p<nparticle; p++)
  {
    a = (x1[p] – x1s) ∗ dx1 + isg;
    ig = (int)(a);
    is = ig – 1;
    d = a – ig;
    wei1[0] = 0.5 ∗ (1.0 – d) ∗ (1.0 – d);
    wei1[1] = 0.75 – (d – 0.5) ∗ (d – 0.5);
    wei1[2] = 0.5 ∗ d ∗ d;

    a = (x2[p] – x2s) ∗ dx2 + jsg;
    ig = (int)(a);
    js = ig – 1;
    d = a – ig;
    wei2[0] = 0.5 ∗ (1.0 – d) ∗ (1.0 – d);
    wei2[1] = 0.75 – (d – 0.5) ∗ (d – 0.5);
    wei2[2] = 0.5 ∗ d ∗ d;


    a = (x3[p] – x3s) ∗ dx3 + ksg;
    ig = (int)(a);
    ks = ig – 1;
    d = a – ig;
    wei3[0] = 0.5 ∗ (1.0 – d) ∗ (1.0 – d);
    wei3[1] = 0.75 – (d – 0.5) ∗ (d – 0.5);
    wei3[2] = 0.5 ∗ d ∗ d;


    bfld1 = 0.0; bfld2 = 0.0; bfld3 = 0.0;
    efld1 = 0.0; efld2 = 0.0; efld3 = 0.0;
    totwei=0; eb=0.0;

    // interpolate from grid to particle (gather)
    for (k0=0; k0<=2; k0++){
      for (j0=0; j0<=2; j0++){
        for (i0=0; i0<=2; i0++){
          w = wei3[k0] ∗ wei2[j0] ∗ wei1[i0];
          totwei += w;
          bfld1 += w ∗ fcoup(0,ks+k0,js+j0,is+i0);
          bfld2 += w ∗ fcoup(1,ks+k0,js+j0,is+i0);
          bfld3 += w ∗ fcoup(2,ks+k0,js+j0,is+i0);
          efld1 += w ∗ fcoup(3,ks+k0,js+j0,is+i0);
          efld2 += w ∗ fcoup(4,ks+k0,js+j0,is+i0);
          efld3 += w ∗ fcoup(5,ks+k0,js+j0,is+i0);
          eb    += w ∗ fcoup(6,ks+k0,js+j0,is+i0);
        }
      }
    }

    bsq   = std::max(bfld1 ∗ bfld1 + bfld2 ∗ bfld2 +     bfld3 ∗
bfld3, TINY_NUMBER);
    edotb = efld1 ∗ bfld1 + efld2 ∗ bfld2 + efld3 ∗ bfld3;
    diff = (eb∗totwei – edotb)/bsq;
    efld1 += diff∗bfld1;
    efld2 += diff∗bfld2;
    efld3 += diff∗bfld3;
    …

    // update particle position and velocity
    v1[p] = v1n + efld1 + vp2 ∗ s3 – vp3 ∗ s2;
    v2[p] = v2n + efld2 + vp3 ∗ s1 – vp1 ∗ s3;
    v3[p] = v3n + efld3 + vp1 ∗ s2 – vp2 ∗ s1;

    x1[p] = x1n + v1[p] ∗ 0.5 ∗ dt;
    x2[p] = x2n + v2[p] ∗ 0.5 ∗ dt;
    x3[p] = x3n + v3[p] ∗ 0.5 ∗ dt;
}
```

move.optrpt

```
LOOP BEGIN at src/particle/move.cpp(69,3)
<Peeled loop for vectorization>
   remark #15389: vectorization support: reference this->x1[p] has unaligned access   [ src/particle/move.cpp(73,13) ]
   remark #15389: vectorization support: reference this->x2[p] has unaligned access   [ src/particle/move.cpp(74,13) ]
   remark #15389: vectorization support: reference this->x3[p] has unaligned access   [ src/particle/move.cpp(75,13) ]
   remark #15389: vectorization support: reference this->v1[p] has unaligned access   [ src/particle/move.cpp(76,13) ]
   remark #15389: vectorization support: reference this->v2[p] has unaligned access   [ src/particle/move.cpp(77,13) ]
   remark #15389: vectorization support: reference this->v3[p] has unaligned access   [ src/particle/move.cpp(78,13) ]
   remark #15389: vectorization support: reference this->x1[p] has unaligned access   [ src/particle/move.cpp(155,5) ]
   remark #15389: vectorization support: reference this->x2[p] has unaligned access   [ src/particle/move.cpp(156,5) ]
   remark #15389: vectorization support: reference this->x3[p] has unaligned access   [ src/particle/move.cpp(157,5) ]
   remark #15389: vectorization support: reference this->v1[p] has unaligned access   [ src/particle/move.cpp(158,5) ]
   remark #15389: vectorization support: reference this->v2[p] has unaligned access   [ src/particle/move.cpp(159,5) ]
   remark #15389: vectorization support: reference this->v3[p] has unaligned access   [ src/particle/move.cpp(160,5) ]
   remark #15381: vectorization support: unaligned access used inside loop body
   remark #15335: peel loop was not vectorized: vectorization possible but seems inefficient. Use vector always directive or -vec-threshold0 to override
   remark #15305: vectorization support: vector length 2
   remark #15309: vectorization support: normalized vectorization overhead 0.135
   remark #25015: Estimate of max trip count of loop=1
LOOP END

   remark #15328: vectorization support: irregularly indexed load was emulated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup>,
om memory   [ src/particle/move.cpp(120,29) ]
   remark #15328: vectorization support: irregularly indexed load was emulated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup>,
om memory   [ src/particle/move.cpp(121,29) ]
   remark #15328: vectorization support: irregularly indexed load was emulated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup>,
om memory   [ src/particle/move.cpp(122,29) ]
   remark #15305: vectorization support: vector length 2
   remark #15309: vectorization support: normalized vectorization overhead 0.299
   remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
   remark #15321: Compiler has chosen to target XMM/YMM vector. Try using -qopt-zmm-usage=high to override
   remark #15450: unmasked unaligned unit stride loads: 6
   remark #15451: unmasked unaligned unit stride stores: 6
   remark #15462: unmasked indexed (or gather) loads: 189
   remark #15475: --- begin vector cost summary ---
   remark #15476: scalar cost: 2089
   remark #15477: vector cost: 3212.000
   remark #15478: estimated potential speedup: 0.630
   remark #15486: divides: 3
   remark #15487: type converts: 6
   remark #15488: --- end vector cost summary ---
```

1. Peel loop exists

2. Unaligned access

3. No potential speed up

Second Attempt:

- Using **posix_memalign** to allocate particle arrays with alignment
- Telling the compiler that memory accesses are aligned

move.cpp

Ensure Alignment

```
Real *x1, *x2, *x3, *v1, *v2, *v3;
posix_memalign(&x1,…,64);
…
posix_memalign(&v3,…,64);

#pragma omp simd aligned(x1,x2,x3,v1,v2,v3 :64) private(…)
for (long p=0; p<nparticle; p++)
  {
    a = (x1[p] - x1s) * dx1 + isg;
    ig = (int)(a);
    is = ig - 1;
    d = a - ig;
    wei1[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei1[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei1[2] = 0.5 * d * d;

    a = (x2[p] - x2s) * dx2 + jsg;
    ig = (int)(a);
    js = ig - 1;
    d = a - ig;
    wei2[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei2[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei2[2] = 0.5 * d * d;


    a = (x3[p] - x3s) * dx3 + ksg;
    ig = (int)(a);
    ks = ig - 1;
    d = a - ig;
    wei3[0] = 0.5 * (1.0 - d) * (1.0 - d);
    wei3[1] = 0.75 - (d - 0.5) * (d - 0.5);
    wei3[2] = 0.5 * d * d;


    bfld1 = 0.0; bfld2 = 0.0; bfld3 = 0.0;
    efld1 = 0.0; efld2 = 0.0; efld3 = 0.0;
    totwei=0; eb=0.0;

    // interpolate from grid to particle (gather)
    for (k0=0; k0<=2; k0++){
      for (j0=0; j0<=2; j0++){
        for (i0=0; i0<=2; i0++){
          w = wei3[k0] * wei2[j0] * wei1[i0];
          totwei += w;
          bfld1 += w * fcoup(0,ks+k0,js+j0,is+i0);
          bfld2 += w * fcoup(1,ks+k0,js+j0,is+i0);
          bfld3 += w * fcoup(2,ks+k0,js+j0,is+i0);
          efld1 += w * fcoup(3,ks+k0,js+j0,is+i0);
          efld2 += w * fcoup(4,ks+k0,js+j0,is+i0);
          efld3 += w * fcoup(5,ks+k0,js+j0,is+i0);
          eb    += w * fcoup(6,ks+k0,js+j0,is+i0);
        }
      }
    }

    bsq   = std::max(bfld1 * bfld1 + bfld2 * bfld2 +     bfld3 *
bfld3, TINY_NUMBER);
    edotb = efld1 * bfld1 + efld2 * bfld2 + efld3 * bfld3;
    diff = (eb*totwei - edotb)/bsq;
    efld1 += diff*bfld1;
    efld2 += diff*bfld2;
    efld3 += diff*bfld3;
    …

    // update particle position and velocity
    v1[p] = v1n + efld1 + vp2 * s3 - vp3 * s2;
    v2[p] = v2n + efld2 + vp3 * s1 - vp1 * s3;
    v3[p] = v3n + efld3 + vp1 * s2 - vp2 * s1;

    x1[p] = x1n + v1[p] * 0.5 * dt;
    x2[p] = x2n + v2[p] * 0.5 * dt;
    x3[p] = x3n + v3[p] * 0.5 * dt;

}
```

move.optrpt

```
LOOP BEGIN at src/particle/move.cpp(75,3)
   remark #25096: Loop Interchange not done due to: Imperfect Loop Nest (Either at Source or due to other Compiler Transformations)
   remark #25451: Advice: Loop Interchange, if possible, might help loopnest. Suggested Permutation : ( 1 2 3 4 ) --> ( 2 3 1 4 )
   remark #25456: Number of Array Refs Scalar Replaced In Loop: 81
   remark #15388: vectorization support: reference this->x1[p] has aligned access   [ src/particle/move.cpp(79,13) ]
   remark #15388: vectorization support: reference this->x2[p] has aligned access   [ src/particle/move.cpp(80,13) ]
   remark #15388: vectorization support: reference this->x3[p] has aligned access   [ src/particle/move.cpp(81,13) ]
   remark #15388: vectorization support: reference this->v1[p] has aligned access   [ src/particle/move.cpp(82,13) ]
   remark #15388: vectorization support: reference this->v2[p] has aligned access   [ src/particle/move.cpp(83,13) ]
   remark #15388: vectorization support: reference this->v3[p] has aligned access   [ src/particle/move.cpp(84,13) ]
   remark #15388: vectorization support: reference this->x1[p] has aligned access   [ src/particle/move.cpp(161,5) ]
   remark #15388: vectorization support: reference this->x2[p] has aligned access   [ src/particle/move.cpp(162,5) ]
   remark #15388: vectorization support: reference this->x3[p] has aligned access   [ src/particle/move.cpp(163,5) ]
   remark #15388: vectorization support: reference this->v1[p] has aligned access   [ src/particle/move.cpp(164,5) ]
   remark #15388: vectorization support: reference this->v2[p] has aligned access   [ src/particle/move.cpp(165,5) ]
   remark #15388: vectorization support: reference this->v3[p] has aligned access   [ src/particle/move.cpp(166,5) ]

    remark #15328: vectorization support: irregularly indexed load was emulated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx
  om memory   [ src/particle/move.cpp(126,29) ]
    remark #15328: vectorization support: irregularly indexed load was emulated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx
  om memory   [ src/particle/move.cpp(127,29) ]
    remark #15328: vectorization support: irregularly indexed load was emulated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx
  om memory   [ src/particle/move.cpp(128,29) ]
    remark #15305: vectorization support: vector length 2
    remark #15309: vectorization support: normalized vectorization overhead 0.294
    remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
    remark #15321: Compiler has chosen to target XMM/YMM vector. Try using -qopt-zmm-usage=high to override
    remark #15448: unmasked aligned unit stride loads: 6
    remark #15449: unmasked aligned unit stride stores: 6
    remark #15462: unmasked indexed (or gather) loads: 189
    remark #15475: --- begin vector cost summary ---
    remark #15476: scalar cost: 2089
    remark #15477: vector cost: 3199.500
    remark #15478: estimated potential speedup: 0.640
    remark #15486: divides: 3
    remark #15487: type converts: 6
    remark #15488: --- end vector cost summary ---
```

1. No peel loop anymore

2. Aligned access

3. Still no potential speed up, unfortunately

Third Attempt

- Use **loop fission** to expose more parallelism
- Use **strip mining** to reduce memory requirement to pass values from the first loop to the second

move.cpp

Two nested loops

```
Real bfld1v[SIMD_WIDTH] __attribute__((aligned(64)));
Real bfld2v[SIMD_WIDTH] __attribute__((aligned(64)));
Real bfld3v[SIMD_WIDTH] __attribute__((aligned(64)));
Real efld1v[SIMD_WIDTH] __attribute__((aligned(64)));
Real efld2v[SIMD_WIDTH] __attribute__((aligned(64)));
Real efld3v[SIMD_WIDTH] __attribute__((aligned(64)));
Real ebv[SIMD_WIDTH] __attribute__((aligned(64)));
Real totweiv[SIMD_WIDTH] __attribute__((aligned(64)));

for (int p=0; p<nparticle; p+=SIMD_WIDTH){

    Real *__restrict__ x1p = x1 + p;
    Real *__restrict__ x2p = x2 + p;
    Real *__restrict__ x3p = x3 + p;
    Real *__restrict__ v1p = v1 + p;
    Real *__restrict__ v2p = v2 + p;
    Real *__restrict__ v3p = v3 + p;

    #pragma omp simd aligned(x1p,x2p,x3p,v1p,v2p,v3p :64) simdlen(SIMD_WIDTH) private(…)
    for (int pp=0; pp<SIMD; pp++) {

        x1tmp = x1p[pp];
        x2tmp = x2p[pp];
        x3tmp = x3p[pp];
        v1tmp = v1p[pp];
        v2tmp = v2p[pp];
        v3tmp = v3p[pp];

        a = (x1tmp - x1s) * dx1 + isg;
        ig = (int)(a);
        is = ig - 1;
        d = a - ig;
        wei1[0] = 0.5 * (1.0 - d) * (1.0 - d);
        wei1[1] = 0.75 - (d - 0.5) * (d - 0.5);
        wei1[2] = 0.5 * d * d;

        a = (x2tmp - x2s) * dx2 + jsg;
        ig = (int)(a);
        js = ig - 1;
        d = a - ig;
        wei2[0] = 0.5 * (1.0 - d) * (1.0 - d);
        wei2[1] = 0.75 - (d - 0.5) * (d - 0.5);
        wei2[2] = 0.5 * d * d;

        a = (x3tmp - x3s) * dx3 + ksg;
        ig = (int)(a);
        ks = ig - 1;
        d = a - ig;
        wei3[0] = 0.5 * (1.0 - d) * (1.0 - d);
        wei3[1] = 0.75 - (d - 0.5) * (d - 0.5);
        wei3[2] = 0.5 * d * d;
```

```
bfld1v[pp] = 0.0; bfld2v[pp] = 0.0; bfld3v[pp] = 0.0;
efld1v[pp] = 0.0; efld2v[pp] = 0.0; efld3v[pp] = 0.0;
ebv[pp] = 0.0; totweiv[pp]=0.0;

for (k0=0; k0<=2; k0++){
  for (j0=0; j0<=2; j0++){
    for (i0=0; i0<=2; i0++){
       w = wei3[k0] * wei2[j0] * wei1[i0];
       totweiv[pp] += w;
       bfld1v[pp] += w * fcoup(0,ks+k0,js+j0,is+i0);
       bfld2v[pp] += w * fcoup(1,ks+k0,js+j0,is+i0);
       bfld3v[pp] += w * fcoup(2,ks+k0,js+j0,is+i0);
       efld1v[pp] += w * fcoup(3,ks+k0,js+j0,is+i0);
       efld2v[pp] += w * fcoup(4,ks+k0,js+j0,is+i0);
       efld3v[pp] += w * fcoup(5,ks+k0,js+j0,is+i0);
       ebv[pp]    += w * fcoup(6,ks+k0,js+j0,is+i0);
    }
  }
}

    #pragma omp simd aligned(x1p,x2p,x3p,v1p,v2p,v3p :64)   simdlen(SIMD_WIDTH)
private(…)
    for (int pp=0; pp<SIMD; pp++) {
      x1tmp = x1p[pp];
      x2tmp = x2p[pp];
      x3tmp = x3p[pp];
      v1tmp = v1p[pp];
      v2tmp = v2p[pp];
      v3tmp = v3p[pp];

      bsq   = std::max(bfld1v[pp] * bfld1v[pp] + bfld2v[pp] * bfld2v[pp] + bfld3v[pp]*
bfld3v[pp], TINY_NUMBER);
      edotb = efld1v[pp] * bfld1v[pp] + efld2v[pp] * bfld2v[pp] + efld3v[pp] *
bfld3v[pp];
      diff = (ebv[pp]*totweiv[pp] - edotb)/bsq;
      efld1v[pp] += diff*bfld1v[pp];
      efld2v[pp] += diff*bfld2v[pp];
      efld3v[pp] += diff*bfld3v[pp];

      …

      x1p[pp] = x1n + v1tmp * halfdt;
      x2p[pp] = x2n + v2tmp * halfdt;
      x3p[pp] = x3n + v3tmp * halfdt;
      v1p[pp] = v1tmp;
      v2p[pp] = v2tmp;
      v3p[pp] = v3tmp;
    }
  }
```

Loop fission

move.optrpt (1/2)

```
LOOP BEGIN at src/particle/move.cpp(79,3)
   remark #25084: Preprocess Loopnests: Moving Out Store    [ src/particle/move.cpp(86,30) ]
   remark #25084: Preprocess Loopnests: Moving Out Store    [ src/particle/move.cpp(87,30) ]
   remark #25084: Preprocess Loopnests: Moving Out Store    [ src/particle/move.cpp(88,30) ]
   remark #15542: loop was not vectorized: inner loop was already vectorized

   LOOP BEGIN at src/particle/move.cpp(93,59)
      remark #25096: Loop Interchange not done due to: Imperfect Loop Nest (Either at Source or due to other Compiler Transformations)
      remark #25451: Advice: Loop Interchange, if possible, might help loopnest. Suggested Permutation : ( 1 2 3 4 ) --> ( 2 3 1 4 )
      remark #15388: vectorization support: reference x1p[pp] has aligned access   [ src/particle/move.cpp(95,13) ]
      remark #15388: vectorization support: reference x2p[pp] has aligned access   [ src/particle/move.cpp(96,13) ]
      remark #15388: vectorization support: reference x3p[pp] has aligned access   [ src/particle/move.cpp(97,13) ]
```

Aligned access

```
      remark #15415: vectorization support: irregularly indexed load was generated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup>, part of index
e.cpp(144,27) ]
      remark #15415: vectorization support: irregularly indexed load was generated for the variable <fcoup.pdata_[?-1+i0+fcoup.nx1_*(?-1+j0+fcoup.nx2_*(ig-1+k0+fcoup>, part of index
e.cpp(145,27) ]
      remark #15305: vectorization support: vector length 16
      remark #15309: vectorization support: normalized vectorization overhead 0.034
      remark #26012: vectorization support: data layout of a private variable wei1 was optimized, converted to SoA
      remark #26012: vectorization support: data layout of a private variable wei2 was optimized, converted to SoA
      remark #26012: vectorization support: data layout of a private variable wei3 was optimized, converted to SoA
      remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
      remark #15448: unmasked aligned unit stride loads: 193
      remark #15449: unmasked aligned unit stride stores: 224
      remark #15462: unmasked indexed (or gather) loads: 189
      remark #15475: --- begin vector cost summary ---
      remark #15476: scalar cost: 2182
      remark #15477: vector cost: 2413.930
      remark #15478: estimated potential speedup: 0.870
      remark #15487: type converts: 6
      remark #15488: --- end vector cost summary ---
      remark #25015: Estimate of max trip count of loop=1
```

No potential speed up (but it is ok)

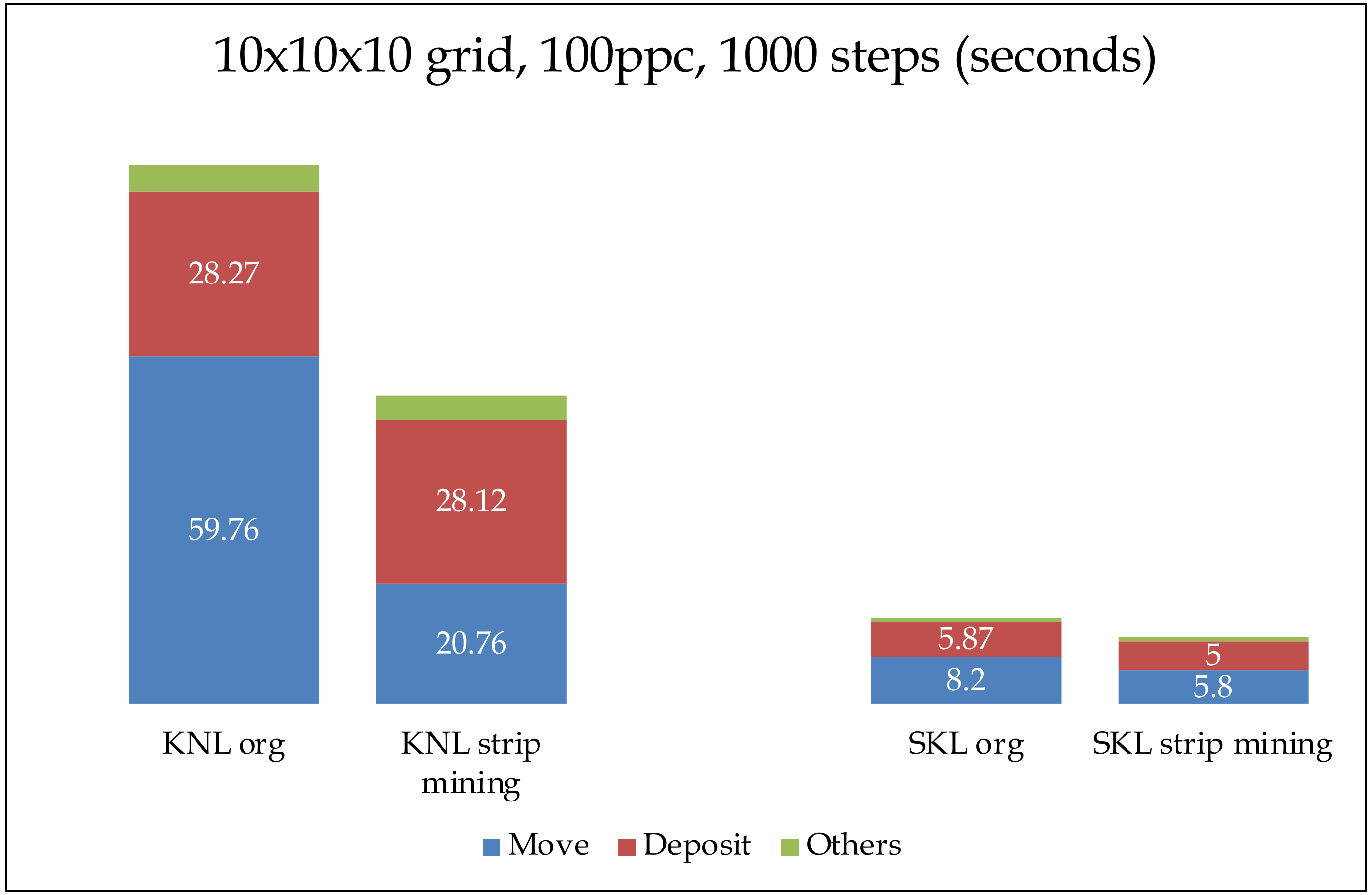
move.optrpt (2/2)

```
LOOP BEGIN at src/particle/move.cpp(153,59)
   remark #15388: vectorization support: reference x1p[pp] has aligned access   [ src/particle/move.cpp(154,15) ]
   remark #15388: vectorization support: reference x2p[pp] has aligned access   [ src/particle/move.cpp(155,15) ]
   remark #15388: vectorization support: reference x3p[pp] has aligned access   [ src/particle/move.cpp(156,15) ]
   remark #15388: vectorization support: reference v1p[pp] has aligned access   [ src/particle/move.cpp(157,15) ]
   remark #15388: vectorization support: reference v2p[pp] has aligned access   [ src/particle/move.cpp(158,15) ]
   remark #15388: vectorization support: reference v3p[pp] has aligned access   [ src/particle/move.cpp(159,15) ]
   remark #15388: vectorization support: reference bfld1v[pp] has aligned access   [ src/particle/move.cpp(165,24) ]
   remark #15388: vectorization support: reference bfld1v[pp] has aligned access   [ src/particle/move.cpp(165,37) ]
   remark #15388: vectorization support: reference bfld2v[pp] has aligned access   [ src/particle/move.cpp(165,50) ]
   remark #15388: vectorization support: reference bfld2v[pp] has aligned access   [ src/particle/move.cpp(165,63) ]
   remark #15388: vectorization support: reference bfld3v[pp] has aligned access   [ src/particle/move.cpp(165,76) ]
   remark #15388: vectorization support: reference bfld3v[pp] has aligned access   [ src/particle/move.cpp(165,88) ]

   remark #15388: vectorization support: reference x1p[pp] has aligned access   [ src/particle/move.cpp(193,7) ]
   remark #15388: vectorization support: reference x2p[pp] has aligned access   [ src/particle/move.cpp(194,7) ]
   remark #15388: vectorization support: reference x3p[pp] has aligned access   [ src/particle/move.cpp(195,7) ]
   remark #15388: vectorization support: reference v1p[pp] has aligned access   [ src/particle/move.cpp(196,7) ]
   remark #15388: vectorization support: reference v2p[pp] has aligned access   [ src/particle/move.cpp(197,7) ]
   remark #15388: vectorization support: reference v3p[pp] has aligned access   [ src/particle/move.cpp(198,7) ]
   remark #15305: vectorization support: vector length 16
   remark #15309: vectorization support: normalized vectorization overhead 0.057
   remark #15301: OpenMP SIMD LOOP WAS VECTORIZED
   remark #15448: unmasked aligned unit stride loads: 49
   remark #15449: unmasked aligned unit stride stores: 16
   remark #15475: --- begin vector cost summary ---
   remark #15476: scalar cost: 367
   remark #15477: vector cost: 69.620
   remark #15478: estimated potential speedup: 4.980
   remark #15486: divides: 3
   remark #15488: --- end vector cost summary ---
   remark #25015: Estimate of max trip count of loop=1
LOOP END
```

Aligned access

~5x potential speed up

Performance Comparison



	Move	Deposit
KNL	2.87x	1.00x
SKL	1.41x	1.17x

Strip-Mining Lessons Learned

Strip-mining is useful because it:

1. Helps the compiler detects data alignment
   - Data alignment typically means two things:
   - Aligning the base-pointer where the space is allocated for the array (no peel loop)
   - Making sure the starting indices have alignment properties for each vectorized loop
2. Allows loop splitting to expose vectorization (without additional memory footprint)
   - The compiler refuses to vectorize a loop because a non-vectorizable operation is present in it
   - Split the loop to two loops, one contains non-vectorizable operations and one contains vectorizable ones
3. Allows vectorization to co-exist with multi-threading and tiling

https://software.intel.com/sites/default/files/parallel-universe-issue-36.pdf

Good References

- Theoretical peak FLOPS per instruction set: a tutorial, Domain Dolbeau, J Supercomput, 74: 1341-1377, 2018
- Demystifying Vectorization, Colfax Interational, Webinar, June 2017
- Exploiting Parallelism for Intel Xeon Processors, J.D.Patel, Intel Skylake Training at Princeton, 2018
- Vector Parallelism on Multi-Core Processors, Steve Lantz, CoDas-HEP Summer School, July 2019
- https://cvw.cac.cornell.edu/vector/default
- Compiling and Tuning for Performance using Intel Advanced Vector Extensions 512, Carlos Rosales-Fernandez, SC18, Intel Speakership Tutorial
- Improving Performance by Vectorization for Particle-In-Cell Codes, Bei Wang, Carlos Rosales-Fernandez, and William Tang, The Parallel Universe, issue 36, 2018