

Optimization

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Outline

What to expect from this course

- A look at some example-driven, hands-on techniques for optimizing computational kernels
- The techniques will be motivated by specific codes which we will optimize step-by-step
- Techniques might seem problem-specific, but will (hopefully) demonstrate an overall strategy for optimizing kernels
- We will be using CPUs (e.g. not GPUs), but the strategies are generalizable

Lecture section

- Introduction and refresh of notation, definitions, etc. (some overlap with "Performance Analysis" sessions)
- Finding a code's asymptotically achievable performance
- Understanding a code's current performance
- Steps to take to optimize, motivated by examples/exercises

Outline

Exercises

Three exercises to demonstrate some optimization strategies

1. Simple data-layout transformations

- "AoS to SoA" (*Array of Structures* to *Structure of Arrays*)

2. Optimizing matrix-matrix multiplications

- Blocking of data for mitigating cache misses

3. 3D laplacian-stencil code

- Multi-threading (OpenMP)
- Data layout transformations
- Blocking (or tiling)

Hardware characteristics

Peak floating point rate

- The theoretical, highest number of floating point operations that can be carried out by a computational unit
- Depends on: clock rate, vector length, FPUs per core, cores per socket

Peak bandwidth

- The theoretical, highest number of bytes that can be read/written from/to some level of memory (L1,2,3 cache, RAM, etc.)
- For RAM: data rate, channels, ranks, banks

When optimizing, it is important to have these numbers in mind for the machine you're running on

Julia

E.g. Julia compute nodes have the following characteristics:

- Peak FP (γ_{FP})
 - 64-cores per node (1 KNL), clock: 1.3 GHz
 - Best case: two 512-bit fused multiply-and-adds per cycle (AVX-512)
- In double precision: $2 \times (8 \text{ mul} + 8 \text{ add})$ per cycle = 32 flop/cycle
 - Therefore: $1.3 \times 10^9 \text{ cycles/s} \times 32 \text{ flop/cycle} = 41.6 \text{ Gflop/s per core}$
 - 2662.4 Gflop/s per node
- Peak BW (γ_{IO})
 - 115.2 GB/s to 96 GB DDR4 RAM assuming all channels populated
 - 400 GB/s to 16 GB MCDRAM
- Some (semi-)standard tools
 - On Linux, you can obtain processor details via `cat /proc/cpuinfo`.
 - You can obtain topology and memory info e.g. `hwloc`, `dmidecode` (latter requires access to `/dev/mem`)

Julia

On Linux, you can obtain processor details via `cat /proc/cpuinfo`. For a Julia compute node:

```
processor      : 0
vendor_id     : GenuineIntel
...
model name    : Intel(R) Xeon Phi(TM) CPU 7230 @ 1.30GHz
...
cpu MHz       : 1261.914
cache size    : 1024 KB
physical id   : 0
siblings       : 256
core id        : 0
cpu cores     : 64
...
cpuid level   : 13
...
flags          : fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca cmov pat
                  pse36 clflush dts acpi mmx fxsr sse sse2 ss ht tm pbe syscal...
```

Computational kernels

Sustained performance

- Sustained FP-rate: the measured, average number of floating point operations carried out by the kernel per unit time
 - `add`, `sub`, and `mul` count as 1 flop
 - `dev`, `sqrt`, `sin`, etc. count ≥ 2 flops. Depends on architecture
 - Count number of flops in kernel and divide by runtime
 - Alternatively, or for more complex codes, use performance counters

In our examples we will see cases of kernels where the flops are countable

- Sustained BW: the measured, average bytes read/written from main memory per unit time
 - As in the case of FP-rate, count bytes needed to be read and bytes needed to be written to and from RAM and divide by run time
 - **Maximum data reuse** assumption: once data is read from RAM, it never needs to be re-read

An example

- Consider the following kernel operation:

$$Y_i^{ab} = A^{ac} \cdot X_i^{cb},$$

with: $i = 0, \dots, L - 1, a, b, c = 0, \dots, N - 1, L \gg N$

- Naive implementation:

```
double Y[L][N][N];
double X[L][N][N];
double A[N][N];

/* ...
 * Initialize X[][][] and A[][]
 */
for(int i=0; i<L; i++) {
    for(int a=0; a<N; a++) {
        for(int b=0; b<N; b++) {
            Y[i][a][b] = 0;
            for(int c=0; c<N; c++) {
                Y[i][a][b] += A[a][c]*X[i][c][b];
            }
        }
    }
}
```

Number of fp operations

- $N_{FP} = L \cdot 2 \cdot N^3$

Number of bytes of I/O

- $N_{IO} = w \cdot (2 \cdot L \cdot N^2 + N^2)$
- w : word-length in bytes, e.g. $w = 4$ for single precision, 8 for double, etc.
- $2LN^2 \rightarrow O(L)$ if $L \gg N$
- In any case, if N small enough, A should be kept in low-level cache

An example

Note the assumption of data reuse

```
Y[i][0][0] = A[0][0]*X[i][0][0] + A[0][1]*X[i][1][0] + ... + A[0][N-1]*X[i][N-1][0];
Y[i][0][1] = A[0][0]*X[i][0][1] + A[0][1]*X[i][1][1] + ... + A[0][N-1]*X[i][N-1][1];
...
Y[i][1][0] = A[1][0]*X[i][0][0] + A[1][1]*X[i][1][0] + ... + A[1][N-1]*X[i][N-1][0];
Y[i][1][1] = A[1][0]*X[i][0][1] + A[1][1]*X[i][1][1] + ... + A[1][N-1]*X[i][N-1][1];
...
```

Elements of X and A are required multiple times. However we only count their loads once.

- Given some measurement of the run-time \bar{T}

- FP-rate: $\beta_{\text{FP}} = \frac{N_{\text{FP}}}{\bar{T}}$

- IO-rate: $\beta_{\text{IO}} = \frac{N_{\text{IO}}}{\bar{T}}$

- This motivates defining an *intensity* $I = \frac{N_{\text{FP}}}{N_{\text{IO}}}$

```
for(int i=0; i<L; i++) {
    for(int a=0; a<N; a++) {
        for(int b=0; b<N; b++) {
            Y[i][a][b] = 0;
            for(int c=0; c<N; c++) {
                Y[i][a][b] += A[a][c]*X[i][c][b];
            }
        }
    }
}
```

Intensities

Computational kernel intensity

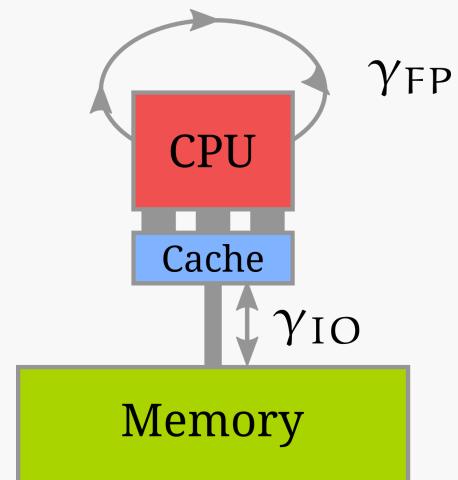
- Ratio of kernel floating point operations to bytes of I/O
- For our previous example:

$$\circ \quad I_k = \frac{N_{FP}}{N_{IO}} = \frac{2LN^3}{2wLN^2} = N/w$$

- Note how the problem size L drops out \Rightarrow constant I_k irrespective of problem size
- E.g. for $N = 3$ and double precision, $I_k = 0.375$ flops/byte

Machine flop/byte ratio

- Similarly to I_k , we can define the machine flop/byte ratio (I_m)
- $I_m = \frac{\gamma_{FP}}{\gamma_{IO}}$
- E.g. for a Julia (compute node): $I_m \simeq 23 \frac{\text{flop}}{\text{byte}}$



Intensities

Balance between kernel / hardware intensities

- $I_k \gg I_m$: Kernel is "compute-bound" on this architecture. Higher γ_{FP} would lead to higher performance, but higher γ_{IO} would not.
- $I_k \ll I_m$: Kernel is "bandwidth-" or "memory-bound" on this architecture. Higher γ_{IO} would lead to higher performance, but higher γ_{FP} would not.
- $I_k \simeq I_m$: Kernel is balanced on this architecture. Ideal situation.

For the example kernel of the previous slides, on Julia

- $I_k \ll I_m \Rightarrow$ the kernel is memory-bound on Julia

Note the assumptions that enter I_k and I_m

- γ_{FP} considers all operations can be a sequence of multiply-and-add
- β_{IO} assumes maximum data reuse
- I_k constant if problem size L drops out

Kernel computational intensity

Another example: matrix-matrix multiplication

- Consider a matrix-matrix multiplication: $C_{M \times K} = A_{M \times N} \cdot B_{N \times K}$

```
double C[M][K];
double A[M][N];
double B[N][K];

for(int m=0; m<M; m++) {
    for(int k=0; k<K; k++) {
        C[m][k] = 0;
        for(int n=0; n<N; n++) {
            C[m][k] += A[m][n]*B[n][k];
        }
    }
}
```

- $N_{FP} = 2 \cdot M \cdot K \cdot N$
- $N_{IO} = w \cdot (M \cdot K + M \cdot N + N \cdot K)$
- $I_k = \frac{2}{w} \frac{1}{\frac{1}{M} + \frac{1}{N} + \frac{1}{K}}$
- E.g. for a square problem $M = N = K$,
 $\Rightarrow I_k = \frac{2}{3} \frac{N}{w}$

- This is an example of a kernel where I_k depends on the problem size.
- On a given architecture with I_m , the kernel transitions from bandwidth-bound to compute-bound as N increases.
- On Julia, the kernel is balanced when $N \geq 12 \Rightarrow$ when the matrices are too large to fit in cache the problem is compute-bound.

Optimization

Given a code you wish to optimize, for an architecture with I_m

- What is N_{FP} and N_{IO} and what is the resulting I_k ?
- Is the kernel memory or compute bound on this architecture?
- What do you obtain for β_{FP} and β_{IO}
 - For this one requires measuring the performance on the targeted architecture
- What are the ratios $\frac{\beta_{FP}}{\gamma_{FP}}$ and $\frac{\beta_{IO}}{\gamma_{IO}}$?

These are questions you need to answer before considering optimization

- After answering the above, we can start considering targeted optimizations for our kernel on the given machine
 - If your kernel is **memory-bound**, we should be trying to optimize for **memory I/O**. Ideally we try to achieve a $\frac{\beta_{IO}}{\gamma_{IO}} \rightarrow 1$.
 - If your kernel is **compute-bound**, we should be trying to optimize for a higher **FP-rate**. Ideally we try to achieve a $\frac{\beta_{FP}}{\gamma_{FP}} \rightarrow 1$.
- In practice, however, we will see how these two strategies in general are combined to optimize both memory- and compute-bound kernels.

Optimization

On modern systems, the compiler and the architecture will do a lot for you

- Loop unrolling, prefetching, out-of-order execution, auto-vectorization, etc.

We will motivate our optimizations by considering specific examples where a significant speedup can be achieved on top of `-O3`

Vectorization

- We will see how to use *vector intrinsic functions* which compile to Single Instruction Multiple Data (SIMD) instructions
- At first sight, this optimization seems to target compute bound kernels
- However the data transformations required to efficiently vectorize a compute kernel also prove beneficial for the I/O efficiency

Optimization

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Data layout transformations

- Transformations for mitigation of cache misses (improve temporal and spatial cache locality)
- Transformations which can assist vectorization or auto-vectorization

Cache awareness

- Similar to the above, this optimization will allow us to modify code parameters according to cache characteristics (*blocking* or *tiling*)

Optimization

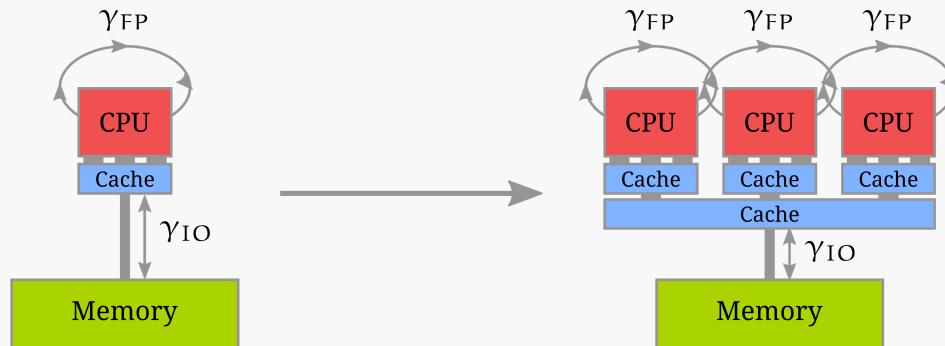
On modern systems, the compiler and the architecture will do a lot for you

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We will motivate our optimizations by considering specific examples where a significant speedup can be achieved on top of `-O3`

Multi-threading

- Some simple `OpenMP` can go a long way



- For compute-bound kernels, this effectively multiplies γ_{FP}
- For memory-bound kernels, allows better saturation of γ_{IO}

Vectorization

Most modern processors have some vectorization capabilities

- SSE, AVX, AltiVec, QPX, NEON
- Single Instruction Multiple Data -- SIMD

```
for(int i=0; i<L; i++)
    y[i] = a*x[i] + y[i];
```

Vectorization

Most modern processors have some vectorization capabilities

- SSE, AVX, AltiVec, QPX, NEON
- Single Instruction Multiple Data -- SIMD

```
for(int i=0; i<L; i++)
    y[i] = a*x[i] + y[i];
```

```
for(int i=0; i<L; i+=4) {
    y[i] = a*x[i] + y[i];
    y[i+1] = a*x[i+1] + y[i+1];
    y[i+2] = a*x[i+2] + y[i+2];
    y[i+3] = a*x[i+3] + y[i+3];
}
```

Vectorization

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- SSE, AVX, AltiVec, QPX, NEON
- Single Instruction Multiple Data -- SIMD

```
for(int i=0; i<L; i++)  
    y[i] = a*x[i] + y[i];
```

```
float4 va = {a,a,a,a};  
for(int i=0; i<L; i+=4) {  
    float4 vy;  
    float4 vx;  
    load4(vx, &x[i]);  
    load4(vy, &y[i]);  
    vy = va*vx + vy;  
    store4(&y[i], vy);  
}
```

```
for(int i=0; i<L; i+=4) {  
    y[i] = a*x[i] + y[i];  
    y[i+1] = a*x[i+1] + y[i+1];  
    y[i+2] = a*x[i+2] + y[i+2];  
    y[i+3] = a*x[i+3] + y[i+3];  
}
```

Note: the above is pseudo-code, namely `load4`,
`float4`, etc. are simplifications.

Vectorization

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- SSE, AVX, AltiVec, QPX, NEON
- Single Instruction Multiple Data -- SIMD

```
for(int i=0; i<L; i++)  
    y[i] = a*x[i] + y[i];
```

```
float4 va = {a,a,a,a};  
for(int i=0; i<L; i+=4) {  
    float4 vy;  
    float4 vx;  
    load4(vx, &x[i]);  
    load4(vy, &y[i]);  
    vy = va*vx + vy;  
    store4(&y[i], vy);  
}
```

```
for(int i=0; i<L; i+=4) {  
    y[i] = a*x[i] + y[i];  
    y[i+1] = a*x[i+1] + y[i+1];  
    y[i+2] = a*x[i+2] + y[i+2];  
    y[i+3] = a*x[i+3] + y[i+3];  
}
```

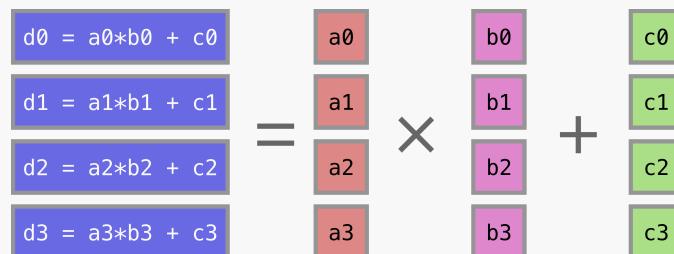
Note: the above is pseudo-code, namely `load4`, `float4`, etc. are simplifications.

- In many cases, the compiler will generate vector instructions (auto-vectorization)
- If not, we will learn here how to explicitly program using these vector instructions, via *intrinsic functions*

Vectorization

Intrinsics

- These are extensions to C and architecture-specific
- Here we will see some Intel intrinsics, though most of what we will learn is generalizable to other architectures. In the best case, they differ in the function naming convention
- For an exhaustive reference on Intel intrinsics, the best resource is at:
<https://software.intel.com/sites/landingpage/IntrinsicsGuide>
 - Lists intrinsics for all versions of SSE to AVX and KNL
 - Note the header requirements depending on the extension version under which the function you would like to use is defined (e.g. `<xmmmintrin.h>`, `<immintrin.h>`, etc.)



```
d = _mm256_fmaddd_pd(a, b, c)
```

Vectorization

Intrinsics - short intro

- Vector types defined in `<?mmmintrin.h>`:
 - `_m128`: 128-bit single precision ⇒ can pack four
 - `_m128d`: 128-bit double precision ⇒ can pack two
 - `_m256` (`_m256d`): 256-bit float (double), packs eight (four)
- `_mm_load_pd()`: "load packed double", e.g.:

```
double *x;
posix_memalign(&x, 32, L*sizeof(double));
double __attribute__((aligned(32))) a;
_m128d vx, va;
_mm_load_pd(vx, &x[i]);
_mm_load_pd(va, &a);
```

- **Alignment restrictions:** `&x[i]` must be a multiple of the vector length.
- Use `posix_memalign()` to allocate
- Use `__attribute__((aligned(32)))` for static
- `_mm_load_ps()`, `_mm256_load_ps()`, etc.

Vectorization

Intrinsics - short intro

- Store:
 - `_mm_store_ps()`, `_mm256_store_ps()`, `_mm_store_pd()`, etc.
 - Same restriction on alignment as in the case of load
- Arithmetic:
 - `c = _mm_add_pd(a, b);`, $c = a + b$ with a, b, c of type `_m128d`
 - `c = _mm256_mul_ps(a, b);`, $c = a \times b$ with a, b, c of type `_m256`
 - In general, `_mm_` prepends 128-bit vector instructions (SSE) and `_mm256_` prepends 256-bit instructions (AVX)
 - If processor supports fused-multiply-add (`fma` flag in `/proc/cpuinfo`), then:
`d = _mm256_fmadd_pd(a, b, c);`, $d = a \times b + c$ with a, b, c, d of type `_m256d`

Vectorization

Intrinsics - short intro

- Shuffles, swizzles,
 - Instructions which allow permuting the elements within a vector
- One classical demonstration is when doing complex multiplications, e.g.:
$$z_n = x_n \cdot y_n, \text{ with } x, y, z \text{ complex, e.g: } x_n = x_n^r + i x_n^i \Rightarrow$$
$$z_n^r = x_n^r \cdot y_n^r - x_n^i \cdot y_n^i$$
$$z_n^i = x_n^r \cdot y_n^i + x_n^i \cdot y_n^r$$
- A complex type is typically implemented as an array of two elements:

```
for(int n=0; n<N; n++) {  
    z[n][0] = x[n][0]*y[n][0] - x[n][1]*y[n][1]; /* z[n][0]: real part of z[n] */  
    z[n][1] = x[n][1]*y[n][0] + x[n][0]*y[n][1]; /* z[n][1]: imag part of z[n] */  
}
```

Vectorization

Intrinsics - short intro

```
for(int n=0; n<N; n++) {
    z[n][0] = x[n][0]*y[n][0] - x[n][1]*y[n][1]; /* z[n][0]: real part of z[n] */
    z[n][1] = x[n][1]*y[n][0] + x[n][0]*y[n][1]; /* z[n][1]: imag part of z[n] */
}
```

- One (naive) way to implement this in intrinsics:

```
_m256d vx0, vx1, vy0, vy1, aux0, aux1;
_m256d mp = {-1.0, +1.0};
for(int n=0; n<N; n++) {
    _mm_load_pd(vx0, &x[n][0]);
    _mm_load_pd(vy0, &y[n][0]);
    vx1 = _mm_shuffle_pd(vx0, vx0, 0b10); /* swap real and imag of vx0 and put into vx1 */
    vy1 = _mm_shuffle_pd(vy0, vy0, 0b11); /* put the imag of vy0 into both elems of vy1 */
    vy0 = _mm_shuffle_pd(vy0, vy0, 0b00); /* put the real of vy0 into both elems of vy0 */
    vx1 = _mm_mul_pd(mp, vx1);           /* flip sign of 1st elem of vx1 and store in vx1 */
    aux0 = _mm_mul_pd(vx0, vy0);
    aux1 = _mm_mul_pd(vx1, vy1);
    vz = _mm_add_pd(aux0, aux1);
    _mm_store_pd(&z[n][0], vz);
}
```

Vectorization

Intrinsics - short intro

- General form of shuffle: `c = _mm_shuffle_pd(a, b, mask)`
-

<code>mask = 0b00</code> → <code>c = {a[0], b[0]}</code>	<code>mask = 0b01</code> → <code>c = {a[1], b[0]}</code>
<code>mask = 0b10</code> → <code>c = {a[0], b[1]}</code>	<code>mask = 0b11</code> → <code>c = {a[1], b[1]}</code>

- In general, rightmost bits of `mask` select elements of `a` and leftmost bits select elements of `b`
- A better implementation may be (SSE3):

```
for(int n=0; n<N; n++) {
    z[n][0] = x[n][0]*y[n][0];
    z[n][0] -= x[n][1]*y[n][1];
    z[n][1] = x[n][1]*y[n][0];
    z[n][1] += x[n][0]*y[n][1];
}
```

`c = hadd(a, b) →`
`c[0] = a[0]+a[1],`
`c[1] = b[0]+b[1]`

```
m128d mp = {+1.0, -1.0};
for(int n=0; n<N; n++) {
    _mm_load_pd(vx0, &x[n][0]);
    _mm_load_pd(vy0, &y[n][0]);
    vx1 = _mm_shuffle_pd(vx0, vx0, 0b10); /* swap re-im */
    vx0 = _mm_mul_pd(mp, vx0);
    aux0 = _mm_mul_pd(vx0, vy0);
    aux1 = _mm_mul_pd(vx1, vy0);
    vz = _mm_hadd_pd(aux0, aux1);
    _mm_store_pd(&z[n][0], vz);
}
```

Data layout

Data layout transformations

- Better cache locality
 - The data are ordered in a way as close to the order in which they will be accessed in your kernels as possible
 - The data are reordered such that when an element needs to be accessed multiple times, these multiple accesses are issued very close to each other
 - Optimizes for temporal and for spatial locality
- Easier vectorization
 - The data are ordered such that the same operation can be applied to consecutive elements
 - Assists the compiler in detecting auto-vectorization opportunities
 - Assists the programmer in implementing the intrinsics

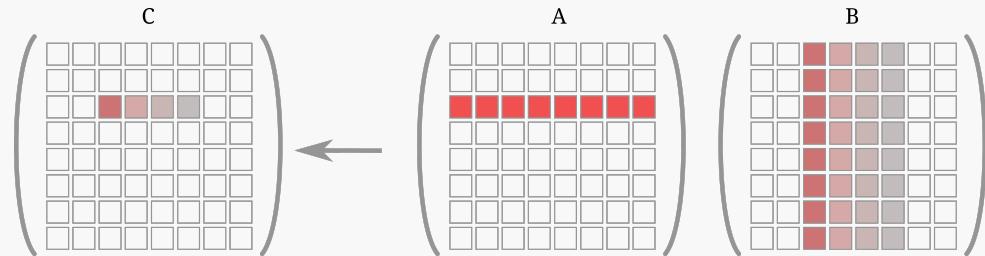
Data layout

1. Matrix-matrix multiplication

$$C_{ij} = \sum_{k=0}^{N-1} A_{ik} \cdot B_{kj}$$

$A_{M \times N}, B_{N \times M}, C_{M \times M}$

```
for(int i=0; i<M; i++) {  
    for(int j=0; j<M; j++) {  
        C[i*M + j] = 0;  
        for(int k=0; k<N; k++) {  
            C[i*M + j] += A[i*N + k]*B[k*M + j];  
        }  
    }  
}
```



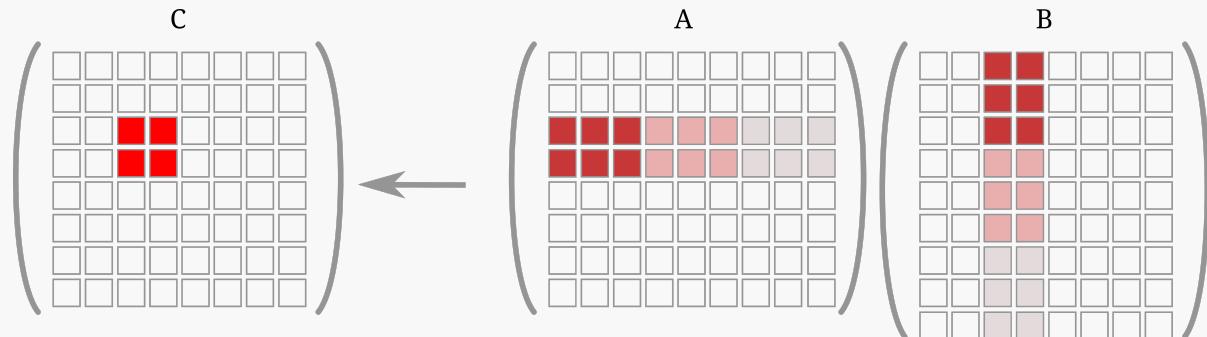
- Repeated reading of columns of B
- If N too large, a whole row of A may not fit into L2 cache

Data layout

1. Matrix-matrix multiplication

Consider a blocked version

```
for(int i=0; i<M; i+=BM)
    for(int j=0; j<M; j+=BM) {
        Cb [:BM] [:BM] = 0;
        for(int k=0; k<N; k++) {
            Ab [:BM] [:BN] = A[i:i+BM] [k:k+BN];
            Bb [:BN] [:BM] = B[k:k+BN] [j:j+BM];
            for(int ib=0; ib<BM; ib++)
                for(int jb=0; jb<BM; jb++)
                    for(int kb=0; kb<BN; kb++)
                        Cb[ib][jb] += Ab[ib][kb] * Bb[kb][jb];
            C[i:i+BM] [j:j+BM] = Cb [:BM] [:BM];
        }
    }
```

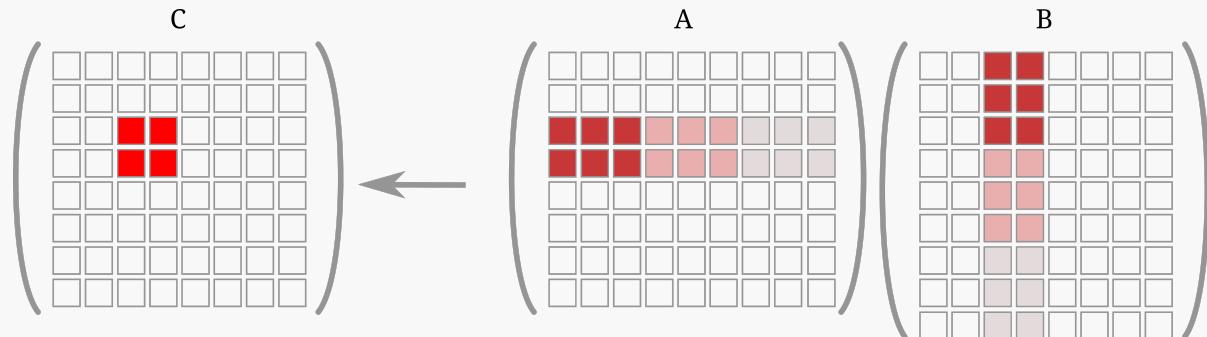


Data layout

1. Matrix-matrix multiplication

Consider a blocked version

```
for(int i=0; i<M; i+=BM)
    for(int j=0; j<M; j+=BM) {
        Cb[:BM] [:BM] = 0;
        for(int k=0; k<N; k++) {
            Ab[:BM] [:BN] = A[i:i+BM] [k:k+BN];
            Bb[:BM] [:BN] = B[j:j+BM] [k:k+BN]; /* Transpose B! */
            for(int ib=0; ib<BM; ib++)
                for(int jb=0; jb<BM; jb++)
                    for(int kb=0; kb<BN; kb++)
                        Cb[ib][jb] += Ab[ib][kb] * Bb[jb][kb];
            C[i:i+BM] [j:j+BM] = Cb[:BM] [:BM];
        }
    }
```



Data layout

2. AoS to SoA

AoS: Array of structures

Arrays of structures arise naturally when mapping physical problems to code. E.g. say you want to define an array of coordinates:

```
typedef struct {
    float x;
    float y;
    float z;
} coords;
```

You can now allocate an array of `coords`:

```
size_t L = 1000;
coords *arr = malloc(sizeof(coords)*L);
```

Now assume you would like to get an array of the distances of the coordinates from the origin:

```
for(int i=0; i<L; i++)
    r[i] = sqrt(arr[i].x*arr[i].x +
                arr[i].y*arr[i].y +
                arr[i].z*arr[i].z);
```

You can see how the choice of data layout makes auto-vectorization difficult. A common way around this is to use a Structure of Arrays (SoA) rather than an Array of Structures.

Data layout

2. AoS to SoA

Define a structure of arrays, this is similar to how one programs for GPUs:

```
typedef struct {  
    float *x;  
    float *y;  
    float *z;  
} coords;
```

And now allocate each element of `coords` separately:

```
coords arr;  
arr.x = malloc(sizeof(float)*L);  
arr.y = malloc(sizeof(float)*L);  
arr.z = malloc(sizeof(float)*L);
```

You can see how it is more obvious vectorize the distance calculation after unrolling:

```
for(int i=0; i<L; i+=4) {  
    r[i] = sqrt(arr.x[i]*arr.x[i]+arr.y[i]*arr.y[i]+arr.z[i]*arr.z[i]);  
    r[i+1] = sqrt(arr.x[i+1]*arr.x[i+1]+arr.y[i+1]*arr.y[i+1]+arr.z[i+1]*arr.z[i+1]);  
    r[i+2] = sqrt(arr.x[i+2]*arr.x[i+2]+arr.y[i+2]*arr.y[i+2]+arr.z[i+2]*arr.z[i+2]);  
    r[i+3] = sqrt(arr.x[i+3]*arr.x[i+3]+arr.y[i+3]*arr.y[i+3]+arr.z[i+3]*arr.z[i+3]);  
}
```

Data layout

3. Stencil codes

Another application of the data re-ordering is in stencil codes. Consider a 2-D stencils operation:

$$\phi_{x,y} \leftarrow 4\psi_{x,y} - (\psi_{x+1,y} + \psi_{x-1,y} + \psi_{x,y+1} + \psi_{x,y-1})$$

```
for(int y=0; y<L; y++)  
for(int x=0; x<L; x++) {  
    B[y][x] = 4*A[y][x] - (A[y][x+1] + A[y][x-1] + A[y+1][x] + A[y-1][x]);  
}
```

Consider an unrolled implementation of this, with `x` running fastest and `y` slowest:

```
for(int y=0; y<L; y++)  
for(int x=0; x<L; x+=4) {  
    B[y][x] = 4*A[y][x] - (A[y][x+1] + A[y][x-1] + A[y+1][x] + A[y-1][x]);  
    B[y][x+1] = 4*A[y][x+1] - (A[y][x+2] + A[y][x] + A[y+1][x+1] + A[y-1][x+1]);  
    B[y][x+2] = 4*A[y][x+2] - (A[y][x+3] + A[y][x+1] + A[y+1][x+2] + A[y-1][x+2]);  
    B[y][x+3] = 4*A[y][x+3] - (A[y][x+4] + A[y][x+2] + A[y+1][x+3] + A[y-1][x+3]);  
}
```

If $A[y][x:x+4]$ is fit into a vector register, you can see how many shuffles of the elements are required to vectorize this operations.

Data layout

3. Stencil codes

```
for(int y=0; y<L; y++)  
for(int x=0; x<L; x+=4) {  
    B[y][x] = 4*A[y][x] - (A[y][x+1] + A[y][x-1] + A[y+1][x] + A[y-1][x]);  
    B[y][x+1] = 4*A[y][x+1] - (A[y][x+2] + A[y][x] + A[y+1][x+1] + A[y-1][x+1]);  
    B[y][x+2] = 4*A[y][x+2] - (A[y][x+3] + A[y][x+1] + A[y+1][x+2] + A[y-1][x+2]);  
    B[y][x+3] = 4*A[y][x+3] - (A[y][x+4] + A[y][x+2] + A[y+1][x+3] + A[y-1][x+3]);  
}
```

An alternative is to change the data layout so that we vectorize over distant elements.
I.e. we can reshape the data layout:

from: $A[y][x] \leftarrow A + y*L + x$

to: $vA[y0][x][y1] = A[y0+y1*L/4][x]$, and re-write the kernel:

```
for(int y=0; y<L/4; y++)  
for(int x=0; x<L; x++) {  
    vB[y][x][0] = 4*vA[y][x][0] - (vA[y][x+1][0] + vA[y][x-1][0] + vA[y+1][x][0] + vA[y-1][x][0]);  
    vB[y][x][1] = 4*vA[y][x][1] - (vA[y][x+1][1] + vA[y][x-1][1] + vA[y+1][x][1] + vA[y-1][x][1]);  
    vB[y][x][2] = 4*vA[y][x][2] - (vA[y][x+1][2] + vA[y][x-1][2] + vA[y+1][x][2] + vA[y-1][x][2]);  
    vB[y][x][3] = 4*vA[y][x][3] - (vA[y][x+1][3] + vA[y][x-1][3] + vA[y+1][x][3] + vA[y-1][x][3]);  
}
```

Data layout

3. Stencil codes

Shuffling of the elements is still required but restricted to the boundaries. E.g. for periodic boundary conditions, the original code at the $y=0$ boundary would be:

```
y = 0;
for(int x=0; x<L; x++) {
    B[0][x] = 4*A[0][x] - (A[0][x+1] + A[0][x-1] + A[1][x] + A[L-1][x]);
}
```

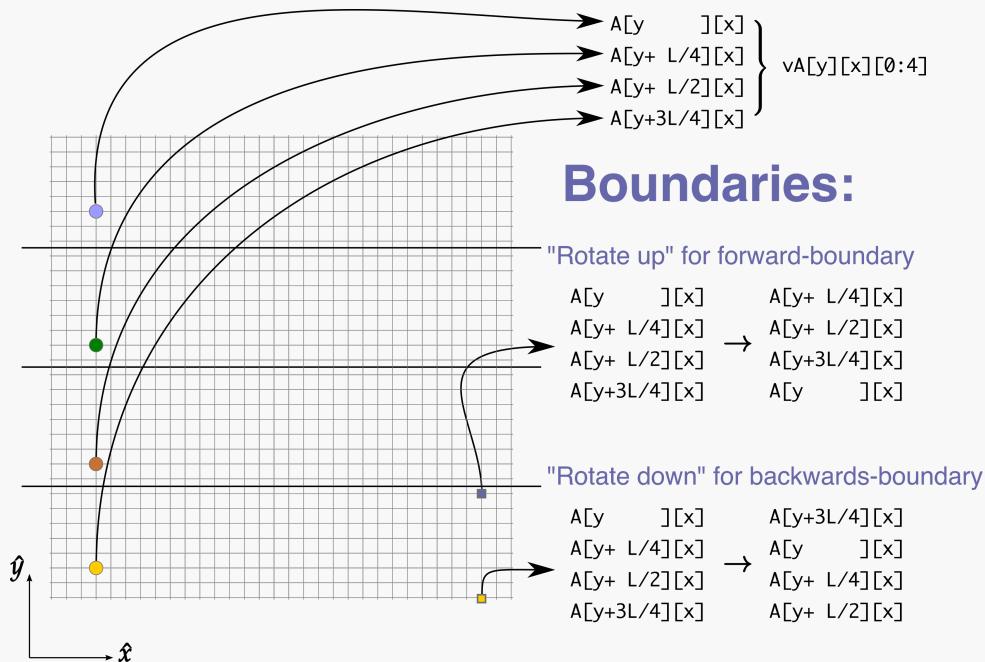
which requires shuffling of the boundary element at $y=L/4-1$ of vA :

```
y = 0;
for(int x=0; x<L; x++) {
    vB[0][x][0] = 4*vA[0][x][0] - (vA[0][x+1][0] + vA[0][x-1][0] + vA[1][x][0] + vA[L/4-1][x][3]);
    vB[0][x][1] = 4*vA[0][x][1] - (vA[0][x+1][1] + vA[0][x-1][1] + vA[1][x][1] + vA[L/4-1][x][2]);
    vB[0][x][2] = 4*vA[0][x][2] - (vA[0][x+1][2] + vA[0][x-1][2] + vA[1][x][2] + vA[L/4-1][x][1]);
    vB[0][x][3] = 4*vA[0][x][3] - (vA[0][x+1][3] + vA[0][x-1][3] + vA[1][x][3] + vA[L/4-1][x][0]);
}
```

Data layout

3. Stencil codes

```
y = 0;  
for(int x=0; x<L; x++) {  
    vB[0][x][0] = 4*vA[0][x][0] - (vA[0][x+1][0] + vA[0][x-1][0] + vA[1][x][0] + vA[L/4-1][x][3]);  
    vB[0][x][1] = 4*vA[0][x][1] - (vA[0][x+1][1] + vA[0][x-1][1] + vA[1][x][1] + vA[L/4-1][x][2]);  
    vB[0][x][2] = 4*vA[0][x][2] - (vA[0][x+1][2] + vA[0][x-1][2] + vA[1][x][2] + vA[L/4-1][x][1]);  
    vB[0][x][3] = 4*vA[0][x][3] - (vA[0][x+1][3] + vA[0][x-1][3] + vA[1][x][3] + vA[L/4-1][x][0]);  
}
```



Exercises

```
git clone -n https://github.com/g-koutsou/CDS-1.git  
cd CDS-1  
git checkout trainee
```

The exercises are prepared for: `julia.fz-juelich.de`

For compiling codes, use Intel's C compiler: `module load openmpi`

For plotting, use Python 3: `module load python/3.6.1 matplotlib/2.1.0`

AoS to SoA

In the first exercise we will look into two optimizations:

1. Going from an Array-of-Structures to a Structure-of-Arrays,
2. which will assist the (auto-)vectorization of our kernel

The kernel does the following: assuming an array of 4-vectors: $a_i = (ct_i, x_i, y_i, z_i)$ compute the squared "norm": $s_i = (ct_i)^2 - (x_i^2 + y_i^2 + z_i^2)$

Navigate to: [CDS-1/0ptim/Ex/AoS-to-SoA/](#).

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Navigate to: [CDS-1/0ptim/Ex/AoS-to-SoA/](#).

```
while(1) {
    double t0 = stop_watch(0);
    for(int i=0; i<NREP; i++)
        comp_s(arr, L);
    t0 = stop_watch(t0)/(double)NREP;
    t0acc += t0;
    t1acc += t0*t0;
    if(n > 2) {
        double ave = t0acc/n;
        double err = sqrt(t1acc/n -
                           ave*ave)/sqrt(n);
        if(err/ave < 0.1) {
            t0acc = ave;
            t1acc = err;
            break;
        }
    }
    n++;
}
```

`stop_watch()` is just a system timer:

```
double
stop_watch(double t0) {
    struct timeval tp;
    gettimeofday(&tp, NULL);
    double t1 = tp.tv_sec + tp.tv_usec*1e-6;
    return t1-t0;
}
```

- Call the kernel `NREP` times
- Do this repeatedly. Stop when variation in time to call kernel `NREP` times is smaller than 10%

AoS to SoA

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Navigate to: [CDS-1/0ptim/Ex/AoS-to-SoA/](#).

`stop_watch()` is just a system timer:

```
double  
stop_watch(double t0) {  
    struct timeval tp;  
    gettimeofday(&tp, NULL);  
    double t1 = tp.tv_sec + tp.tv_usec*1e-6;  
    return t1-t0;  
}
```

`x`, `y`, `z`, `t`, and `s` are elements of a `struct`

```
typedef struct {  
    float x, y, z, t;  
    float s;  
} st_coords;
```

The computation of `s` is a loop over an array of `st_coords`:

```
void  
comp_s(st_coords *arr, int L)  
{  
#pragma omp parallel for  
    for(int i=0; i<L; i++) {  
        float x = arr[i].x;  
        float y = arr[i].y;  
        float z = arr[i].z;  
        float t = arr[i].t;  
        float s = t*t - (x*x + y*y + z*z);  
        arr[i].s = s;  
    }  
    return;  
}
```

Note that we are using OpenMP and parallelizing over 128 threads

AoS to SoA

For the first task you will modify `space-time-aos.c`. You have instructions tagged with `_TODO_A_`.

After correcting for `beta_fp` and `beta_io`, you need to compile:

```
module load openmpi  
make A
```

and submit the prepared job script:

```
sbatch sub-A.job
```

```
void  
comp_s(st_coords *arr, int L)  
{  
#pragma omp parallel for  
    for(int i=0; i<L; i++) {  
        float x = arr[i].x;  
        float y = arr[i].y;  
        float z = arr[i].z;  
        float t = arr[i].t;  
        float s = t*t - (x*x + y*y + z*z);  
        arr[i].s = s;  
    }  
    return;  
}  
...  
double beta_fp = 0 /* _TODO_A_: insert number of */  
/* Gflop/sec based on timing */;  
double beta_io = 0 /* _TODO_A_: insert number of */  
/* Gbyte/sec based on timing */;
```

This will run the code for various lengths `L`. The output is in `aos.txt`. There is a Python script so that you can visualize the output. You will need to:

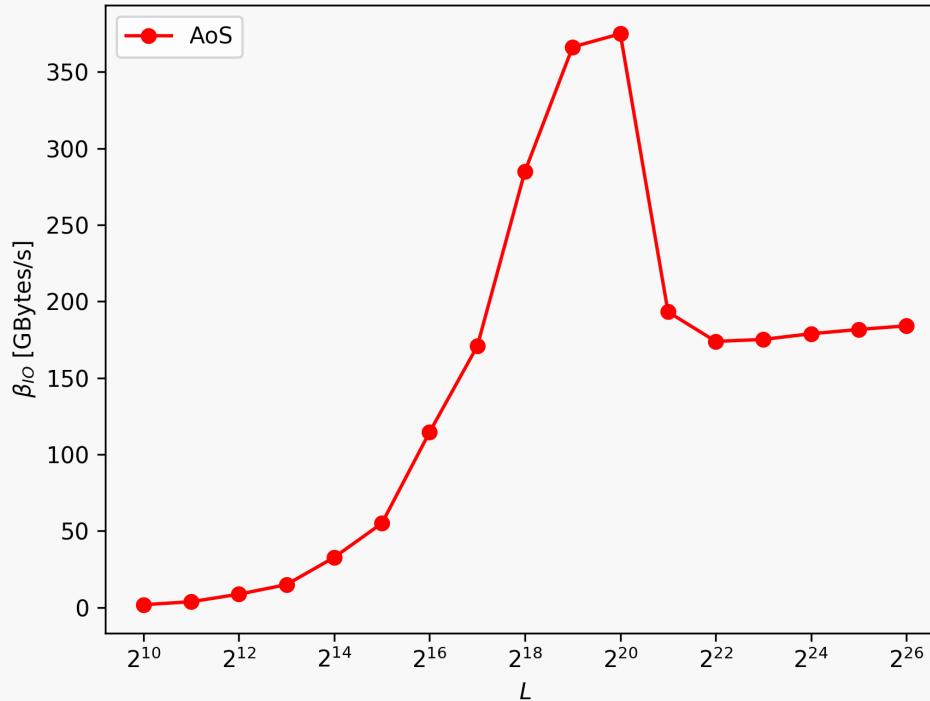
```
module load python/3.6.1 matplotlib/2.1.0,
```

run: `python3 plot-A.py` and then this will produce `A.png`.

AoS to SoA

Task A

The resulting plot should look like:



AoS to SoA

In Task B you need to modify `space-time-soa.c`. First transfer your modifications from `space-time-aos.c`, tagged with `_TODO_A_`.

`space-time-soa.c` implements a structure of arrays of length `VL` rather than an array of structures:

```
typedef struct {
    float x[VL];
    float y[VL];
    float z[VL];
    float t[VL];
    float s[VL];
} st_coords;
```

Once done, as in Task A, make and submit:

```
make B
sbatch sub-B.job
```

and plot the result using: `python3 plot-B.py` to produce `B.png`.

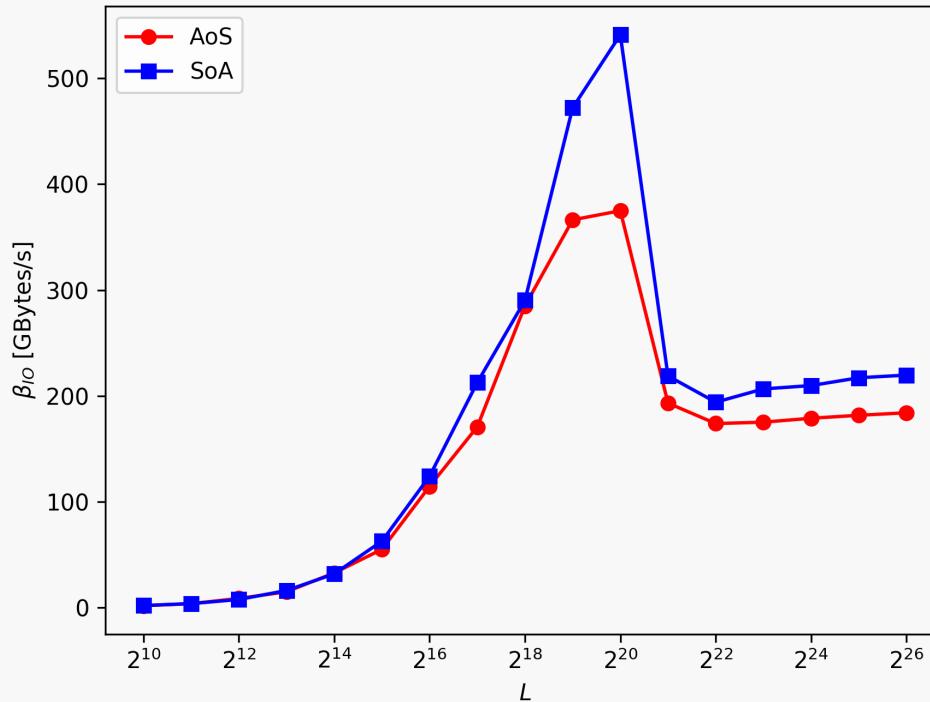
For the pieces tagged with `_TODO_B_` you need to implement `comp_s()` to operate on this new data layout:

```
/*
 * compute: s = t**2 - x**2 - y**2 - z**2,
 * with s, t, x, y, z member variables of
 * length VL of the st_coords structure
 */
void
comp_s(st_coords *arr, int L)
{
    /* _TODO_B_: complete the kernel */
    #pragma omp parallel for
    ...
```

AoS to SoA

Task B

The resulting plot should look like:



AoS to SoA

Task C

In Task C, you will use the same program, `space-time-soa.c`. But you will run it multiple times, varying `VL`.

You are not required to modify code. Look at `sub-C.job`:

```
#!/bin/bash
#SBATCH -J soa
#SBATCH -N 1
#SBATCH -o soa-%j.out
#SBATCH -e soa-%j.err
module load openmpi

export OMP_NUM_THREADS=128

for VL in 2 4 8 16 32 64 128 256; do
    make -B VL=${VL} B
    for L in 1024 2048 4096 8192 16384 32768 65536 131072 262144 524288 1048576 2097152 4194304 8388608 167772
        srun numactl --membind 1 ./space-time-soa $L
    done | tee soa-vl${VL}.txt
done
```

This will compile and run the program for all values of `VL` in the list. Submit with:

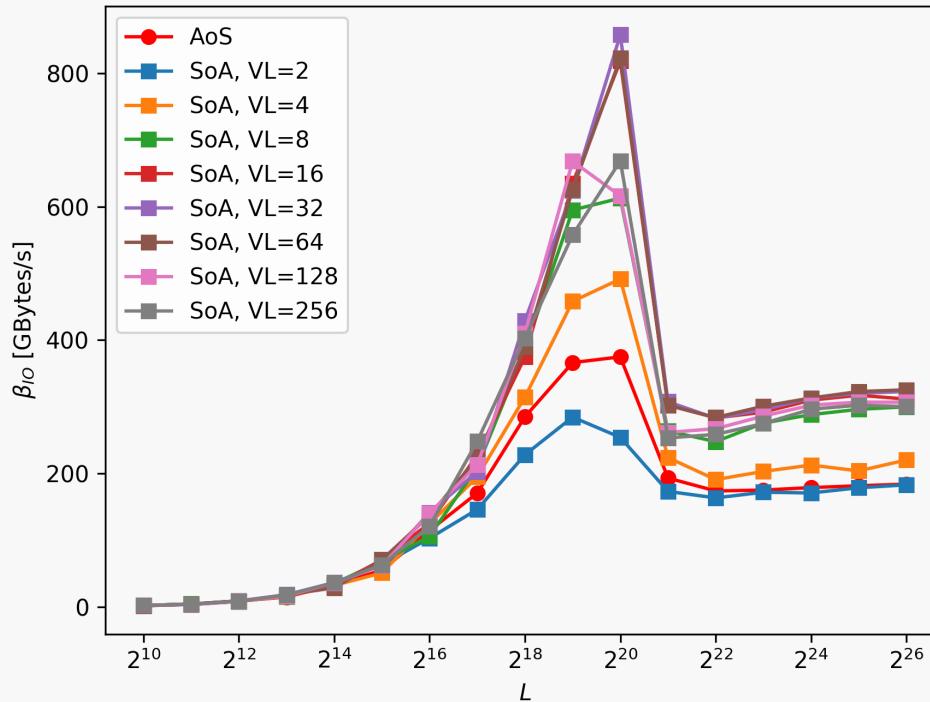
```
sbatch sub-C.job
```

and run: `python3 plot-C.py`. This will produce `C.png`.

AoS to SoA

Task C

The resulting plot should look like:



For which value of VL do we achieve best performance? Why?

AoS to SoA

In Task D you need to modify `space-time-soa-v.c`. First transfer your modifications from `space-time-aos.c`, tagged with `_TODO_A_`.

`space-time-soa-v.c` implements the same structure of arrays as in `space-time-soa.c`

For the pieces tagged with `_TODO_D_` you need to implement `comp_s()` in intrinsics. Once done, as in the previous tasks, make and submit:

```
make D  
sbatch sub-D.job
```

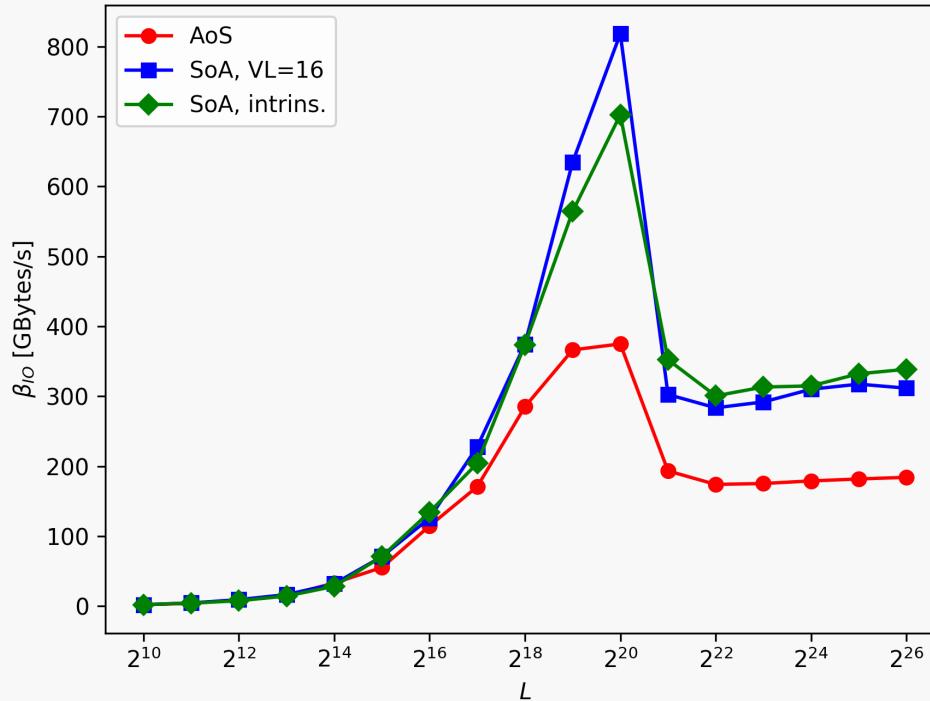
and plot: `python3 plot-D.py`.

```
void  
comp_s(st_coords *arr, int L)  
{  
#pragma omp parallel for  
for(int i=0; i<L/VL; i++) {  
    register __m512 x = _mm512_load_ps(&arr[i].x[0]);  
    register __m512 y = _mm512_load_ps(&arr[i].y[0]);  
    register __m512 z = _mm512_load_ps(&arr[i].z[0]);  
    register __m512 t = _mm512_load_ps(&arr[i].t[0]);  
    register __m512 s0;  
    /*  
     _TODO_D_  
  
     Complete this function using  
     intrinsics so that it computes:  
  
     arr[i].s[:] = arr[i].t[:]**2 - (  
         arr[i].x[:]**2 +  
         arr[i].y[:]**2 +  
         arr[i].z[:]**2  
     )  
  
     You will use:  
  
     _mm512_mul_ps();  
     _mm512_fmadd_ps();  
     _mm512_fmsub_ps();  
  
     and the temporary variable s0.  
    */  
  
    /*  
     Store s0 to arr[i].s[:]  
    */  
    _mm512_stream_ps(&arr[i].s[0], s0);  
}  
  
return;  
}
```

AoS to SoA

Task D

The resulting plot should look like:



MatMul

This exercise deals with a matrix-matrix multiplication

Navigate to CDS-1/0ptim/Ex/MatMul/. There is only one file `mm.c`.

In the first task (task A), you will need to complete the `_TODO_A_` tags. Here this requires:

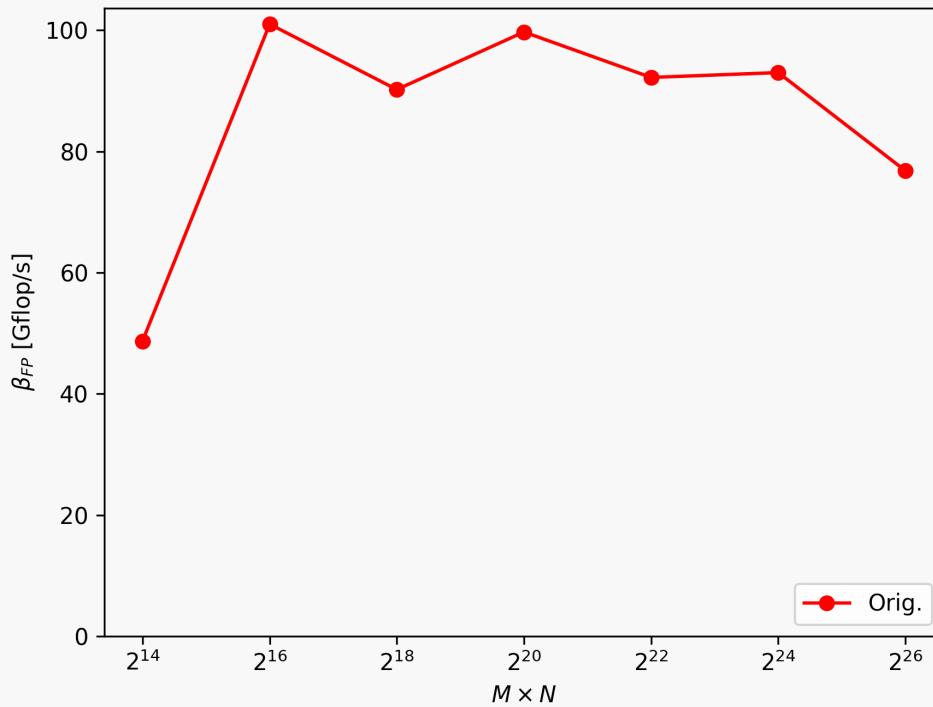
1. Computing `N_fp`, so that the flops are reported correctly.
2. Implement naively the matrix matrix multiplication in `mat_mul()`.

```
void
mat_mul(double *C, int M, int N, double *A, double *B)
{
#pragma omp parallel for collapse(2)
    for(int i=0; i<M; i++)
        for(int j=0; j<N; j++)
            C[i*M + j] = 0;

#pragma omp parallel for collapse(2)
    for(int i=0; i<M; i++)
        for(int k=0; k<N; k++)
            for(int j=0; j<N; j++)
/*
    _TODO_A_
    Implement the matrix-matrix multiplication naively
*/
    ...
}
```

MatMul

When done: `make A`, `sbatch sub-A.` job, and then you can plot the result with `python3 plot-A.py`. The job script runs the `mm-orig` program for multiple values of `M` and `N` with `M == N`. The result should look like:



MatMul

In Task B you will implement a blocked version of the matrix-matrix multiplication.
Find the tags with `_TODO_B_`.

```
void
mat_mul_blocked(double *C, int M, int N, double *A, double *B)
{
    double Ab[BM*BN];
    double Bb[BM*BN];
    double Cb[BM*BM];
    for(int i=0; i<M; i+=BM)
        for(int j=0; j<N; j+=BM) {

            /* Set Cb to zero */
            for(int ib=0; ib<BM; ib++)
                for(int jb=0; jb<BN; jb++) {
                    Cb[ib*BN + jb] = 0;
                }

            /*
             * _TODO_B_
             *
             * Implement the blocked matrix-matrix multiplication
             * Steps:
             *
             * 0. Loop over k-blocks
             * 1. Fill Ab with the block that begins from A[i:][k:]
             * 2. Fill Bb with the block that begins from B[k:][j:]
             * 3. Do the little matrix matrix multiplication Cb = Ab*Bb
             *
             */
            /*
             * Copy Cb to C[i][j];
             */
            ...
        }
}
```

MatMul

While developing the matrix-matrix multiplication, you can make `B` and run for a small `M, N`, e.g.:

```
./mm-blck 64 64
```

The code checks that the two versions (blocked and original) produce the same result and will print to the screen if there is a discrepancy, e.g.:

```
ORIG: M = 128, N = 128, took: 5.25e-04 sec, P = 7.99e+03 Mflop/s
BLCK: M = 128, N = 128, took: 4.79e-04 sec, P = 8.76e+03 Mflop/s, BM = 16, BN = 16
Non zero diff: 6.559491e-02
```

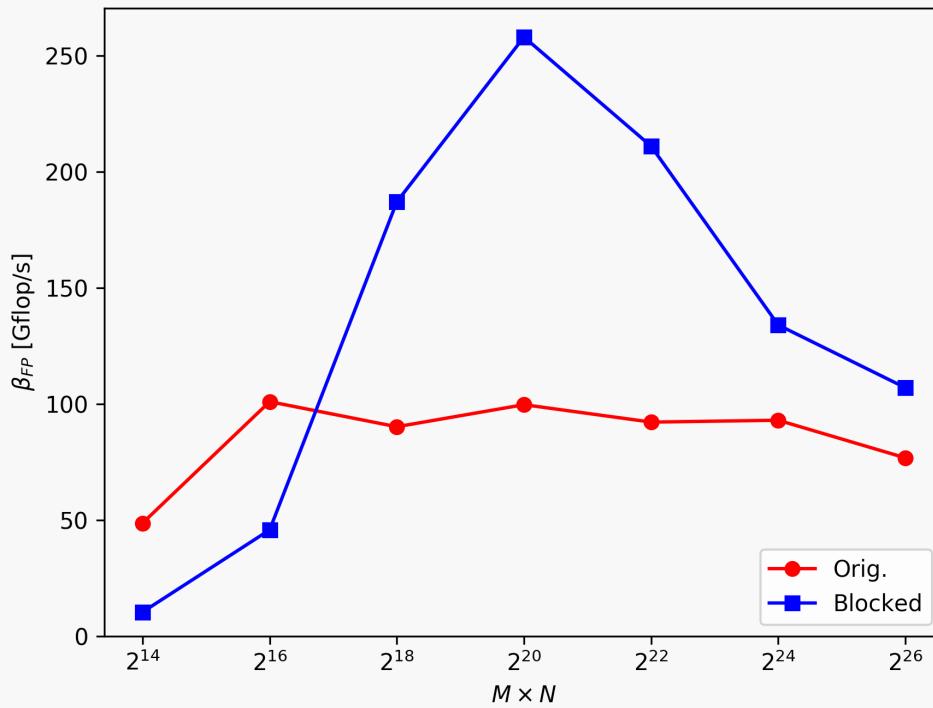
When done, and the two versions agree, submit with: `sbatch sub-B.job`, and after the job completes you can plot the result with `python3 plot-B.py`. Note that the block lengths are defined at compile time. They are defined at the beginning:

```
/*
 * Block length in M direction
 */
#ifndef BM
#define BM 64
#endif
```

```
/*
 * Block length in N direction
 */
#ifndef BN
#define BN 64
#endif
```

MatMul

The resulting plot should look like:



3D Laplacian

- Consider the 3D "gauge" Laplacian.

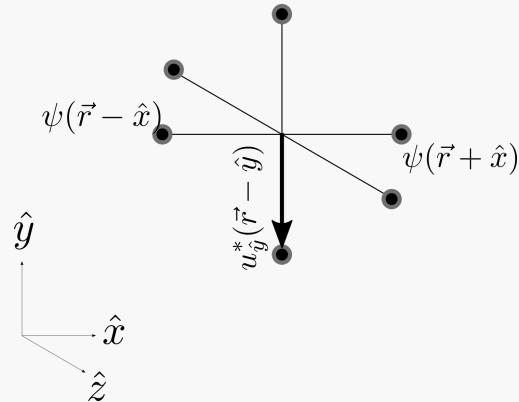
$$\phi(\vec{r}) = \nabla \psi(\vec{r}) = 6\psi(\vec{r}) - \sum_{i=1}^{N_d} [u_i^\wedge(\vec{r})\psi(\vec{r} + \hat{i}) + u_i^*(\vec{r} - \hat{i})\psi(\vec{r} - \hat{i})]$$

with $N_d = 3$ the number of dimensions,

$u_i^\wedge(\vec{r}) \in \mathbb{C}$, and $|u_i^\wedge(\vec{r})| = 1$

$\psi(\vec{r}) \in \mathbb{C}$

- $2 \cdot N_d$ "u"s at each site \vec{r} , but only N_d unique "u"s
- Conjugation flips the direction of u, i.e. $u_{-\hat{i}}^\wedge(\vec{r}) = u_i^*(\vec{r})$



-
- \hat{i} unit vector in direction i , $(u_0^\wedge(\vec{r}), u_1^\wedge(\vec{r}), u_2^\wedge(\vec{r}))$, or $(u_z^\wedge(\vec{r}), u_y^\wedge(\vec{r}), u_x^\wedge(\vec{r}))$

3D Laplacian

- Conjugate gradient (CG) to solve

$$\nabla x = b$$

initial guess x

$$r_0 = b - \nabla x$$

$$p = r_0$$

loop until $\|r_0\|$ small enough

$$\alpha = \frac{r_0^\dagger r_0}{p^\dagger \nabla p}$$

$$x = \alpha p + x$$

$$r_1 = -\alpha \nabla p + r_0$$

$$\beta = \frac{r_1^\dagger r_1}{r_0^\dagger r_0}$$

$$p = \beta p + r_1$$

$$r_0 = r_1$$

Linear algebra already implemented
in exercise: `xdotx()`, `xdoy()`, `axpy()`,
`aypx()`, `xmy()`

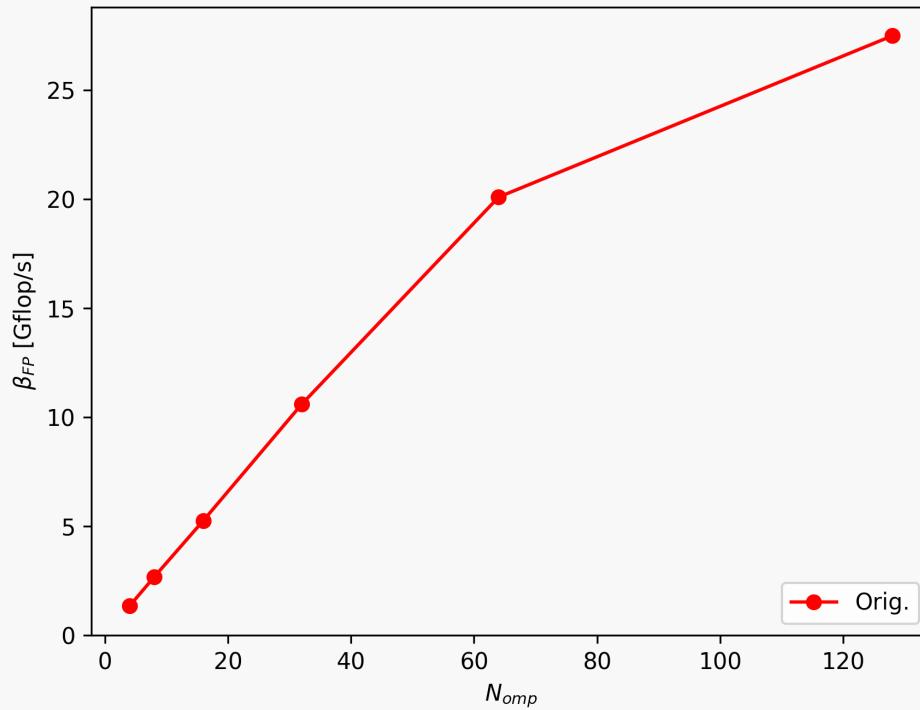
```
$ srun numactl --membind 1 ./lapl 128
 0, res = +1.000000e+00
 1, res = +1.669268e-01
 2, res = +3.343321e-02
 3, res = +6.682492e-03
 4, res = +1.339953e-03
 5, res = +2.682193e-04
 6, res = +5.365824e-05
 7, res = +1.079675e-05
 8, res = +2.181284e-06
 9, res = +4.423248e-07
10, res = +9.009035e-08
11, res = +1.844173e-08
12, res = +3.792212e-09
13, res = +7.814874e-10
14, res = +1.617658e-10
15, res = +3.366356e-11
16, res = +7.020740e-12
17, res = +1.470992e-12
18, res = +3.094643e-13
19, res = +6.524311e-14
20, res = +1.382112e-14
21, res = +2.943272e-15
22, res = +6.290599e-16
23, res = +1.345215e-16
24, res = +2.883775e-17
25, res = +6.205892e-18
26, res = +1.337031e-18
27, res = +2.886712e-19
```

Converged after 27 iterations, res = +3.781296e-14
Time in lapl(): +7.828e-02 sec/call, 1.34e+00 Gflop/s, 1.0

3D Laplacian

- Navigate to `CDS-1/Optim/Ex/Lapl-3D/`
- `lapl.c` implements a CG algorithm which solves $\nabla x = b$ for a random b and gauge u
- The `_T0D0_A` pieces need completion
- This includes the bulk of the Laplacian operation in function `lapl()` at [`lapl.c:145`](#)
- After you're done compile with `make A` and submit the job `sbatch sub-A.job`. You can then plot with `python3 plot-A.py`

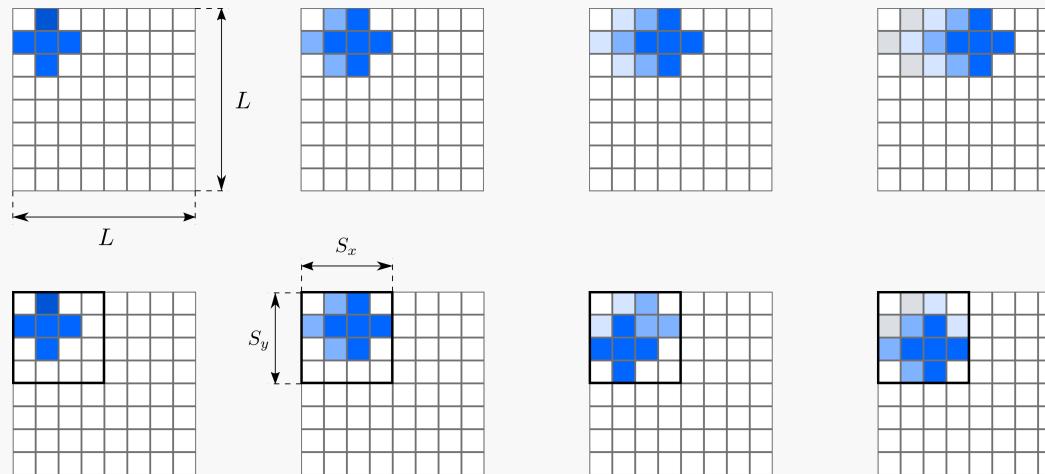
3D Laplacian



The plot is the performance vs the number of OMP threads

3D Laplacian

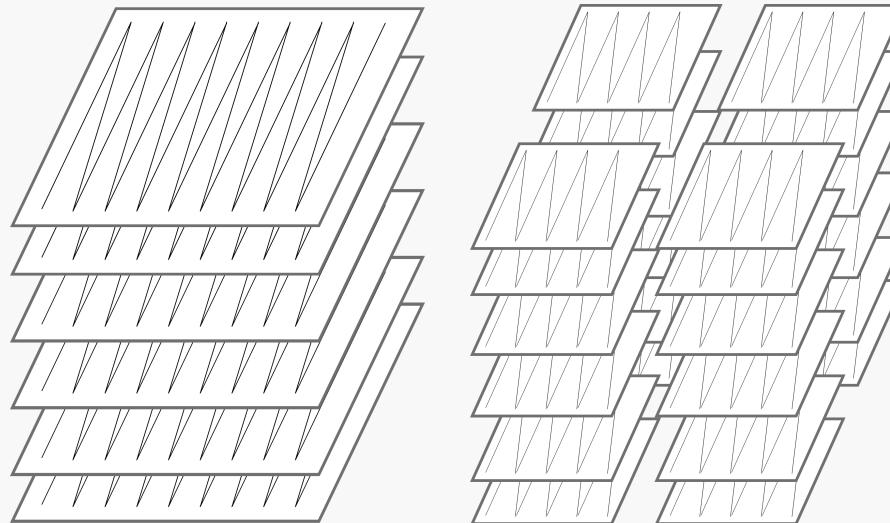
- In Task B, you need to modify `laplt.c` ("t" stands for "tiled")
- This is to implement a "blocked" (or "tiled") version of the stencil operation in `lapl()`



- Block in x and y directions
- Distribute OMP threads so that each thread processes a block
- To check correctness, you should obtain the same CG iterations as the original version

3D Laplacian

- In Task B, you need to modify `laplt.c` ("t" stands for "tiled")
- This is to implement a "blocked" (or "tiled") version of the stencil operation in `lapl()`



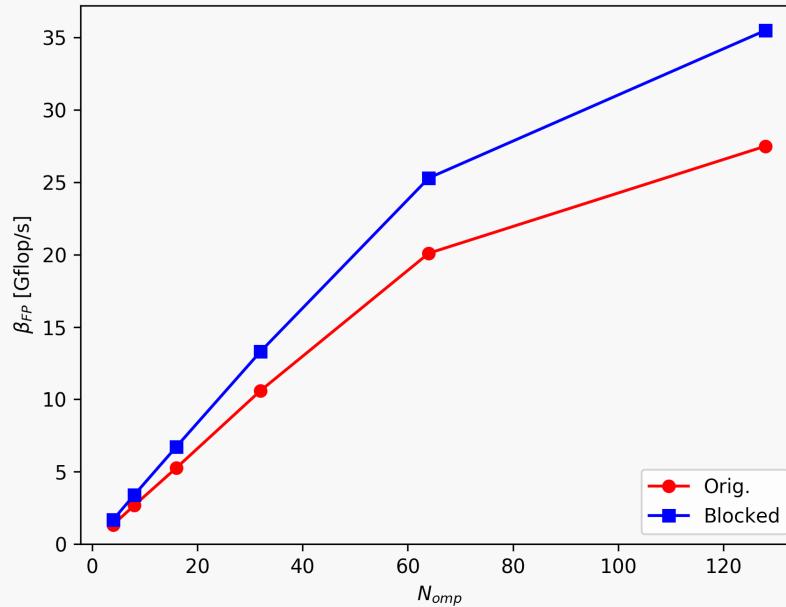
- $A[z][y][x] \rightarrow bA[x_0][y_0][z][y_1][x_1] = A[z][y_1 + y_0 * S_y][x_1 + x_0 * S_x]$
- Distribute OMP threads so that each thread processes a block
- To check correctness, you should obtain the same CG iterations as the original version

3D Laplacian

- The `_TODO_B_` tag the pieces you need to modify in `laplt.c`. This includes:
 - Completing the bulk calculation of `lapl()`, now that the lattices are blocked
[laplt.c:284](#)
- Handling of the boundaries is taken care of [laplt.c:316](#)
- Compile with `make B`, submit with `sbatch sub-B.job`, and plot with `python3 plot-B.py`

3D Laplacian

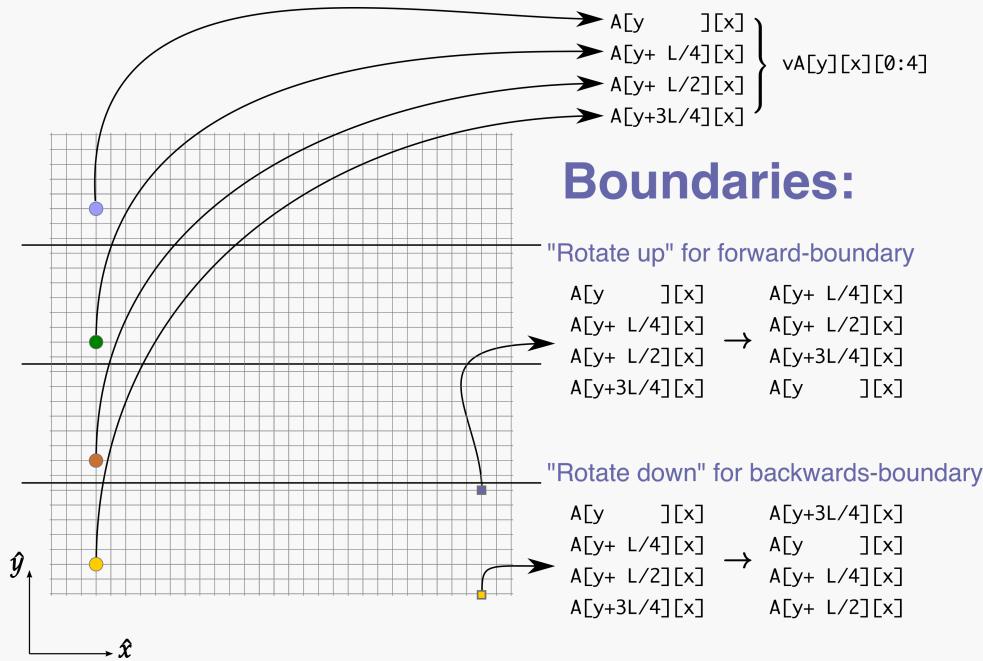
The result of Task B should look like:



Performance of the blocked code compared to the original version

3D Laplacian

- Task C involves implementing a version of `lapl()` which is easier for vectorization



- $A[z][y][x][\text{reim}] \rightarrow$
 $vA[z_0][y][x][\text{reim}][z_1] = A[z_0 + z_1 * L/4][y][x][\text{reim}]$
- Notice shift required on boundaries

3D Laplacian

- Task C involves implementing a version of `lapl()` which is easier for vectorization
- $A[z][y][x][\text{reim}] \rightarrow$
 $vA[z0][y][x][\text{reim}][z1] = A[z0 + z1*L/4][y][x][\text{reim}]$

E.g. for the case of 2D:

```
for(int y=0; y<L/4; y++)  
for(int x=0; x<L; x++) {  
    vB[y][x][0] = 4*vA[y][x][0] - (vA[y][x+1][0] + vA[y][x-1][0] + vA[y+1][x][0] + vA[y-1][x][0]);  
    vB[y][x][1] = 4*vA[y][x][1] - (vA[y][x+1][1] + vA[y][x-1][1] + vA[y+1][x][1] + vA[y-1][x][1]);  
    vB[y][x][2] = 4*vA[y][x][2] - (vA[y][x+1][2] + vA[y][x-1][2] + vA[y+1][x][2] + vA[y-1][x][2]);  
    vB[y][x][3] = 4*vA[y][x][3] - (vA[y][x+1][3] + vA[y][x-1][3] + vA[y+1][x][3] + vA[y-1][x][3]);  
}
```

- Notice shift required on boundaries, e.g. for the $y = 0$ boundary in the 2D problem:

```
y = 0;  
for(int x=0; x<L; x++) {  
    vB[0][x][0] = 4*vA[0][x][0] - (vA[0][x+1][0] + vA[0][x-1][0] + vA[1][x][0] + vA[L/4-1][x][3]);  
    vB[0][x][1] = 4*vA[0][x][1] - (vA[0][x+1][1] + vA[0][x-1][1] + vA[1][x][1] + vA[L/4-1][x][2]);  
    vB[0][x][2] = 4*vA[0][x][2] - (vA[0][x+1][2] + vA[0][x-1][2] + vA[1][x][2] + vA[L/4-1][x][1]);  
    vB[0][x][3] = 4*vA[0][x][3] - (vA[0][x+1][3] + vA[0][x-1][3] + vA[1][x][3] + vA[L/4-1][x][0]);  
}
```

3D Laplacian

- The code to be modified is now `laplv.c`, the parts missing in tagged with `_TODO_C_`
- Modify `laplv.c`, compile with `make C`, run with `sbatch sub-C.job` and plot using `python3 plot-C.py`.
- After completing these parts you should obtain similar CG history as before
- Here the bulk calculation of the Laplacian is implemented. Also the `OpenMP` pragma has been inserted
- You need to complete the pieces that do the shuffling for the boundaries at [laplv.c:254](#)

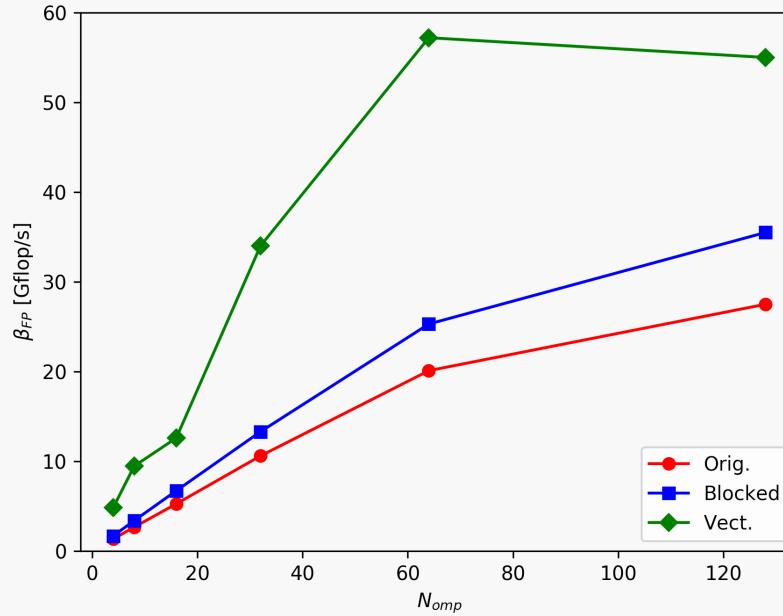
```
if(z == 0) {  
/* _TODO_C_  
*  
* Use shift_dn() or shift_up() to appropriately  
* shift the necessary structures, when on the  
* boundary  
*/  
}
```

```
if(z == lz-1) {  
/* _TODO_C_  
*  
* Use shift_dn() or shift_up() to appropriately  
* shift the necessary structures, when on the  
* boundary  
*/  
}
```

- With `shift_up()` and `shift_dn()` are already defined for you

3D Laplacian

Result of Task C should look like:



Vector-friendly version compared to original and blocked versions