Optimization

Giannis Koutsou

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Outline

Expectations

- Optimization is a very broad subject
- Rather than a broad overview of techniques, we will attempt an in-depth look at some specific optimization strategies
- These techniques will be motivated by a set of example codes which we will optimize step-by-step
- The resulting optimizations may seem problem-specific, but (hopefully) you will take home the general strategy
- Optimizations for CPUs, though they may be generalizable

Lecture section

- Refresh from previous courses (notation, etc.)
- Understanding a code's current performance
- Understanding a code's achievable performance
- Steps to take to optimize, motivate by examples/exercises

Outline

Exercises

Wednesday

- Data layout transformations for easier (auto-)vectorization: AoS to SoA
- Blocking for mitigating cache misses: transformations on matrix-matrix multiplication

Thursday

- 3D laplacian-stencil code:
  - Multi-threading (`OpenMP`)
  - Data layout transformations
  - Blocking

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

Jureca

E.g. Jureca nodes have the following characteristics:

- Peak FP
  - 12-cores per socket, 2 sockets per node, clock: 2.5 GHz
  - Best case: two 256-bit fused multiply-and-adds per cycle (AVX2.0)
  - In double precision: $2 \times (4$ `mul` + 4 `add`$)$ per cycle = 16 flop/cycle
  - Therefore: $2.5 \text{x} 10^9$ cycles/s $\times$ 16 flop/cycle = 40 Gflop/s per core
  - 960 Gflop/s per node
- Peak BW
  - 68 GB/s to RAM assuming all channels populated
  - Good assumption for an HPC system
- 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`)

Jureca

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

```
processor       : 0
vendor_id       : GenuineIntel
...
model name      : Intel(R) Xeon(R) CPU E5-2680 v3 @ 2.50GHz
...
cpu MHz         : 3129.296
cache size      : 30720 KB
physical id     : 0
siblings        : 24
core id         : 0
cpu cores       : 12
...
cpuid level     : 15
...
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 syscall nx pdpe1gb rdtscp lm constant_tsc...
```

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 $\geqslant$ 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. I.e., all cache misses are compulsory

An example

- Say you're running a kernel which performs:

  $$Y_i^{ab} = A^{ac} \cdot X_i^{cb},\ i = 0, \ldots, L-1,\ a, b, c = 0, \ldots, N-1,\ L \gg N$$

- Naive implementation:

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

/* ...
 * 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[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.
    - $w = 4$ bytes for single precision,
    - $w = 8$ bytes for double, etc.
  - $2LN^2$ to $O(L)$
  - 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][0];
...
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: $\beta_{fp} = \frac{N_{fp}}{\bar{T}}$
  - IO-rate: $\beta_{IO} = \frac{N_{IO}}{\bar{T}}$
- This motivates defining an *intensity* $I = \frac{N_{fp}}{N_{IO}}$

```
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[c][b];
      }
    }
  }
}
```

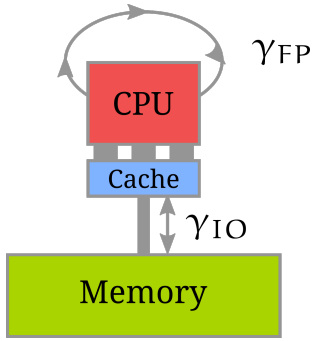
Intensities

Computational kernel intensity

- Ratio of kernel floating point operations to bytes of I/O
- For our previous example:
  - $I_k = \frac{N_{fp}}{N_{IO}} = \frac{2LN^3}{2wLN^2} = N/w$
  - 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 Jureca (compute node): $I_m \simeq 14 \frac{flop}{byte}$



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

For the example we have been studying, and for the case of Jureca

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

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 Jureca, the kernel is balanced when $N \geqslant 12 \Rightarrow$ 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 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

```
float ar = creal(a);
float ai = cimag(a);
float aux0[] = { ar, ar, ar, ar};
float aux1[] = {-ai, ai,-ai, ai};
register __m128 va_re = _mm_load_ps(aux0);
register __m128 va_im = _mm_load_ps(aux1);
register __m128 x0, x1, y0;
...
```

```
for(int i=0; i<L; i+=2) {
  y0 = _mm_load_ps((float *)&y[i]);
  x0 = _mm_load_ps((float *)&x[i]);
  x1 = _mm_shuffle_ps(x0, x0, MASK);
  y0 = _mm_fmadd_ps(va_im, x1, y0);
  y0 = _mm_fmadd_ps(va_re, x0, y0);
  _mm_store_ps((float *)&y[i], y0);
}
```

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

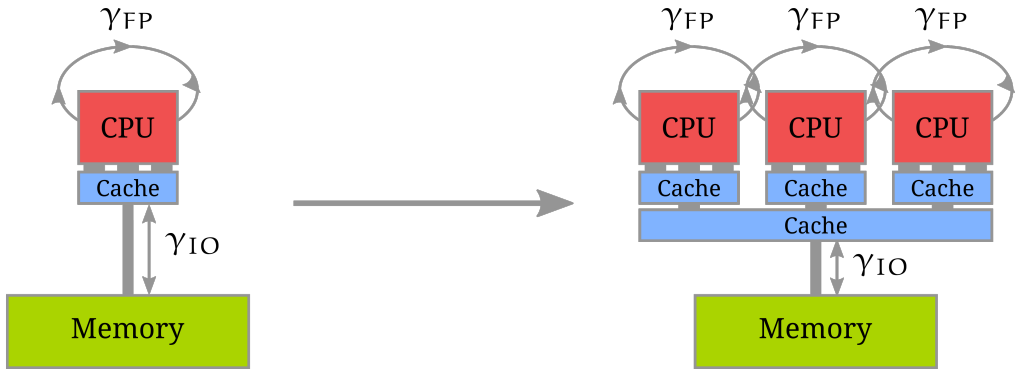
On modern systems, the compiler and the architecture will do a lot for you

- 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`

Mutli-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
- Single Instruction Multiple Data -- SIMD

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

Vectorization

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- SSE, AVX, AltiVec, QPX
- 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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- 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

Most modern processors have some vectorization capabilities

- SSE, AVX, AltiVec, QPX
- 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);
}
```

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

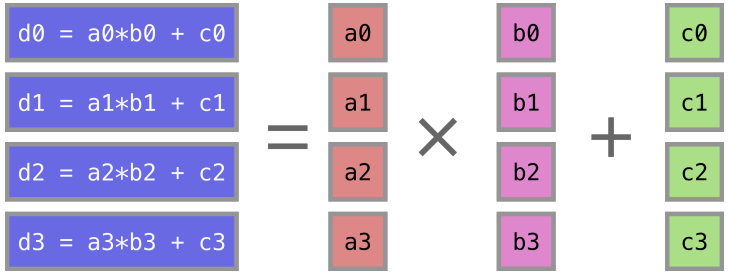
```
for(int i=0; i<L; i+=4) {
  y[i  ] = a*x[i  ] + y[i  ];
  y[i+1] = a*x[i+1] + y[i+1];
  y[i+2] = a*x[i+2] + y[i+2];
  y[i+3] = a*x[i+3] + y[i+3];
}
```

- In many case, 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. `<xmmintrin.h>`, `<immintrin.h>`, etc.)




```
d = _mm256_fmadd_pd(a, b, c)
```

Vectorization

Intrinsics - short intro

- Vector types defined in `<?mmintrin.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.:
  $z_n = x_n \cdot y_n$, with x, y, z complex, e.g: $x_n = x_n^r + ix_n^i \Rightarrow$
  $z_n^r = x_n^r \cdot y_n^r - x_n^r \cdot y_n^r$
  $z_n^i = x_n^r \cdot y_n^i + x_n^i \cdot y_n^r$
- 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)`

`mask = 0b00` ⟶ `c = {a[0], b[0]}` `mask = 0b01` ⟶ `c = {a[1], b[0]}`
`mask = 0b10` ⟶ `c = {a[0], b[1]}` `mask = 0b11` ⟶ `c = {a[1], b[1]}`

- 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

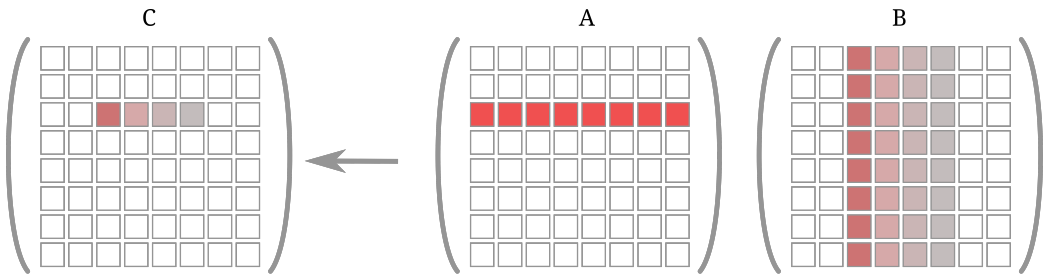
Data layout

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];
    }
  }
}
```



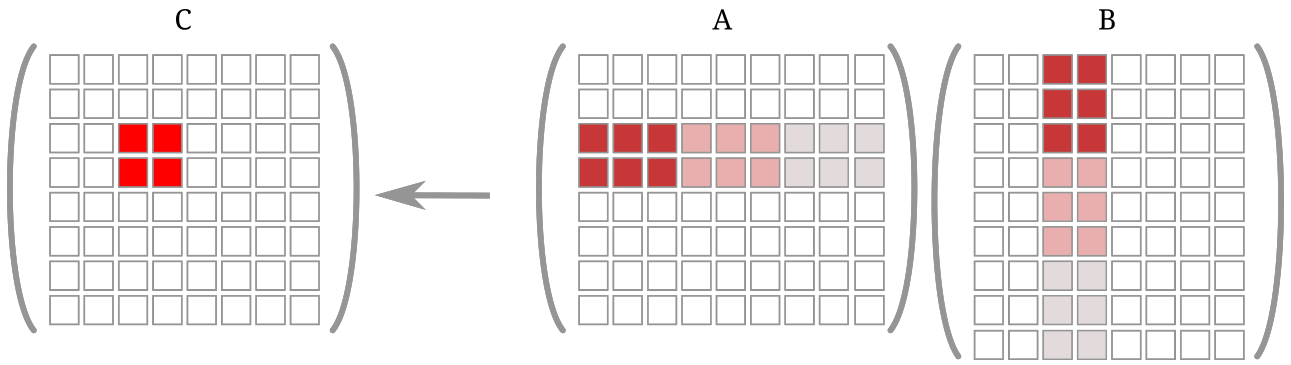
- Repeated reading of columns of B
- If N too large, a whole row of A may not fit into L2 cache

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];
    }
  }
```

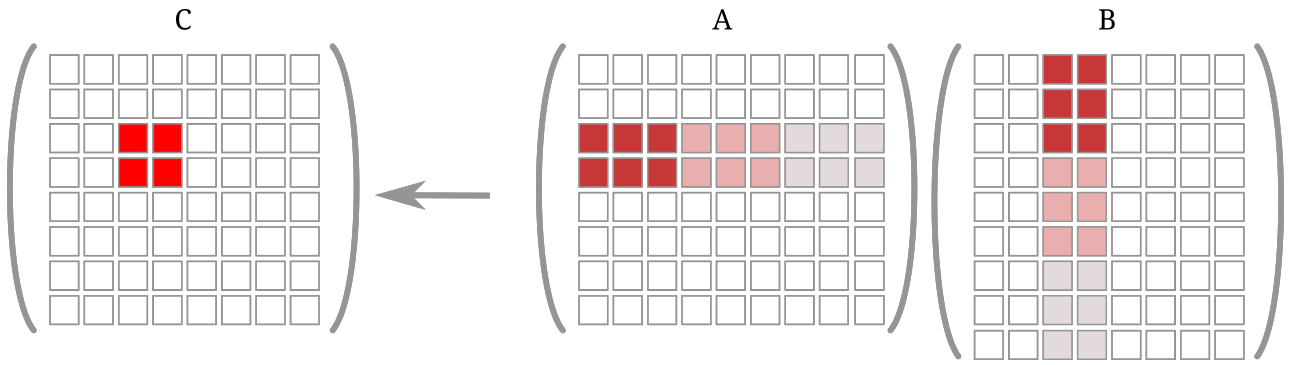


Data layout

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:

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

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] <- 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]);
}
```

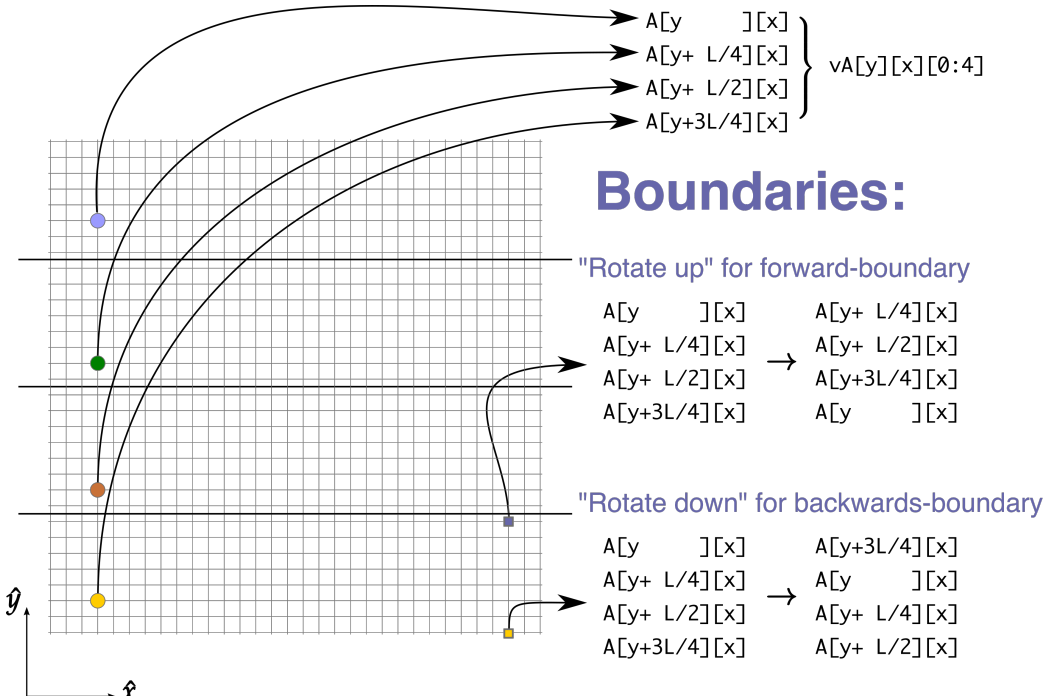
which requires shuffling of the boundary element at `y=L/4-1` of `vA`:

```
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 https://github.com/g-koutsou/CoS-2.git
```

`juropa3.zam.kfa-juelich.de`

AoS to SoA

In the first exercise we will look into two optimizations:

1. Going from an AoS to a SoA,
2. which will assist the vectorization of our kernel with intrinsics

The kernel does the following: assuming an array of 4-vectors: $a_i = (ct_i, x_i, y_i, z_i)$
compute the "norm": $s_i = \sqrt{(ct_i)^2 - (x_i^2 + y_i^2 + z_i^2)}$
Navigate to: `CoS-2/Optim/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;
}
```

AoS to SoA

In the first exercise we will look into two optimizations:

1. Going from an AoS to a SoA,
2. which will assist the vectorization of our kernel with intrinsics

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

`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)
{
  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 = sqrt(s);
  }
  return;
}
```

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 intel-para
make space-time-aos
```

and submit the prepared submit script:

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

This will run the code for various lengths `L`. The output is in `aos.txt`. There is a `gnuplot` script so that you can visualize the output. You'll need to `module load gnuplot`, run `gnuplot` and then from the gnuplot prompt: `load 'plot-A.gpl'`

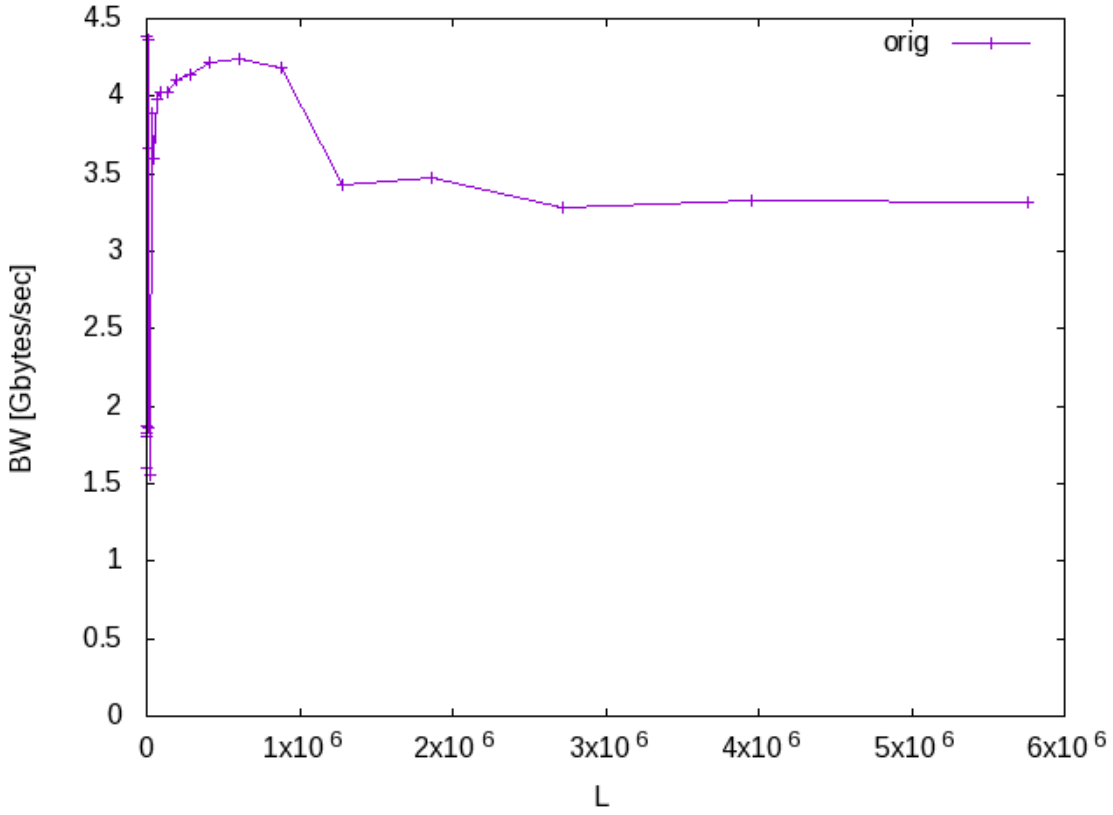
```
void
comp_s(st_coords *arr, int L)
{
  for(int i=0; i<L; i++) {
    float x = arr[i].x;
    float y = arr[i].y;
    float z = arr[i].z;
    float t = arr[i].t;
    float s = t*t - (x*x + y*y + z*z);
    arr[i].s = sqrt(s);
  }
  return;
}
...
double beta_fp = 0 /* _TODO_A_: insert number of */
 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

```
gnuplot
    G N U P L O T
    Version 5.0 patchlevel 0    last modified 2015-01-

    Copyright (C) 1986-1993, 1998, 2004, 2007-2015
    Thomas Williams, Colin Kelley and many others

    gnuplot home:     http://www.gnuplot.info
    faq, bugs, etc:   type "help FAQ"
    immediate help:   type "help"  (plot window: hit

Terminal type set to 'x11'
gnuplot> load 'plot-A.gpl'
```

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 rather than an array of structures:

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

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

```
make space-time-soa
sbatch sub-B.job
```

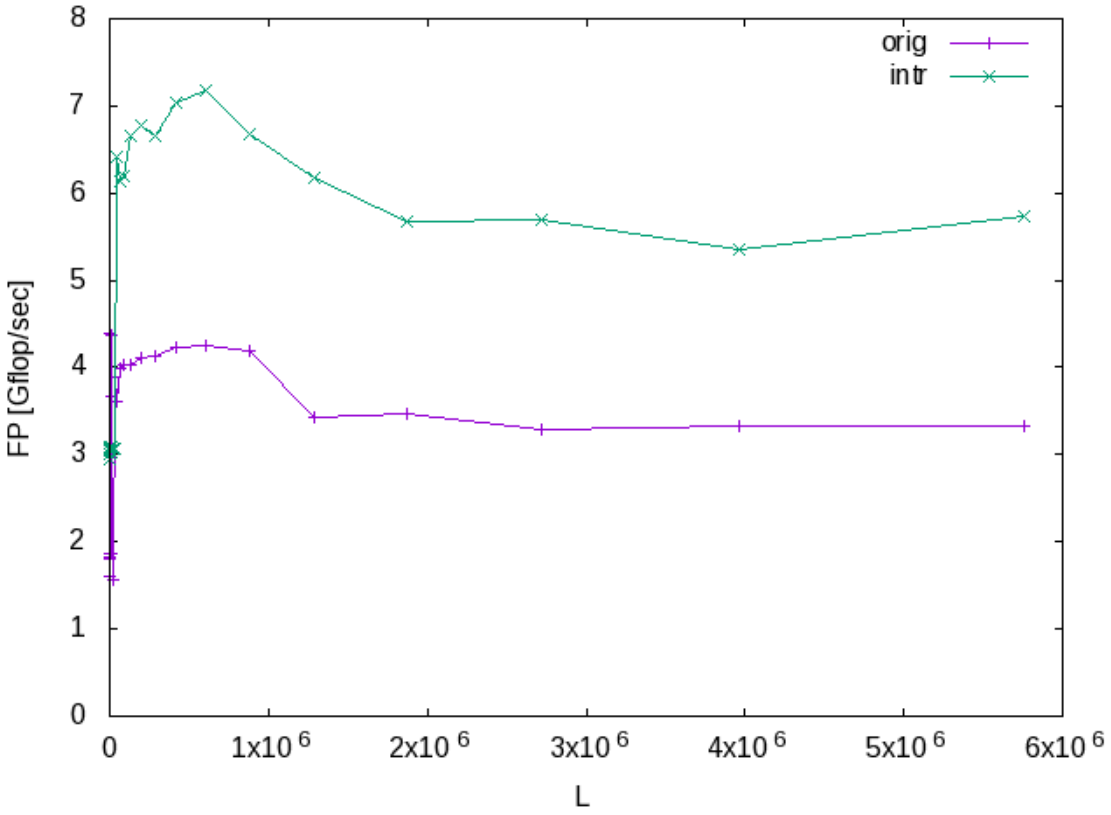
and plot in gnuplot: `load 'plot-B.plt'`.

```
void
comp_s(st_coords arr, int L)
{
  for(int i=0; i<L; i+=8) {
    __m256 x = _mm256_load_ps(&arr.x[i]);
    __m256 y = _mm256_load_ps(&arr.y[i]);
    __m256 z = _mm256_load_ps(&arr.z[i]);
    __m256 t = _mm256_load_ps(&arr.t[i]);
    register __m256 s0, s1; /* Temporaries */
    /*
       _TODO_B_

       Complete this function using intrinsics so that

       s[i:i+8] = sqrt(t[i:i+8]**2 - (
                                      x[i:i+8]**2 +
                                      y[i:i+8]**2 +
                                      z[i:i+8]**2
                                      )
                       )

       where, s, t, x, y, z are members of arr.

       You will use:

       _mm256_mul_ps();
       _mm256_add_ps();
       _mm256_sub_ps();
       _mm256_sqrt_ps();
    */

    _mm256_store_ps(&arr.s[i], s0);
  }
  return;
}
```

AoS to SoA

Task B

The resulting plot should look like:



AoS to SoA

Task C

In Task C, you will use `space-time-soa-r.c`. This is mostly identical to `space-time-soa.c`, just that rather than striding sequentially the array in `comp_s()`, the array is strided randomly.

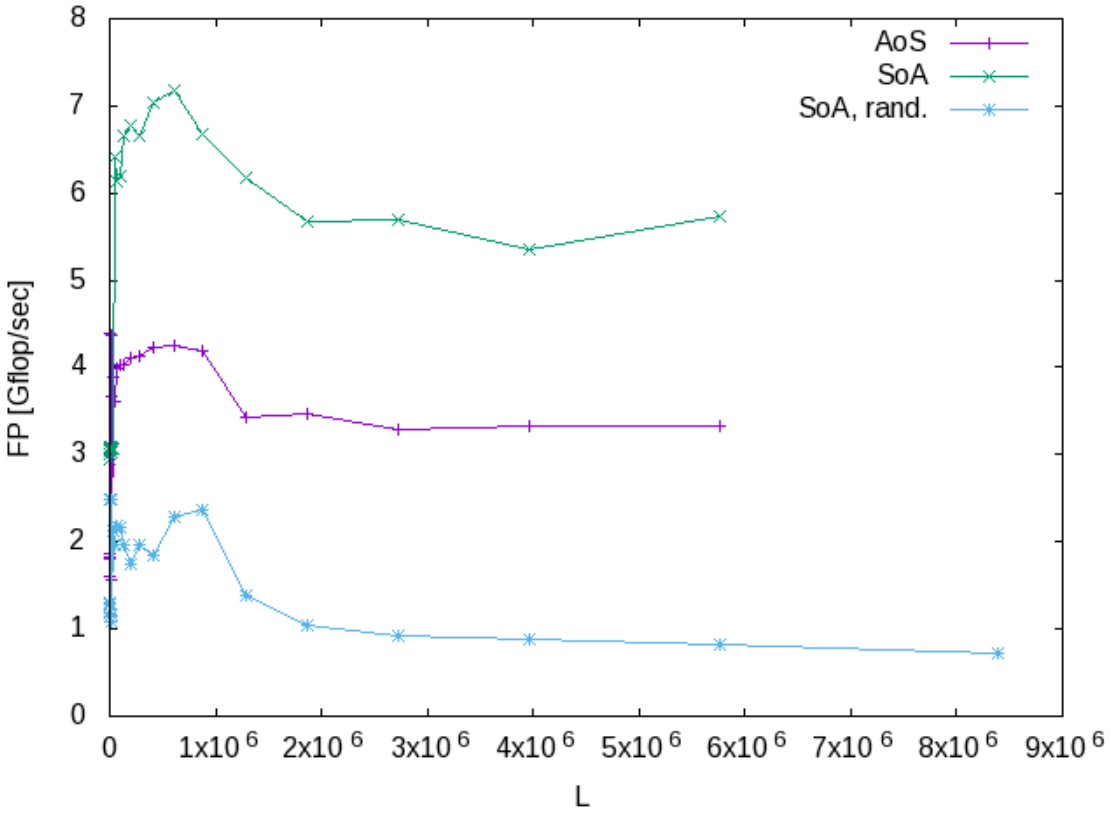
```
void
comp_s(st_coords arr, int L)
{
  for(int j=0; j<L; j+=8) {
    int i = (rand() % (L/8)) * 8;
    __m256 x = _mm256_load_ps(&arr.x[i]);
    ...
```

This makes prefetching unpredictable. Transfer the `_TODO_A_` and `_TODO_B_` tasks you completed in the previous tasks to this task. Compile and run as before, using: `make space-time-soa-r` and `sbatch sub-C.job`. The results can be plotted using `plot-C.gpl`.

AoS to SoA

Task C

The resulting plot should look like:



AoS to SoA

Task D

In Task D, you will use `space-time-aosoa-r.c`. This uses a AoSoA rather than a SoA:

```
typedef struct {
  float __attribute__((aligned(32))) x[VL];
  float __attribute__((aligned(32))) y[VL];
  float __attribute__((aligned(32))) z[VL];
  float __attribute__((aligned(32))) t[VL];
  float __attribute__((aligned(32))) s[VL];
} st_coords;
```

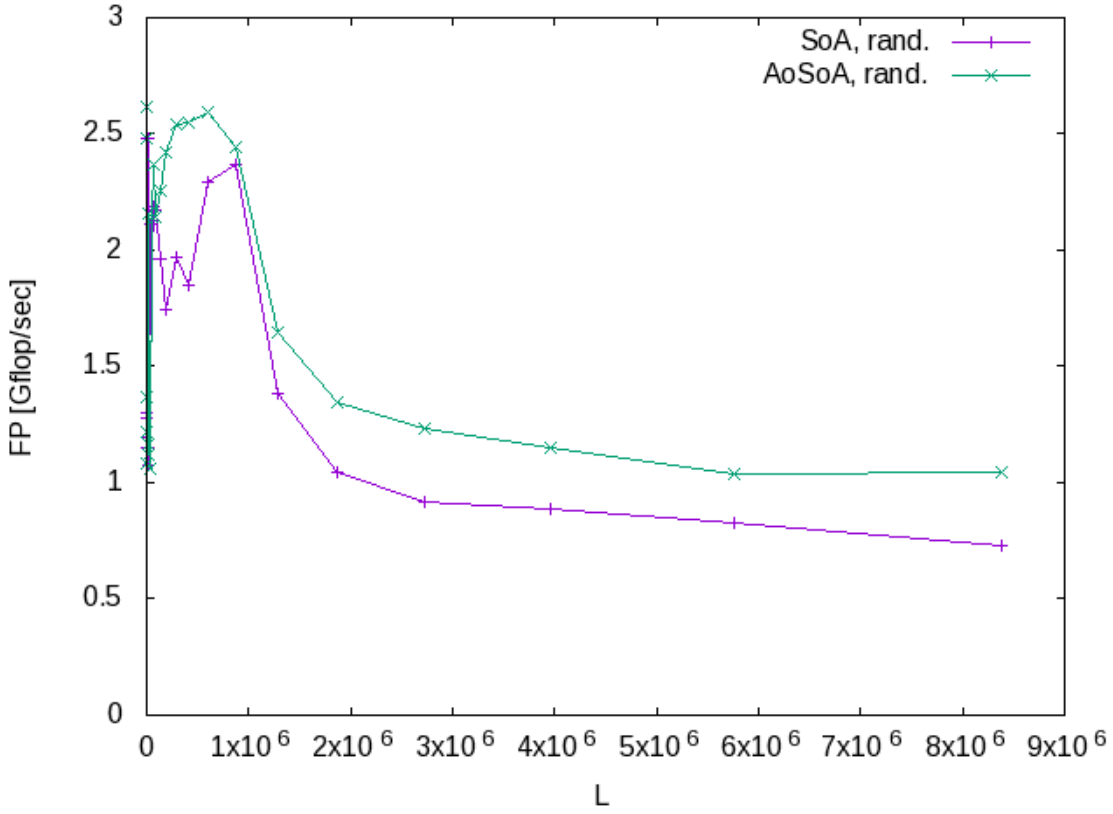
where `VL` is set to the vector length in units of `float`s.

Transfer the `_TODO_A_` and `_TODO_B_` tasks you completed in the previous tasks to this task. Compile and run as before, using: `make space-time-aosoa-r` and `sbatch sub-D.job`. The results can be plotted using `plot-D.gpl`. You will notice that this version is slightly faster than in Task C. Can you explain why?

AoS to SoA

Task D

The resulting plot should look like:



MatMul

This exercise deals with a matrix-matrix multiplication

Navigate to `CoS-2/Optim/Ex/MatMul/`. There is only one file `mm.c`.

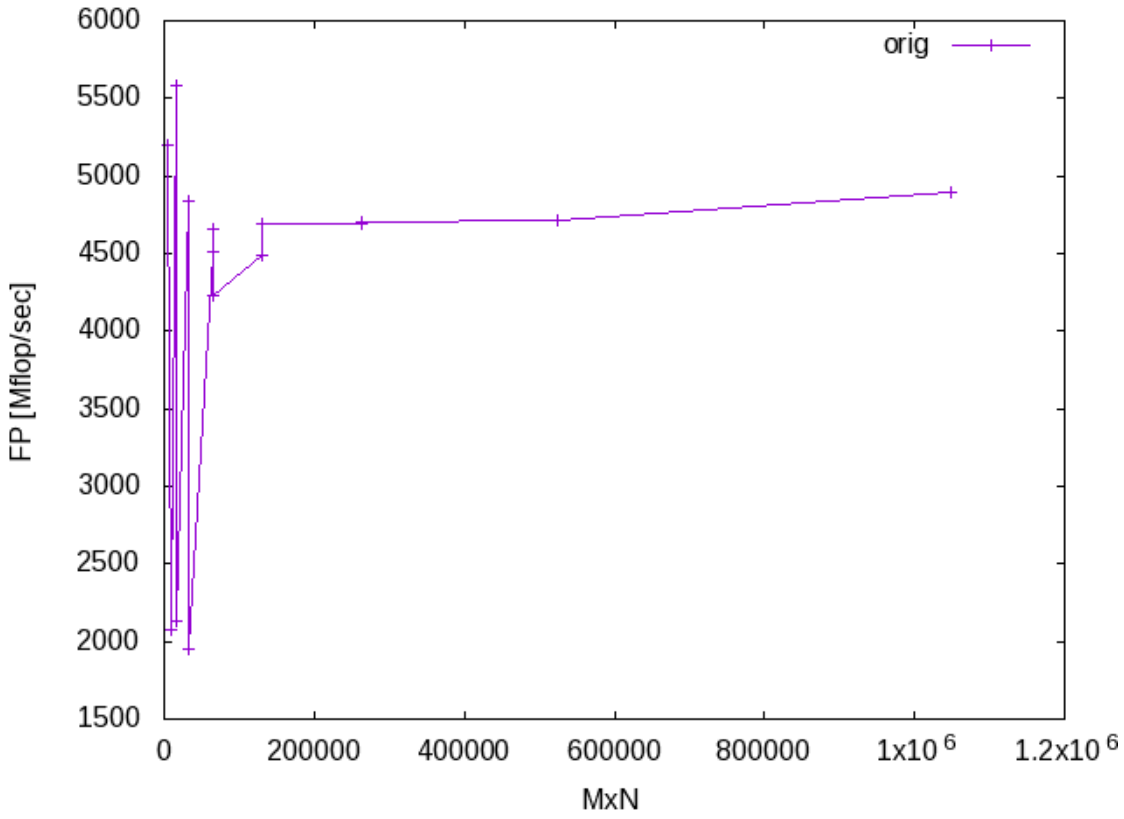
In the first task (task A), you will need to complete the `_TODO_A_` tags. Here this requires:

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

```
void
mat_mul(double *C, int M, int N, double *A, double *B)
{
  for(int i=0; i<M; i++) {
    for(int j=0; j<M; j++)
      C[i*M + j] = 0;
    /*
      _TODO_A_

      Implement the matrix-matrix multiplication naively
     */
  }
  return;
}
```

MatMul

When done: `make mm-orig`, `sbatch sub-A.job`, and then you can plot the result with `plot-A.gpl`. 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<M; j+=BM) {

      /* Set Cb to zero */
      for(int ib=0; ib<BM; ib++)
        for(int jb=0; jb<BM; jb++) {
          Cb[ib*BM + 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 mm-blck` 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
```

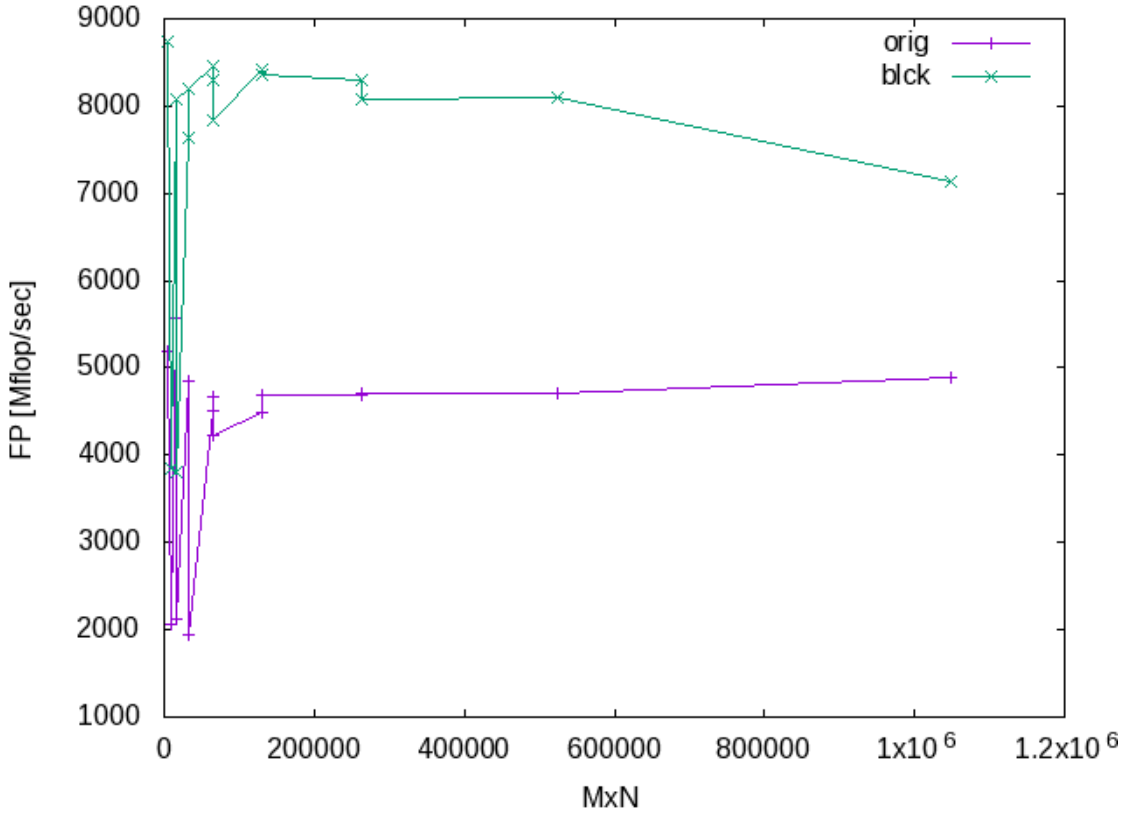
When done, and the two versions agree, submit with: `sbatch sub-B.job`, and after the job completes you can plot the result with `plot-B.gpl`. Note that the block lengths are defined at compile time. They are defined at the beginning:

```
/*
 * Block length in M direction
 */
#ifndef BM
#define BM 16
#endif
```

```
/*
 * Block length in N direction
 */
#ifndef BN
#define BN 16
#endif
```

MatMul

The resulting plot should look like:



3D Laplacian

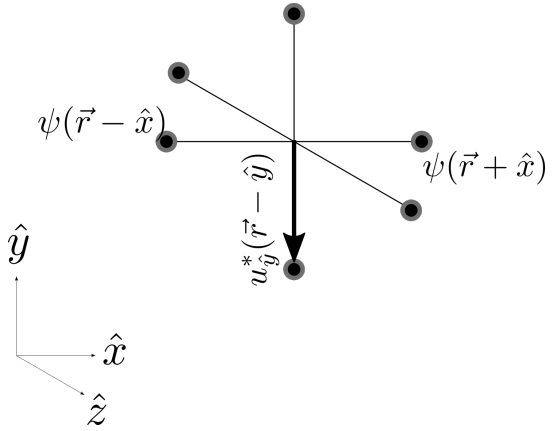
- Consider the 3D "gauge" Laplacian.

$$\phi(\vec{r}) = \nabla\psi(\vec{r}) = 6\psi(\vec{r}) - \sum_{i=1}^{3}[u_{\hat{i}}(\vec{r})\psi(\vec{r}+\hat{i}) + u_{\hat{i}}(\vec{r}-\hat{i})\psi(\vec{r}-\hat{i})]$$

with

$u_{\hat{i}}(\vec{r}) \in \mathbb{C}$, and $|u_{\hat{i}}(\vec{r})| = 1$

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



- 2 us at each site $\vec{r}$
- Conjugation flips the direction of u, i.e. $u_{-\hat{i}}(\vec{x}) = u^*_{\hat{i}}(\vec{x})$

3D Laplacian

- Conjugate gradient (CG) to solve

$$\nabla x = b$$

initial guess x_0
$r_0 = b - \nabla x$
$p = r_0$
loop until $||r_0||$ small enough

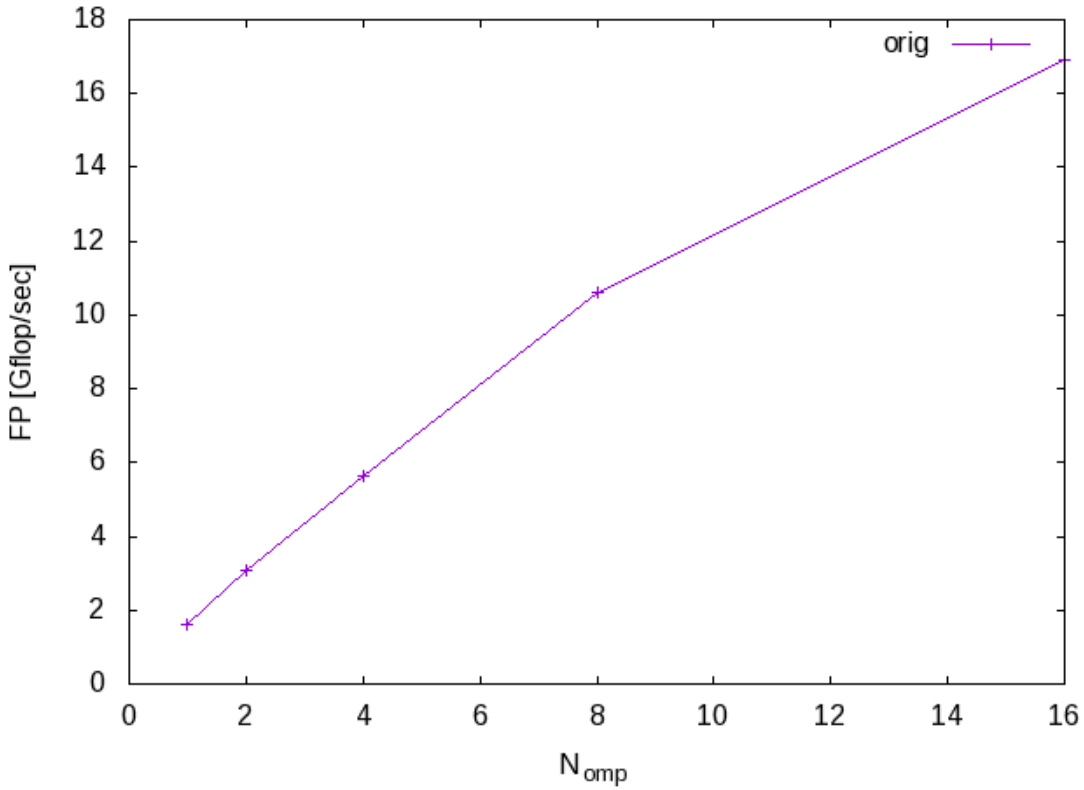
$$\alpha = \frac{r_0^\dagger r_0}{p^\dagger \nabla p}$$
$$x = \alpha p + x$$
$$r_1 = -\alpha \nabla p + r_0$$
$$\beta = \frac{r_1^\dagger r_1}{r_0^\dagger r_0}$$
$$p = \beta p + r_1$$
$$r_0 = r_1$$

```
      0, res = +1.000000e+00
      1, res = +1.665753e-01
      2, res = +3.333299e-02
      3, res = +6.665369e-03
      4, res = +1.333499e-03
      5, res = +2.668942e-04
      6, res = +5.341509e-05
      7, res = +1.074500e-05
      8, res = +2.170688e-06
      9, res = +4.405346e-07
     10, res = +8.984282e-08
     11, res = +1.842731e-08
     12, res = +3.796921e-09
     13, res = +7.870543e-10
     14, res = +1.639781e-10
     15, res = +3.433125e-11
     16, res = +7.228439e-12
     17, res = +1.530630e-12
     18, res = +3.257463e-13
     19, res = +6.973104e-14
     20, res = +1.499168e-14
     21, res = +3.237763e-15
     22, res = +7.021646e-16
     23, res = +1.529374e-16
     24, res = +3.340107e-17
     25, res = +7.319255e-18
     26, res = +1.607249e-18
     27, res = +3.537078e-19
Converged after     27 iterations,
final res = +4.039893e-14
```

3D Laplacian

- Navigate to `CoS-2/Optim/Ex/lapl-3D/`
- `lapl.c` implements a CG algorithm which solves $\nabla \mathfrak{x} = \mathfrak{b}$ for a random $\mathfrak{b}$ and gauge $\mathfrak{u}$
- The `_TODO_A_` pieces need completion
- This includes the bulk of the Laplacian operation in function `lapl()`
- It also includes adding an `OpenMP` pragma over the main loop in `lapl()`
- After you're done compile with `make A` and submit the job `sub-A.job`. You can then plot within gnuplot with `load 'plot-A.gpl'`

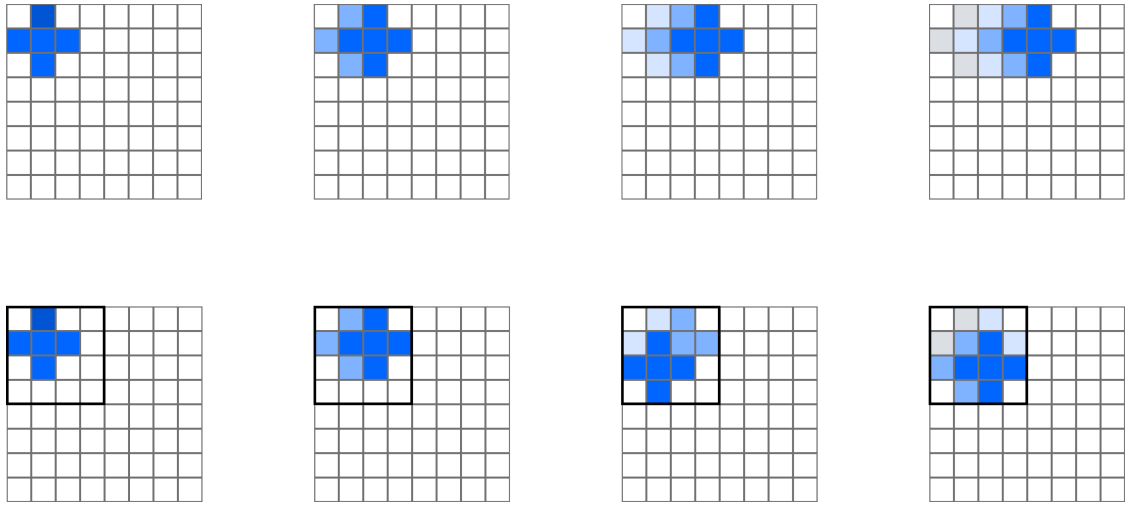
3D Laplacian



The plot is the performance vs the number of OMP threads

3D Laplacian

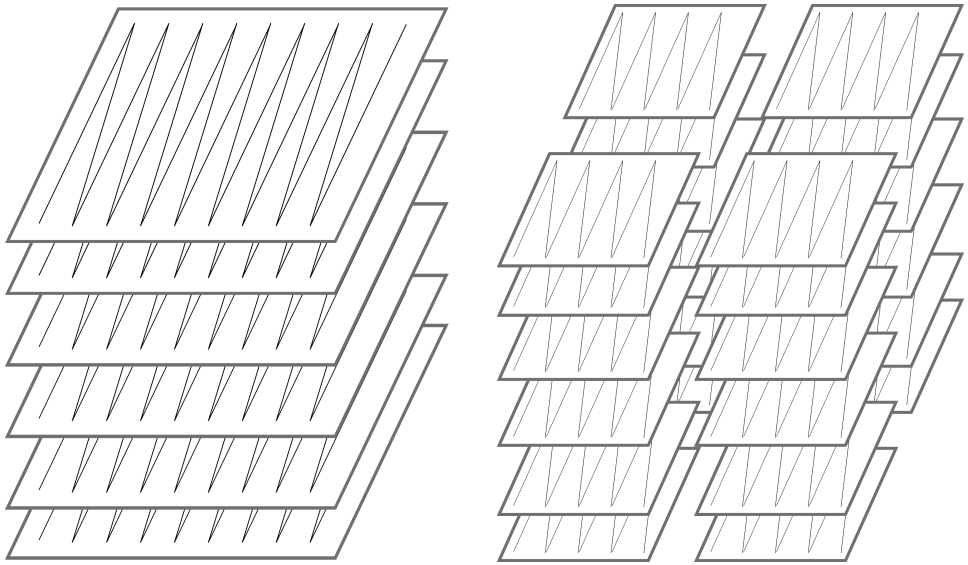
- In Task B, you need to modify `laplb.c`
- This is to implement a "blocked" version of the stencil operation in `lapl()`



- 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

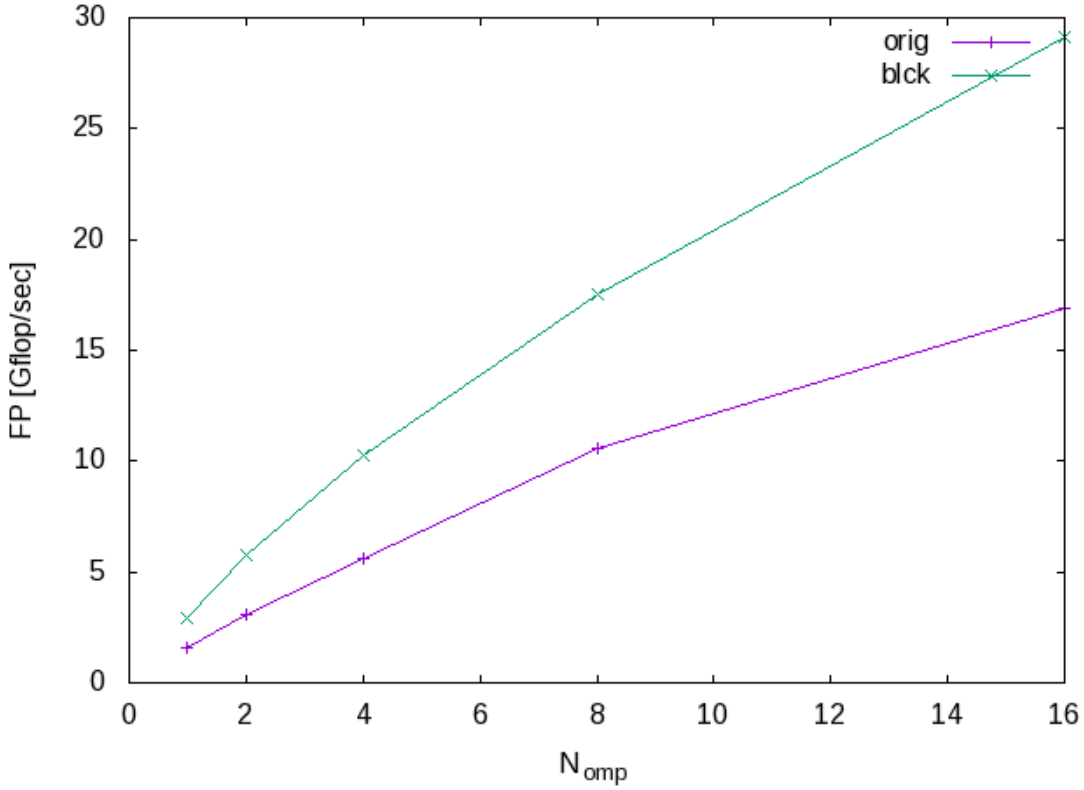
- In Task B, you need to modify `laplb.c`
- This is to implement a "blocked" version of the stencil operation in `lapl()`



- 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

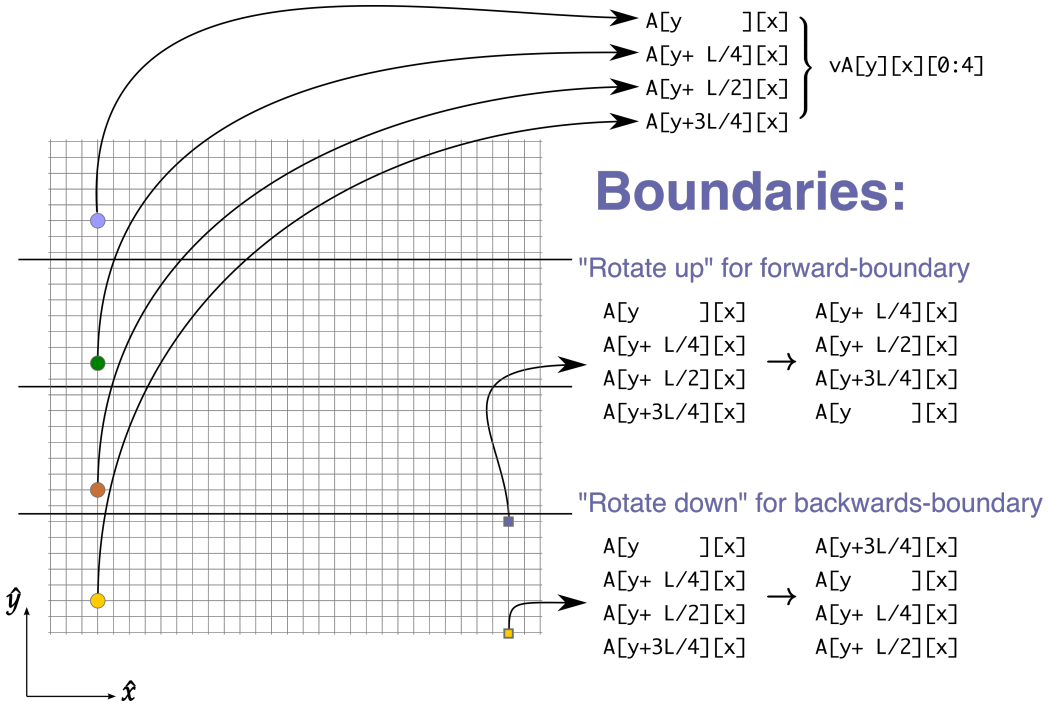
- Compile with `make B`, submit with `sbatch sub-B.job`, and plot in gnuplot with `load 'plot-B.gpl'`



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



- There are parts missing in tagged with `_TODO_C_`
- Modify `laplv.c`, compile with `make C`, run with `sbatch sub-C.job` and plot using `plot-C.gpl`.
- After completing these parts you should obtain similar CG history as before

3D Laplacian

Result of Task D should look like: