High Performance Computing and aspects of Computing in Lattice Gauge Theories

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Lecture 4 (continuation of lecture 3):

Practical exercises

- Data layout transformations for improving performance
    1. Exercise 1: Simple Array-of-Structures to Structure-of-Array transformation
    2. Exercise 2: 2-dimensional stencil operation; "Gauged" laplacian operation
- Practical considerations in implementing LGT
    1. Example: Schwinger fermions

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- Data layout transformations for improving performance
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    2. Exercise 2: 2-dimensional stencil operation; "Gauged" laplacian operation
- Practical considerations in implementing LGT
    1. Example: Schwinger fermions
- Checkout branch `exercises` of repository `EuroPLEx2020` on Github:

```
[user@localhost EuroPLEx2020]$ git fetch
[user@localhost EuroPLEx2020]$ git checkout exercises
```

Data layout optimization

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];
```

```
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)
- However this usually requires an appropriate data layout
- The above is already optimal, but in general this may not be true

Data layout transformations

Facilitating vectorization

- Order the data in arrays such that the same operation can be applied to consecutive elements
  - Assists the compiler in detecting auto-vectorization opportunities
  - Optimized memory accesses
  - Assists the programmer in using *vector intrinsics*

Best practices for optimal data layout

AoS to SoA

AoS: Array of structures

Arrays of structures arise 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;
```

Best practices for optimal data layout

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```
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);
```

Best practices for optimal data layout

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You can now allocate an array of `coords`:

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

Then operations over the coordinates, such as the following, make auto-vectorization difficult.

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

Best practices for optimal data layout

AoS to SoA

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       arr[i].y*arr[i].y +
       arr[i].z*arr[i].z);
```

A common way around this is to use a Structure of Arrays (SoA) rather than an Array of Structures.

Array of Structures to Structure of Arrays

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

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

Array of Structures to Structure of Arrays

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);
```

Array of Structures to Structure of Arrays

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:

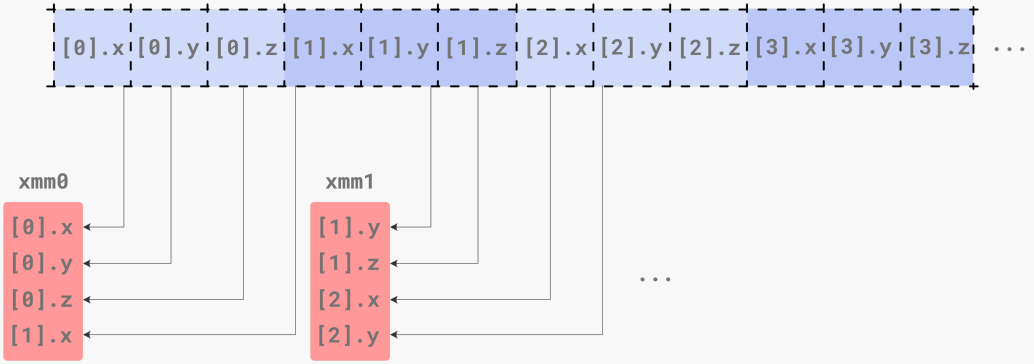
```
coords arr;
arr.x = malloc(sizeof(float)*L);
arr.y = malloc(sizeof(float)*L);
arr.z = malloc(sizeof(float)*L);
```

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

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

AoS to SoA

First elements in AoS, loaded into 4-element vector registers



AoS to SoA

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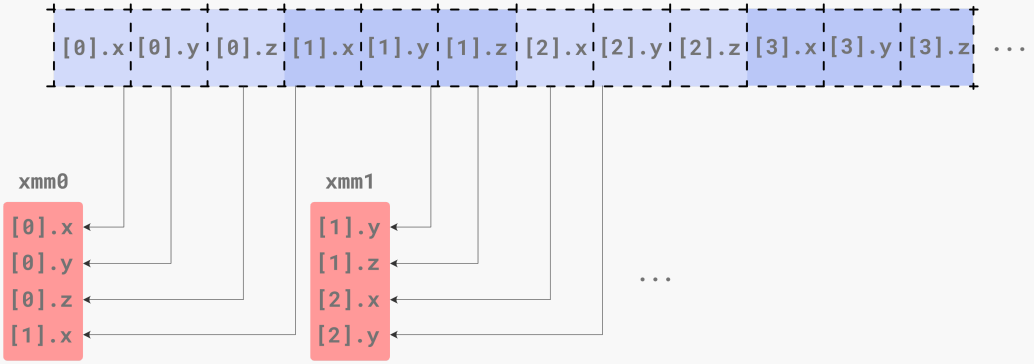

AoS to SoA

In the first exercise we will modify a program that uses an Array-of-Structures to use a Structure-of-Arrays. The main computational kernel in the program does the following:

- Initializes an array of 4-vectors: $a_i = (ct_i, x_i, y_i, z_i)$
- Computes the squared "norm": $s_i = (ct_i)^2 - (x_i^2 + y_i^2 + z_i^2)$ multiple times
- Reports the average time to compute all elements s_i.

To obtain the exercises, pull the `exercises` branch of the Git repository:

- `cd` into the repository on your local system, fetch and checkout the `exercises` branch, and `cd` into the `AoS-to-SoA` directory:

```
[user@localhost ~]$ cd EuroPLEx2020/
[user@localhost EuroPLEx2020]$ git fetch
[user@localhost EuroPLEx2020]$ git checkout exercises
[user@localhost EuroPLEx2020]$ cd AoS-to-SoA/
[user@localhost AoS-to-SoA]$ ls -1
Makefile
plot-A.py
plot-B.py
plot-C.py
run-A.sh
run-B.sh
run-C.sh
space-time-aos.c
space-time-soa.c
```

AoS to SoA

First, look into `space-time-aos.c`

```
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++;
}
```

AoS to SoA

First, look into `space-time-aos.c`

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while(1) {
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     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++;
}
```

- The kernel is (`comp_s()`)
- The kernel is called `NREP` times
- Does this repeatedly. Stops when variation in time to call kernel `NREP` times is smaller than 10%
- `t0acc` holds the average time per `comp_s()` call

AoS to SoA

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     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 -
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      t0acc = ave;
      t1acc = err;
      break;
    }
  }
  n++;
}
```

- The kernel is (`comp_s()`)
- The kernel is called `NREP` times
- Does this repeatedly. Stops when variation in time to call kernel `NREP` times is smaller than 10%
- `t0acc` holds the average time per `comp_s()` call

`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

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

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

AoS to SoA

`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 to parallelize the loop

AoS to SoA

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

```
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  */;
```

Correct `beta_fp` and `beta_io`.

AoS to SoA

After correcting for `beta_fp` and `beta_io`, you need to compile. `make A` should do this for you:

```
[user@localhost AoS-To-SoA]$ make A
cc -O3 -Xpreprocessor -fopenmp -std=gnu99 space-time-aos.c -o space-time-aos -lomp -lm
```

and run the prepared shell script:

```
[user@localhost AoS-To-SoA]$ sh run-A.sh
```

The shell script sets the number of OpenMP threads to four. Modify this if you are on a system that you know has more cores.

AoS to SoA

After correcting for `beta_fp` and `beta_io`, you need to compile. `make A` should do this for you:

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and run the prepared shell script:

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[user@localhost AoS-To-SoA]$ sh run-A.sh
```

The shell script sets the number of OpenMP threads to four. Modify this if you are on a system that you know has more cores.

Running the shell script 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, by running:

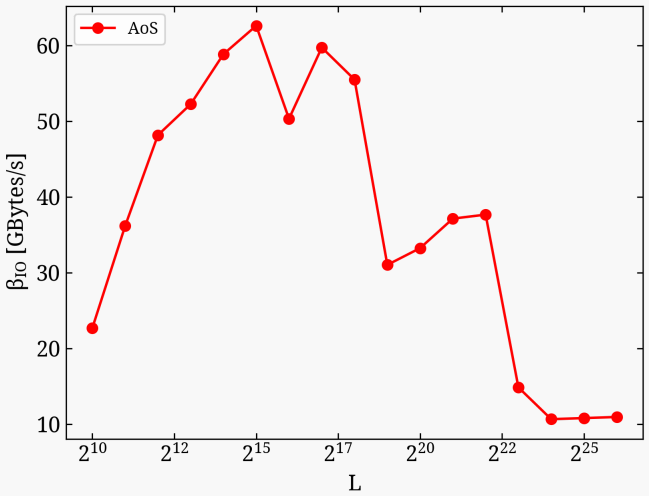
```
[user@localhost AoS-To-SoA]$ python3 plot-A.py
```

which will produce `A.png`.

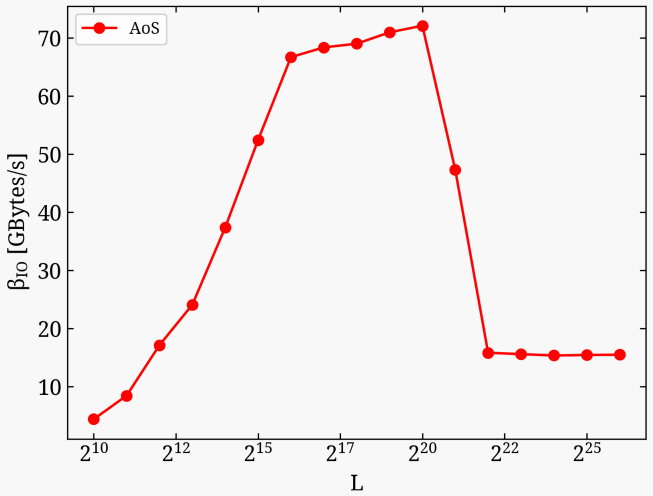
AoS to SoA

Task A

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)

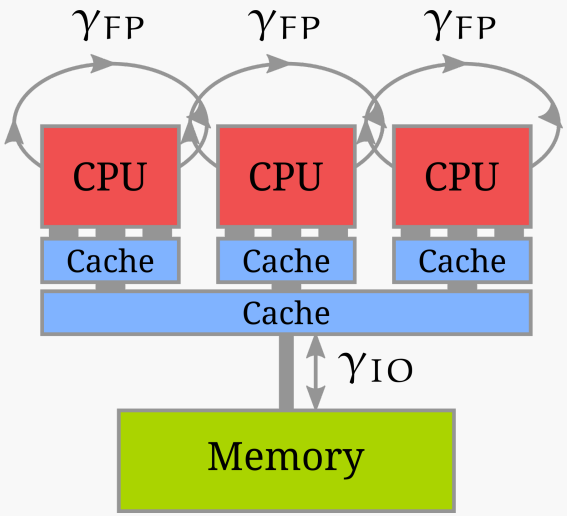


Intel Xeon E5-2650 0 @ 2 GHz
(8 cores, cluster node)



AoS to SoA

Task A



- When $L \ll$, all arrays fit in cache. I/O to cache is at least an order of magnitude faster than I/O to memory
- When $L \gg$ arrays do not fit into cache. Repeated calls to `comp_s()` require repeatedly fetching the arrays from memory. This is more representative of a typical application.

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_`.

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;
```

E.g.: `arr[i].x -> arr[i0].x[i1]`, with:

- `i0 = i/VL = 0,...,N/VL-1` and
- `i1 = i%VL = 0,...,VL-1`

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_`.

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E.g.: `arr[i].x -> arr[i0].x[i1]`, with:

- `i0 = i/VL = 0,...,N/VL-1` and
- `i1 = i%VL = 0,...,VL-1`

For the `_TODO_B_` pieces, 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

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 */
void
comp_s(st_coords *arr, int L)
{
  /* _TODO_B_: complete the kernel */
  #pragma omp parallel for
  ...
```

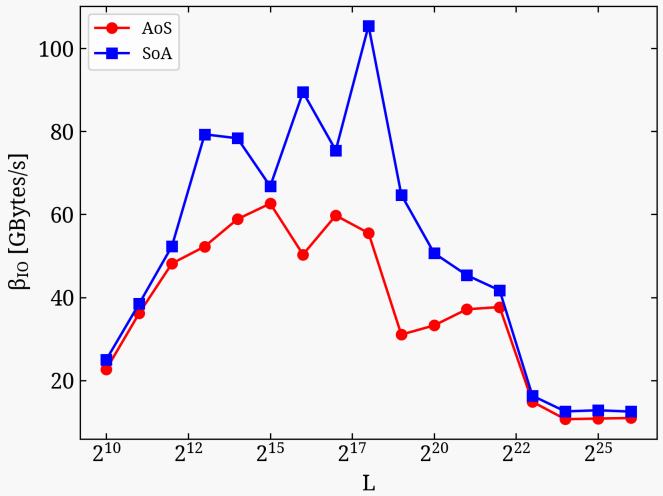
Once done, as in Task A, compile with `make B` and run using the script `run-B.sh`:

```
[user@localhost AoS-To-SoA]$ make B
cc -O3 -Xpreprocessor -fopenmp -std=gnu99 space-time-soa.c -o space-time-soa -lomp -lm
[user@localhost AoS-To-SoA]$ sh run-B.sh
```

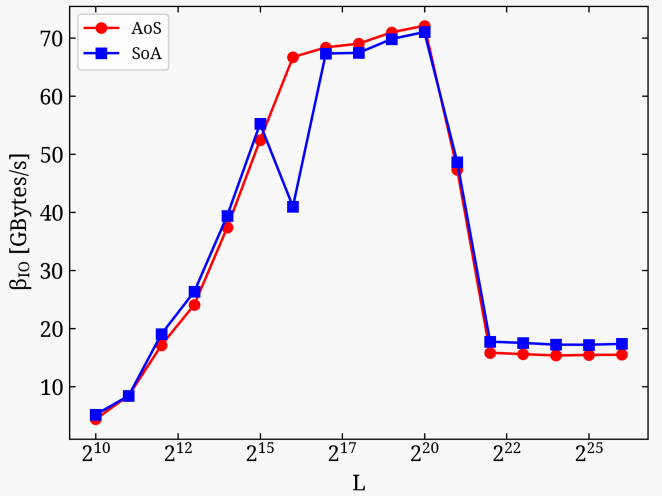
AoS to SoA

Task B

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)



Intel Xeon E5-2650 0 @ 2 GHz
(8 cores, cluster node)



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 `run-C.sh`:

```
export OMP_NUM_THREADS=4
for VL in 2 4 8 16 32 64 128 256; do
    make -B VL=${VL} B
    for ((L=1024; L<=$((64*1024*1024)); L*=2)) ; do
    ./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. Run with:

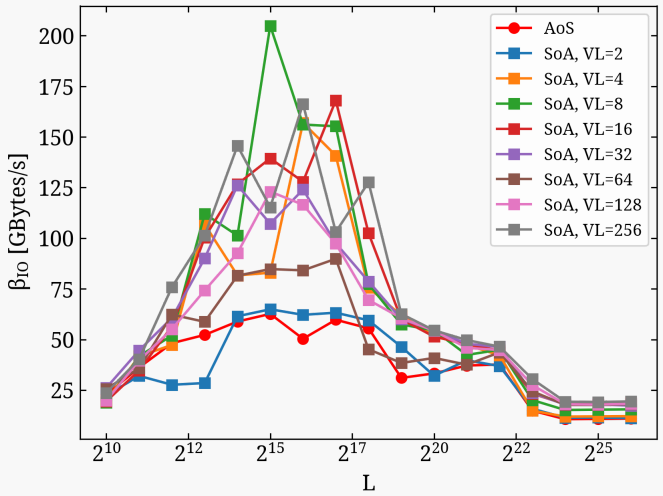
```
[user@localhost AoS-To-SoA]$ sh run-C.sh
```

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

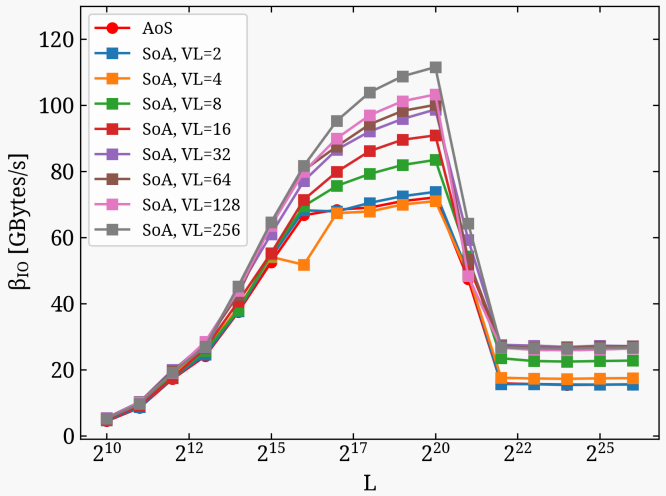
AoS to SoA

Task C

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)



Intel Xeon E5-2650 0 @ 2 GHz
(8 cores, cluster node)

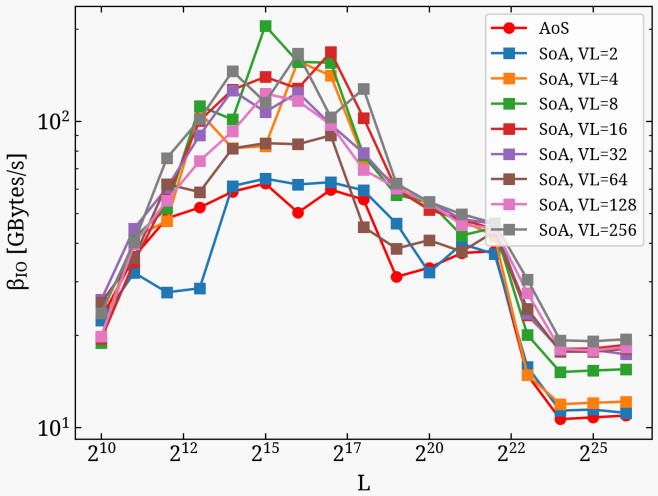


The optimal value of `VL` is in general architecture-dependent. For which value of `VL` do you see best performance?

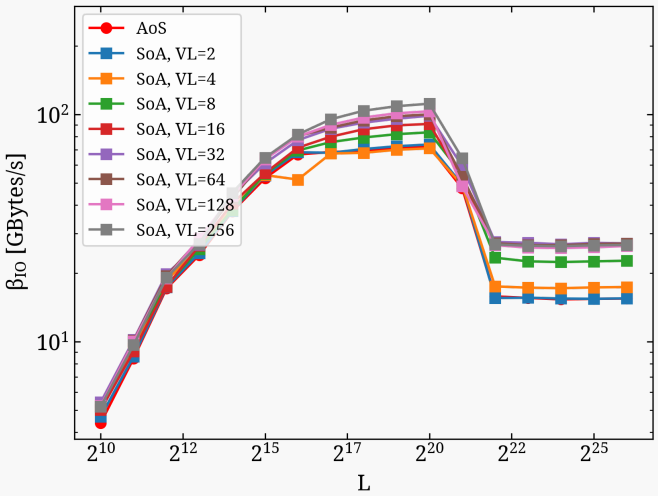
AoS to SoA

Task C

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)



Intel Xeon E5-2650 0 @ 2 GHz
(8 cores, cluster node)



The optimal value of `VL` is in general architecture-dependent. For which value of `VL` do you see best performance?

Data layout in 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]);
  }
```

Data layout in stencil codes

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```
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]);
  }
```

Data layout in 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]);
  }
```

- Operations involve `A[y][x:x+4]`, `A[y][x+1:x+5]`, and `A[y][x-1:x+3]`
- They are badly aligned
- Hard to take advantage of vectorization without inserting multiple *shuffle* and *shift* operations

Data layout in stencil codes

One transformation: change the data layout so that **distant** elements run **fastest**

- If original array is, e.g.

  `A[y][x]`, with `x=0,...,L-1` and `y=0,...,L-1`

- Change to:

  `vA[y0][x][y1]`, with `y0=0,...,L/4-1`, `y1=0,1,2,3`, and `y=y1*(L/4) + y0`

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- Change to:

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- The stencil operation loop will then be:

```
for(int y0=0; y0<L/4; y0++)
  for(int x=0; x<L; x++) {
    vB[y0][x][0] = 4*vA[y0][x][0] - (vA[y0][x+1][0] + vA[y0][x-1][0] + vA[y0+1][x][0] + vA[y0-1][x][0]);
    vB[y0][x][1] = 4*vA[y0][x][1] - (vA[y0][x+1][1] + vA[y0][x-1][1] + vA[y0+1][x][1] + vA[y0-1][x][1]);
    vB[y0][x][2] = 4*vA[y0][x][2] - (vA[y0][x+1][2] + vA[y0][x-1][2] + vA[y0+1][x][2] + vA[y0-1][x][2]);
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}
```

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for(int y0=0; y0<L/4; y0++)
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}
```
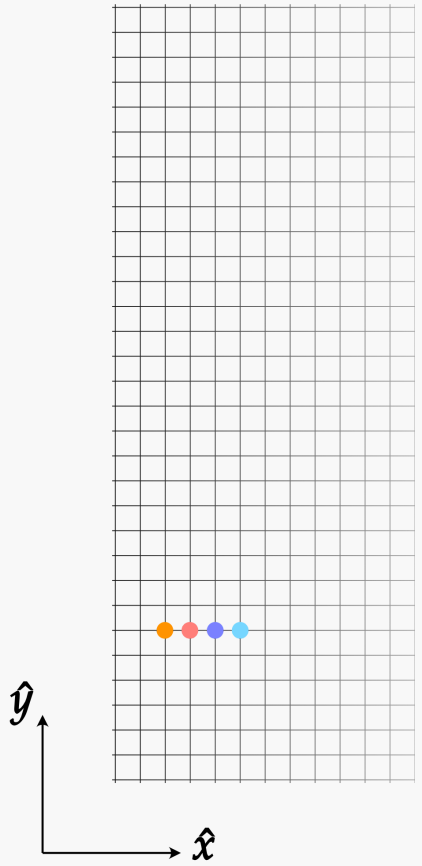

- As long as we keep the data structures ordered this way, the stencil operation will be nicely aligned

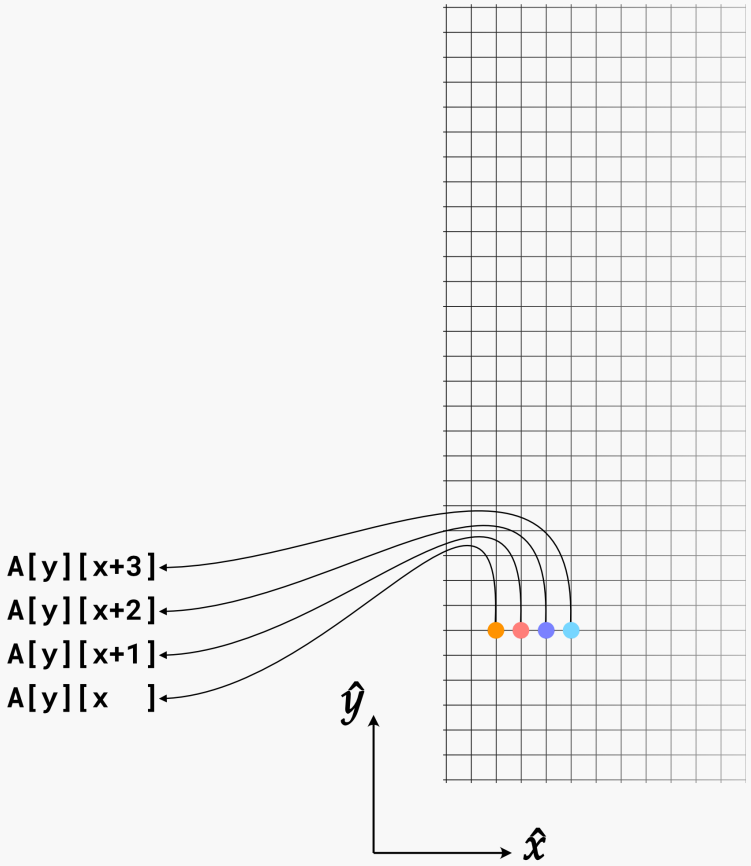
Data layout in stencil codes

Change in data layout so that **distant** elements run **fastest**



Data layout in stencil codes

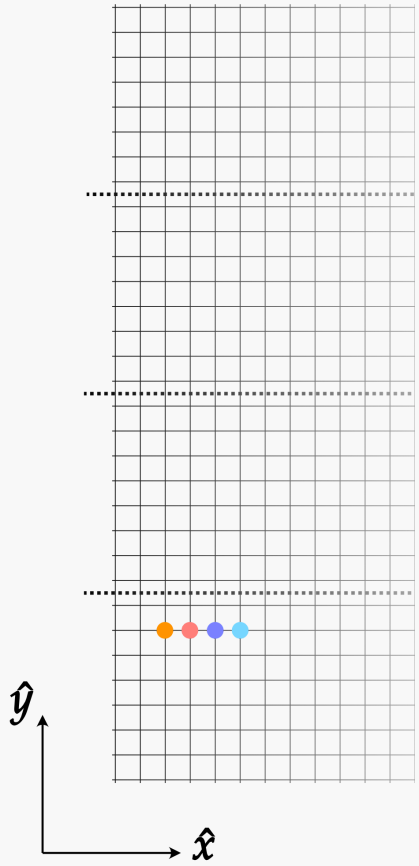
Change in data layout so that **distant** elements run **fastest**



Data layout in stencil codes

Change in data layout so that **distant** elements run **fastest**

```
A[y][x+3]
A[y][x+2]
A[y][x+1]
A[y][x  ]
```



Data layout in stencil codes

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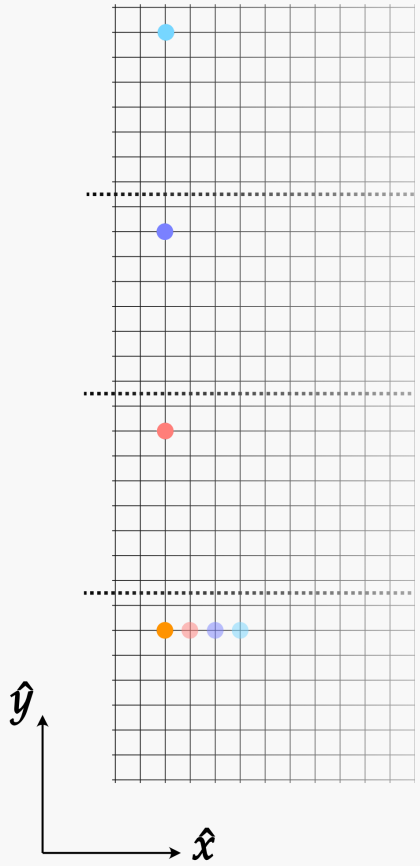

Data layout in stencil codes

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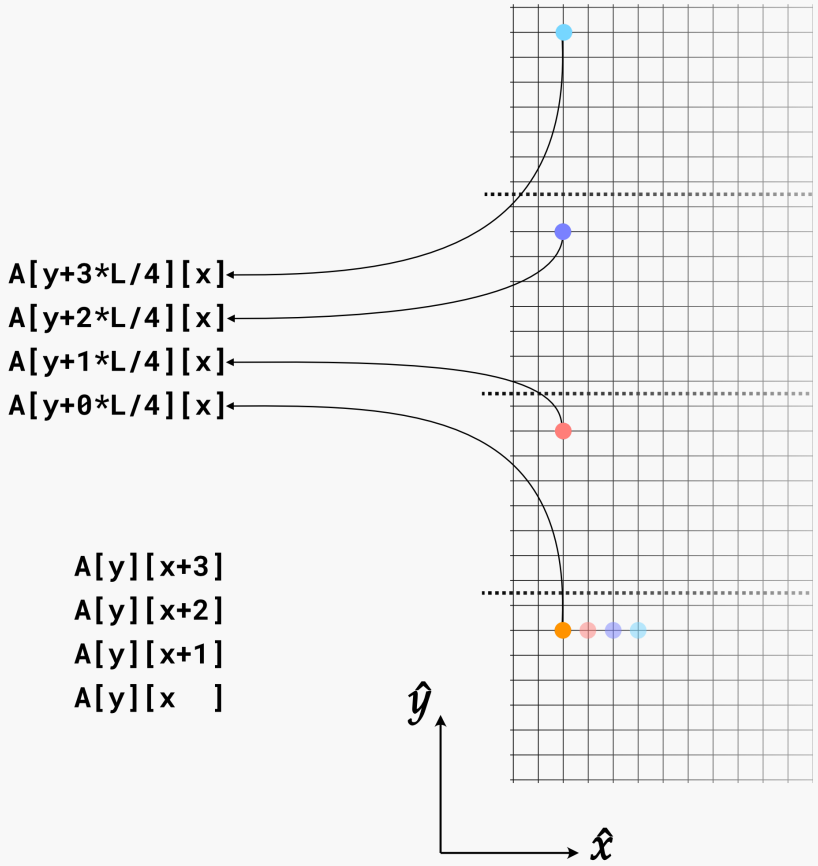

Data layout in stencil codes

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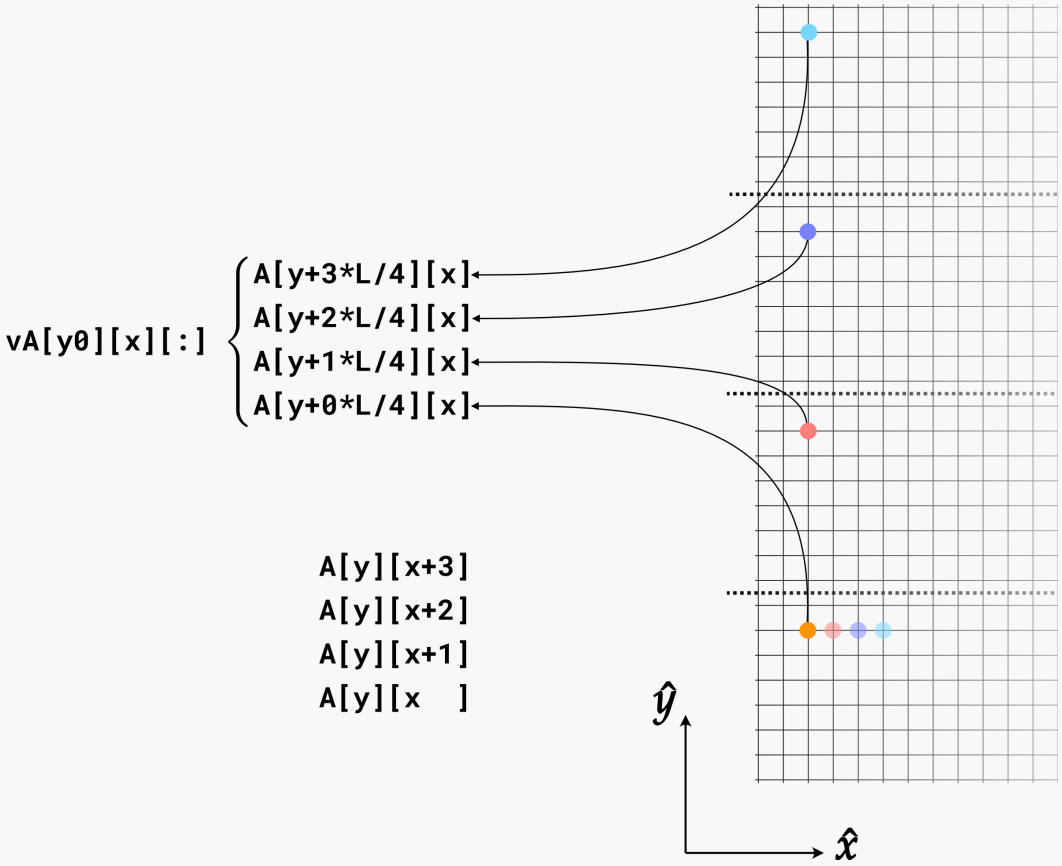

Data layout in stencil codes

- To summarize, reorder the data layout as so (previous slides assumed `VL=4`):

```
for(int y1=0; y1<VL; y1++)
  for(int y0=0; y0<L/VL; y0++)
    for(int x=0; x<L; x++) {
      vA[y0][x][y1] = A[y1*(L/VL) + y0][x];
    }
```

- The stencil operation will then be:

```
for(int y0=0; y0<L/VL; y0++)
  for(int x=0; x<L; x++) {
    vB[y0][x][0] = 4*vA[y0][x][0] - (vA[y0][x+1][0] + vA[y0][x-1][0] + vA[y0+1][x][0] + vA[y0-1][x][0]);
    vB[y0][x][1] = 4*vA[y0][x][1] - (vA[y0][x+1][1] + vA[y0][x-1][1] + vA[y0+1][x][1] + vA[y0-1][x][1]);
    vB[y0][x][2] = 4*vA[y0][x][2] - (vA[y0][x+1][2] + vA[y0][x-1][2] + vA[y0+1][x][2] + vA[y0-1][x][2]);
    vB[y0][x][3] = 4*vA[y0][x][3] - (vA[y0][x+1][3] + vA[y0][x-1][3] + vA[y0+1][x][3] + vA[y0-1][x][3]);
}
```

Data layout in stencil codes

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```
for(int y1=0; y1<VL; y1++)
  for(int y0=0; y0<L/VL; y0++)
    for(int x=0; x<L; x++) {
      vA[y0][x][y1] = A[y1*(L/VL) + y0][x];
    }
```

- The stencil operation will then be:

```
for(int y0=0; y0<L/VL; y0++)
  for(int x=0; x<L; x++) {
    vB[y0][x][0] = 4*vA[y0][x][0] - (vA[y0][x+1][0] + vA[y0][x-1][0] + vA[y0+1][x][0] + vA[y0-1][x][0]);
    vB[y0][x][1] = 4*vA[y0][x][1] - (vA[y0][x+1][1] + vA[y0][x-1][1] + vA[y0+1][x][1] + vA[y0-1][x][1]);
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}
```

- But this is wrong on the boundaries `y0=0` and `y0=L/4-1`!

Data layout in stencil codes

Caution on the boundaries

- In the original data layout:

```
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]);
}
```

Data layout in stencil codes

Caution on the boundaries

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```
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]);
}
```

- In the new data layout:

```
y0 = 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/VL-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/VL-1][x][0]);
 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/VL-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/VL-1][x][2]);
}
```

Data layout in stencil codes

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

- In the new data layout:

```
y0 = 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/VL-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/VL-1][x][0]);
 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/VL-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/VL-1][x][2]);
}
```

- And for the other boundary

```
y0 = L/VL-1;
for(int x=0; x<L; x++) {
 vB[L/VL-1][x][0]=4*vA[L/VL-1][x][0] - (vA[L/VL-1][x+1][0] + vA[L/VL-1][x-1][0] + vA[0][x][1] + vA[L/VL-2][x][0]);
 vB[L/VL-1][x][1]=4*vA[L/VL-1][x][1] - (vA[L/VL-1][x+1][1] + vA[L/VL-1][x-1][1] + vA[0][x][2] + vA[L/VL-2][x][1]);
 vB[L/VL-1][x][2]=4*vA[L/VL-1][x][2] - (vA[L/VL-1][x+1][2] + vA[L/VL-1][x-1][2] + vA[0][x][3] + vA[L/VL-2][x][2]);
 vB[L/VL-1][x][3]=4*vA[L/VL-1][x][3] - (vA[L/VL-1][x+1][3] + vA[L/VL-1][x-1][3] + vA[0][x][0] + vA[L/VL-2][x][3]);
}
```

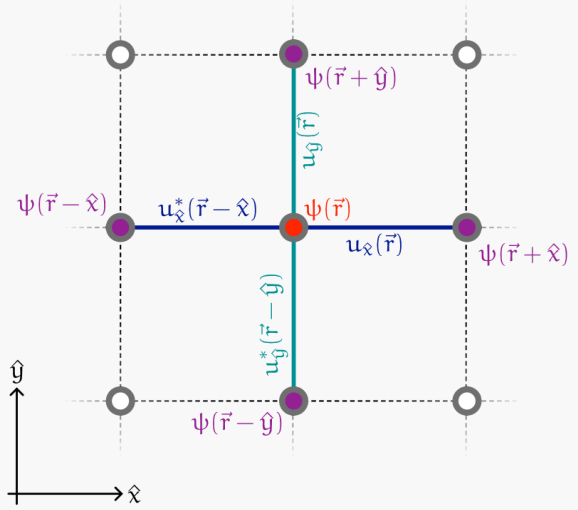
Data layout in stencil codes: Exercise

- Consider the 2D "gauged" Laplacian ($N_d = 2$)

$$\phi(\vec{r}) = \nabla\psi(\vec{r}) = 4\psi(\vec{r}) - \sum_{i=0}^{N_d-1} [u_{\hat{i}}(\vec{r})\psi(\vec{r}+\hat{i}) + u^*_{\hat{i}}(\vec{r}-\hat{i})\psi(\vec{r}-\hat{i})]$$

$u_{\hat{i}}(\vec{r}) \in U(1), \psi(\vec{r}) \in \mathbb{C}$

- $2 \cdot N_d$ "u"s at each site $\vec{r}$, but only N_d unique "u"s
- Conjugation flips the direction of u, i.e. $u_{-\hat{i}}(\vec{r}) = u^*_{\hat{i}}(\vec{r})$
- $\hat{i}$ unit vector in direction i
- Convention: $\hat{x} = \hat{1}, \hat{y} = \hat{0}$



Data layout in stencil codes: Exercise

- The code in the exercise uses 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

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

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

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

$p = \beta p + r_1$
$r_0 = r_1$

```
[koutsou@localhost Lapl]$./lapl 128
      0, res = +1.000000e+00
      1, res = +2.546227e-01
      2, res = +8.557546e-02
      3, res = +2.866554e-02
      4, res = +9.553013e-03
      5, res = +3.151271e-03
      6, res = +1.062331e-03
      7, res = +3.664755e-04
      8, res = +1.269510e-04
      9, res = +4.541719e-05
     10, res = +1.590056e-05
     11, res = +5.618028e-06
     12, res = +1.970783e-06
     13, res = +7.037988e-07
     14, res = +2.475690e-07
     15, res = +8.810894e-08
     16, res = +3.164535e-08
     17, res = +1.140112e-08
     18, res = +4.032213e-09
     19, res = +1.443336e-09
     20, res = +5.135969e-10
     ...
     38, res = +5.274840e-18
     39, res = +1.950025e-18
     40, res = +7.164136e-19
Converged after     40 iterations, res = +1.055927e-13
Time in lapl(): +1.206e-04 sec/call   4.62e+00 Gflop/s   5.43e+00 GB/s
```

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

Data layout in stencil codes: Exercise

- Navigate to directory `./Lapl/`
- `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()` at `lapl.c:146`
- After you're done compile with `make A` and run for varying problem size `L` by running the script `run-A.sh`
- You can then plot the performance with `python3 plot-A.py`

Data layout in stencil codes: Exercise

Some implementation details

- Complex fields don't use the C `_Complex` data type

```
typedef struct {
float phi_re;
float phi_im;
} field;
```

```
typedef struct {
float u_re[ND];
float u_im[ND];
} link;
```

  the reason will become apparent in the next part of the exercise

Data layout in stencil codes: Exercise

Some implementation details

- Complex fields don't use the C `_Complex` data type

```
typedef struct {
float phi_re;
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} field;
```

```
typedef struct {
float u_re[ND];
float u_im[ND];
} link;
```

  the reason will become apparent in the next part of the exercise

- Periodic boundary conditions are implemented via modulo operations:

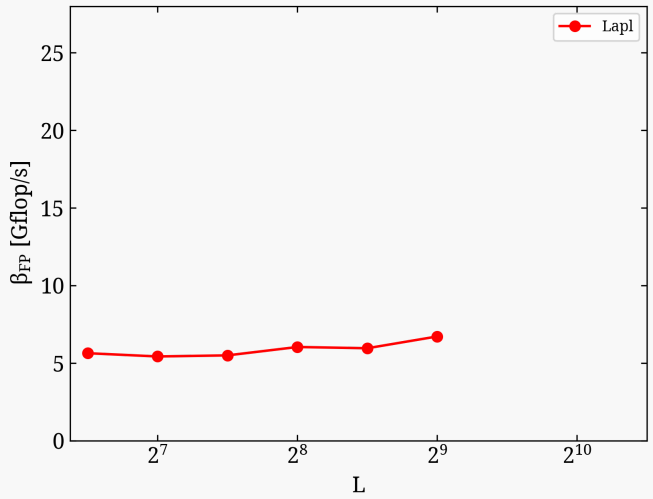
```
int y0 = y*L;
int yp = ((y + 1)%L)*L;
int ym = ((y + L - 1)%L)*L;
```

```
int v0p = (x+1)%L + y0;
int v0m = (L+x-1)%L + y0;
```

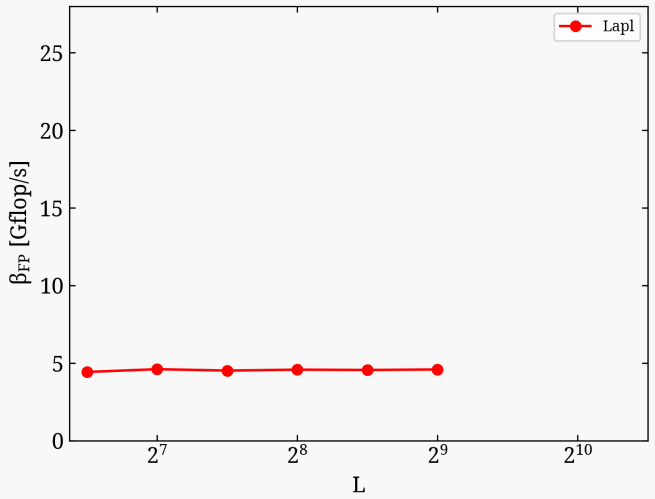
Data layout in stencil codes: Exercise

Task A

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)



Intel Xeon E5-2650 0 @ 2 GHz
(8 cores, cluster node)



Data layout in stencil codes: Exercise

- Task B involves implementing a version of `lapl()` which is easier for vectorization
- The file is `laplv.c` and can be compiled with `make B`

Data layout in stencil codes: Exercise

- Task B involves implementing a version of `lapl()` which is easier for vectorization
- The file is `laplv.c` and can be compiled with `make B`
- The new data structures reflect the new data layout, with `VL` being the "vectorization length":

```
typedef struct {
float phi_re[VL];
float phi_im[VL];
} field;
```

```
typedef struct {
float u_re[ND][VL];
float u_im[ND][VL];
} link;
```

Data layout in stencil codes: Exercise

- Task B involves implementing a version of `lapl()` which is easier for vectorization
- The file is `laplv.c` and can be compiled with `make B`
- The new data structures reflect the new data layout, with `VL` being the "vectorization length":

```
typedef struct {
float phi_re[VL];
float phi_im[VL];
} field;
```

```
typedef struct {
float u_re[ND][VL];
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} link;
```

- The functions `rand_links()` and `rand_field()`, used to initialize with random numbers, are already setup to initialize the arrays in the same order as in `lapl.c`

Data layout in stencil codes: Exercise

- Task B involves implementing a version of `lapl()` which is easier for vectorization
- The file is `laplv.c` and can be compiled with `make B`
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```
typedef struct {
float phi_re[VL];
float phi_im[VL];
} field;
```

```
typedef struct {
float u_re[ND][VL];
float u_im[ND][VL];
} link;
```

- The functions `rand_links()` and `rand_field()`, used to initialize with random numbers, are already setup to initialize the arrays in the same order as in `lapl.c`
- This allows you to check the code: the residuals for each iteration should be exactly the same between `lapl` and `laplv` if you have completed the code correctly

Data layout in stencil codes: Exercise

- Complete the code tagged with `_TODO_B_`. Also, transfer from `lapl` the tasks tagged `_TODO_A_`
- The `_TODO_B_` tasks include:
  - Completing the laplacian main kernel, as before, but now using the new data layout
  - Completing the shift operations required on the boundaries

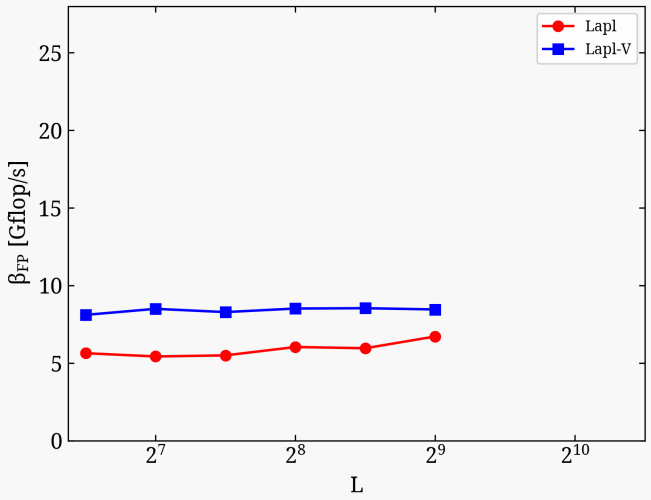
Data layout in stencil codes: Exercise

- Complete the code tagged with `_TODO_B_`. Also, transfer from `lapl` the tasks tagged `_TODO_A_`
- The `_TODO_B_` tasks include:
  - Completing the laplacian main kernel, as before, but now using the new data layout
  - Completing the shift operations required on the boundaries
- Once done, compile with `make B`, run `run-B.sh` and plot with `plot-B.py`

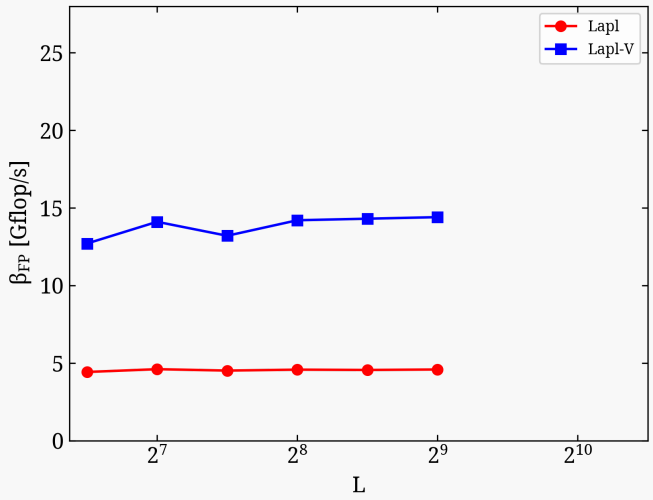
Data layout in stencil codes: Exercise

Task B

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)



Intel Xeon E5-2650 0 @ 2 GHz
(8 cores, cluster node)



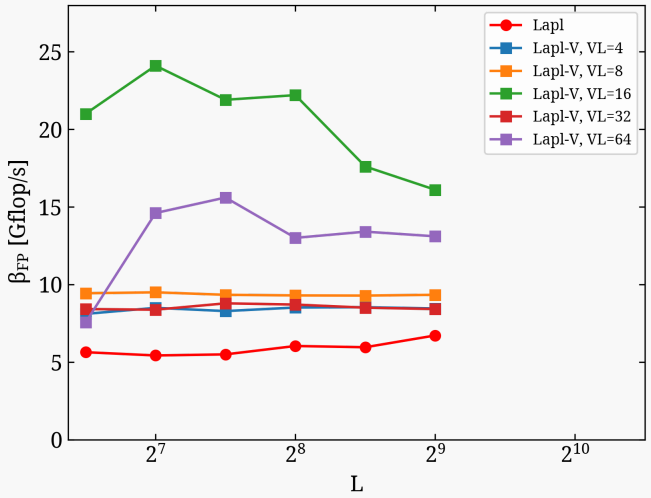
Data layout in stencil codes: Exercise

- Part C of this exercise only requires you to run `run-C.sh`
- As in `AoS-to-SoA`, this runs `laplv` for various values of `VL`
- With `plot-C.py` you can plot and compare with `lapl`

Data layout in stencil codes: Exercise

Task C

Intel Core i5-8259U @ 2.3 GHz
(this 4-core laptop)



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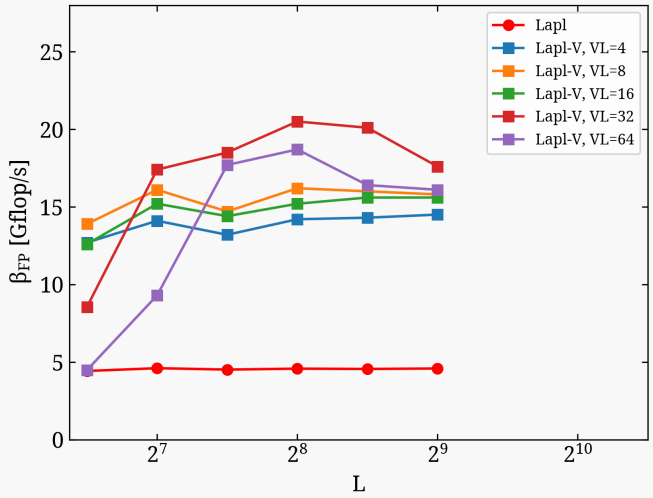

Gauge Theories on the Lattice

Computational intensity example: Schwinger model

- $U(1)$ gauge theory, 2-dimensional, 2-component fermion spinors
- "Wilson" fermion action:

$$\psi'_\alpha(\vec{x}) = M_{\alpha\beta}(\vec{x},\vec{y})\psi_\beta(\vec{y}) = \left[\frac{1}{2}H_{\alpha\beta}(\vec{x},\vec{y}) + (m+2)\delta_{\vec{x},\vec{y}}\delta_{\alpha\beta}\right]\psi_\beta(\vec{y})$$

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- With hopping term:

$$H_{\alpha\beta}(\vec{x},\vec{y})\psi_\beta(\vec{y}) = \sum_{\mu=0}^{1}(1-\sigma_\mu)_{\alpha\beta}u_\mu(\vec{x})\psi_\beta(x+\hat{\mu}) + (1+\sigma_\mu)_{\alpha\beta}u^*_\mu(\vec{x}-\hat{\mu})\psi_\beta(x-\hat{\mu})$$

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- σ are the Pauli matrices:

$$\sigma_0 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_1 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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- The fermion matrix is "σ_z-hermitian"

$$\sigma_z M = M^\dagger \sigma_z \Rightarrow (\sigma_z)_{\alpha\alpha'} M_{\alpha'\beta}(\vec{x},\vec{y}) = M^*_{\alpha'\alpha}(\vec{y},\vec{x})(\sigma_z)_{\alpha'\beta}$$

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- Meaning we can write:

$$M^\dagger M\psi = \sigma_z M \sigma_z M \psi$$

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- E.g., in a Conjugate Gradient, we can get away by only implementing $M\psi$

Gauge Theories on the Lattice

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- Computational intensity of $M\psi$
  - Note the simplifications in multiplying with the Pauli matrices

$$(1 \pm \sigma_0)\psi = \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = \begin{pmatrix} \psi_0 \pm \psi_1 \\ \pm\psi_0 + \psi_1 \end{pmatrix} = \begin{pmatrix} \psi_0 \pm \psi_1 \\ \pm(\psi_0 \pm \psi_1) \end{pmatrix}$$

$$(1 \pm \sigma_1)\psi = \begin{pmatrix} 1 & \mp i \\ \pm i & 1 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = \begin{pmatrix} \psi_0 \mp i\psi_1 \\ \pm i\psi_0 + \psi_1 \end{pmatrix} = \begin{pmatrix} \psi_0 \mp i\psi_1 \\ \pm i(\psi_0 \mp i\psi_1) \end{pmatrix}$$

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- Multiplication by i is an exchange of real and imaginary parts + sign-flip: zero flop!
  - Only one complex addition or subtraction per spinor needed $\longrightarrow$ 2 flops
  - Only one of two components needs to multiply gauge-links

Gauge Theories on the Lattice

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- Computational intensity of $M\psi$
  - Only one complex multiplication per term

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  - Four terms: two terms in each direction ($\mu = 0, 1$)

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  - Four terms: two terms in each direction ($\mu = 0, 1$)
    - Multiplication by Pauli matrix: **2 flop**
    - Multiplication by gauge link: **6 flop**
    - Adding four terms is three complex additions: **6 flop**
  - $\Rightarrow 8_{\text{flop}} \times 4_{\text{terms}} + 6_{\text{flop}} = 38$ flop for hopping term

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  - Mass term: scalar times two-component complex spinor: **+4 flop**

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  - Mass term added to $0.5\times$ hopping term: **+8 flop**

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  - Mass term: scalar times two-component complex spinor: **+4 flop**
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  - **Total**: 50 flop per M application *per lattice site*

Gauge Theories on the Lattice

Computational intensity example: Schwinger model

- Application of $\mathrm{M}\psi$: 50 flop per site
- Data in/out (assuming double precision, 16 bytes per complex):
  - In: 1 gauge field, 1 spinor: 64 bytes per site
  - Out: 1 spinor: 32 bytes per site
- Intensity: $\mathrm{I_k} \simeq 0.52$ flop/byte

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  - Multiplication by σ_z: just a sign-flip of second component: zero flop

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  - Assuming all fields need to be read and written with each application:
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- Hermitian (square) operator: $\sigma_z M \sigma_z M \psi$
  - Multiplication by σ_z: just a sign-flip of second component: zero flop
  - Assuming all fields need to be read and written with each application:
    - Intensity unchanged: $I_k \simeq 0.52$ flop/byte
  - Assuming gauge-field remains available (e.g. in cache):
    - Intensity: $I_k \simeq 0.625$ flop/byte