

# FINM 32950: Intro to HPC in Finance

## Lecture 2

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Vectorization

Using Multicore Nodes

## Vectorization

# Vectorization in Action

- ▶ Last week: we introduced the idea of vectorization.
- ▶ Today: we look at how vectorization works using examples.
- ▶ We will look at 2 ways to introduce vectorization:
  1. Using intrinsics (low-level functions built in to the compiler)<sup>1</sup>.
  2. Auto vectorization (using high-level language constructs).
- ▶ Intrinsics is a powerful technique but we do not use it directly in this course. We use intrinsics mainly to demonstrate/prove vectorization in action.
- ▶ In this course we prefer auto vectorization (for reasons we shall discuss later).

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<sup>1</sup><https://docs.microsoft.com/en-us/cpp/intrinsics/compiler-intrinsics?view=vs-2019>

# Representing Packed Data

- ▶ C++ defines data types for fundamental types.
- ▶ E.g.: int, double, float, short
- ▶ We cannot directly use them to store packed data.
- ▶ We need to use *vector extension types* to store packed data.
- ▶ The register size and fundamental data type determine how many data items we can store in a packed-register:
  - ▶ 128 bit register: can store 4 floats or 2 doubles
  - ▶ 256 bit register: can store 8 floats or 4 doubles
- ▶ Vector extension (packed data) types depend on:
  1. Size of the registers (register size depends on the architecture, SSE2: 128; AVX2: 256; AVX-512: 512)
  2. Fundamental data type (individual data item size depends on type, float: 32; double:64)

# Packed Data Types

- ▶ For 128 bit registers:
  - ▶ `__m128`: stores 4 floats
  - ▶ `__m128d`: stores 2 doubles
  - ▶ `__m128i`: stores 4 ints
  - ▶ ...
- ▶ For 256 bit registers:
  - ▶ `__m256`: stores 8 floats
  - ▶ `__m256d`: stores 4 doubles
  - ▶ `__m256i`: stores 8 ints
  - ▶ ...
- ▶ There's a pattern:
  - ▶ prefix: `__m`
  - ▶ size of the register (e.g. 128, 256)
  - ▶ fundamental data type (i: int; d: double; default: float; ...)

## Operations on Packed Data

- ▶ We must use intrinsic functions (packed instructions) to operate on packed data (i.e., we cannot use regular arithmetic operators (+, -, etc.) with packed types).
- ▶ Intrinsics provide a *family of functions* for a given operation (e.g. addition) for each packed type.
- ▶ Example: for SSE2:
  - ▶ `_mm128_add_epi32`: to add packed (4) integer values stored in a 128 bit packed register
  - ▶ `_mm128_add_epi16`: to add packed (8) short values stored in a 128 bit packed register
  - ▶ ...
- ▶ Example: for AVX2:
  - ▶ `_mm256_add_epi32`: to add packed (8) integer values stored in a 256 bit packed register
  - ▶ `_mm256_add_epi16`: to add packed (16) integer values stored in a 256 bit packed register
  - ▶ ...
- ▶ Ref: <https://software.intel.com/sites/landingpage/IntrinsicsGuide/#=undefined>

# Intrinsics: Example 1

- ▶ Example addition for SSE processors:

```
#include <xmmintrin.h> // for SSE
#include <stdio.h> //for printf

void add_test()
{
    __m128 a = _mm_set_ps(1.0f, 2.0f, 3.0f, 4.0f);
    __m128 b = _mm_set_ps(5.0f, 6.0f, 7.0f, 8.0f);

    __m128 c = _mm_add_ps(a, b);

    // displaying results
    float* f = (float*)&c;
    printf("%f %f %f %f\n", f[0], f[1], f[2], f[3]);
}
```



## Intrinsics: Example 2

- ▶ Let's look at another example to show the power of vectorization.
- ▶ Suppose we want to do a multiply and add operation on vectors:

```
for (int i=0; i<16; i++)  
{  
    d[i] = a[i] * b[i] + c[i];  
}
```

- ▶ This for loop uses 16 additions and 16 multiplications.
- ▶ We can do all of them in one operation:

```
__m512 a = /*packed data*/  
__m512 b = /*packed data*/  
__m512 c = /*packed data*/  
  
__m512 d = _mm512_fmadd_ps(a, b, c);
```

# Vectorization using Intrinsics: Advantages and Disadvantages

- ▶ We briefly looked at intrinsics to show:
  1. How vectorization works
  2. Benefits/power of vectorization
- ▶ Intrinsics has some drawbacks:
  - ▶ Code is difficult to read, write, and maintain (try to write a Black Scholes pricer)
  - ▶ Code is not portable
- ▶ Next, we will look at how to achieve vectorization using high-level programming constructs.

## Auto-Vectorization

# Auto-Vectorization

- ▶ Modern compilers can vectorize code *automatically*. It is known as auto-vectorization.
  - ▶ The compiler generates packed SIMD instructions to replace loops.
- ▶ For auto-vectorization to work:
  - ▶ Code has to satisfy some requirements
  - ▶ Certain directives have to be used to encourage/force the compiler auto-vectorize.
- ▶ We need to understand how we can write code to maximize auto-vectorization:
  - ▶ If auto-vectorization occurred
  - ▶ What if it did not? we need to know why the compiler did not vectorize the loop/loops
  - ▶ So, we can do something to *encourage/force* compiler to auto-vectorize

## Vectorization Using Intel C++ Compiler

- ▶ Modern compilers support auto vectorization, but details are vendor specific.
- ▶ We will limit our discussion to the **Intel C++ compiler** (works on Windows, Linux and Mac).
- ▶ General ideas about vectorization however are not vendor specific.

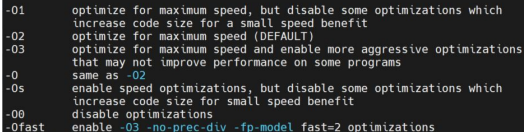
# Auto-Vectorization: Example 1

- ▶ Let's add two vectors:

```
int main()
{
    const int N = 8;
    int a[N] = {1, 2, 3, 4, 5, 6, 7, 8};
    int b[N] = {1, 2, 3, 4, 5, 6, 7, 8};
    int c[N];

    for (int i = 0; i < N; ++i)
        c[i] = a[i] + b[i];
}
```

- ▶ Intel compiler supports following optimizations:

A screenshot of a terminal window showing various Intel compiler optimization flags and their descriptions. The flags are listed on the left, and their descriptions are on the right.

```
-O1      optimize for maximum speed, but disable some optimizations which
         increase code size for a small speed benefit
-O2      optimize for maximum speed (DEFAULT)
-O3      optimize for maximum speed and enable more aggressive optimizations
         that may not improve performance on some programs
-O       same as -O2
-Os      enable speed optimizations, but disable some optimizations which
         increase code size for small speed benefit
-O0      disable optimizations
-Ofast   enable -O3 -no-prec-div -fp-model fast=2 optimizations
```

- ▶ Use help for all available options:  
`icc -help`

- ▶ Compiler is expected to auto-vectorize if optimization level 2 (O2) or higher is used.
- ▶ Will not vectorize if O1 or lower is used.
- ▶ Using O2:  
`icc -O2 example1.cpp -o example1`
- ▶ Is the loop above auto vectorized?



# Vectorization Report

- ▶ A *vectorization-report* shows what loops were vectorized and explains why any loop was not vectorized. To generate a vectorization report:
- ▶ On Linux:

`-qopt-report[=n]`

Generates an optimization report. Default destination is `<target>.optrpt`. Levels of 0 - 5 are valid.

# Vectorization Report

- ▶ Each level provides different amount of information:
  - ▶ n=1: Loops successfully vectorized
  - ▶ n=2: Loops not vectorized; and the reason why not
  - ▶ n=3: Adds dependency information
  - ▶ n=4: Reports only non-vectorized loops
  - ▶ n=5: Reports only non-vectorized loops and adds dependency info
- ▶ The report file has the .REP extension on Windows and .optrpt on Linux.
- ▶ Additionally, we use the following to limit the output to vectorization only as the reports are generally lengthy and difficult to understand at first (you should experiment with and without this flag):  
`-qopt-report-phase=vec`

- ▶ Let's create a vectorization report:  
`icc -qopt-report=1 -O2 example1.cpp -o example1`
- ▶ In the report (example1.optrpt) we see that this loop is vectorized:

```
LOOP BEGIN at example1.cpp(9,2)
    remark #15300: LOOP WAS VECTORIZED
LOOP END
```

- ▶ Let's build the same program with optimizations disabled:  
`icc -qopt-report=1 -O0 example1.cpp -o example1`
- ▶ The loop is not vectorized.
- ▶ Works as advertised.

## Auto-Vectorization: Example 2

- Here's another example<sup>2</sup>:

```
int main()
{
    int sum = 0;
    for (int row = 0; row < ROWS; ++row)
    {
        for (int col = 0; col < COLS; ++col)
        {
            data[row][col] = row + col;
        }
    }
    for (int row = 0; row < ROWS; ++row)
    {
        for (int col = 0; col < COLS; ++col)
        {
            sum += data[row][col] + data[col][row];
        }
    }
}
```

---

<sup>2</sup>This example uses some arbitrary operations on a matrix, just for illustration.

- ▶ We have several (for) loops now.

```
icc -qopt-report=1 -O2 example2.cpp -o example2
```

- ▶ First inner loop is vectorized, but the second inner loop is not vectorized.

```
LOOP BEGIN at example2.cpp(13,7)
    remark #15300: LOOP WAS VECTORIZED
LOOP END
```

```
LOOP BEGIN at example2.cpp(21,7)
    remark #15335: loop was not vectorized:
LOOP END
```

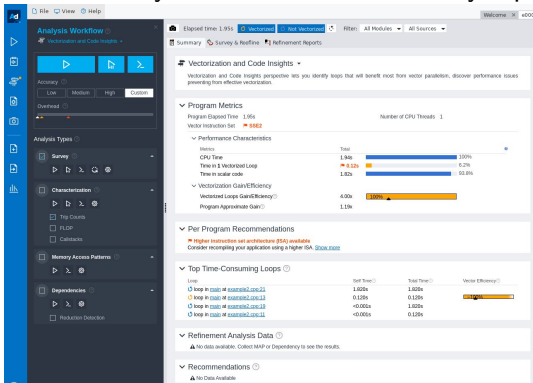
# Intel Advisor

- ▶ Intel toolkit has many features to write performance sensitive code.
- ▶ Intel Advisor helps identify under optimized loops related info.
- ▶ Let's use Advisor to analyse Example 2 above.

## Using Intel Advisor on Midway

- ▶ Load the modules:  
`module use /software/intel/oneapi_hpc_2022.1/modulefiles`  
`module load advisor/2022.0.0`
- ▶ Copy L2Demo.tar from /projects/finm32950/chanaka/ directory and untar (uncompress it).
- ▶ Change directory to L2Demo/advisor directory:  
`cd L2Demo/advisor`
- ▶ Build:  
`make`
- ▶ Collect survey data:  
`advisor --collect=survey --project-dir=. ./example2`
- ▶ Generate survey report:  
`advisor --report=survey --project-dir=.`
- ▶ Examine report:  
`advisor-gui ./`
- ▶ Use "Show Results" to see the results.

► Use summary tab to view the summary report:





## ► Use survey and roofline tab to get details:

The screenshot shows the Visual Studio Code interface with the Analysis Workflow pane on the left and the Performance tab on the right. The Performance tab displays a table of performance metrics for various functions and loops, including CPU Time, Total Time, Self Time, and Type. The table is filtered by 'All Sources' and 'All Threads'. The 'Why No Vectorized?' column shows reasons for non-vectorization, such as 'Scalar loop with instructions that use SIMD registers. Not vectorized; inner loop was unrolled by 4' and 'Scalar loop. Outer loop was not auto-vectorized; consider using SIMD directive'.

Function	Call Sites and Loops	Performance Issues	CPU Time	Total Time	Self Time	Type	Why No Vectorized?
at example2.cpp:13			1.820s	1.820s	0.000s	Scalar	vectorization
at example2.cpp:13			0.020s	0.020s	0.000s	Vectorized (Body)	
			1.840s	0.000s	0.000s	Function	
			1.840s	0.000s	0.000s	Function	

Source: example2.cpp:13 main

Line	Source	Total Time	%	Loop/Function Time
7	int main()			
8	{			
9	int sum = 0;			
10	for (int row = 0; row < ROWS; ++row)			
11	{			
12	loop in main at example2.cpp:11			
13	Scalar loop with instructions that use SIMD registers. Not vectorized; inner loop was unrolled by 4.			
14	No loop transformations applied.			
15	for (int col = 0; col < COLS; ++col)			
16	{			
17	loop in main at example2.cpp:13			
18	Vectorized body loop processor (int32 data type).			
19	Loop was unrolled by 4.			
20	{			
21	data[row][col] = row + col;			
22	}			
23	}			
24	for (int row = 0; row < ROWS; ++row)			
25	{			
26	loop in main at example2.cpp:11			
27	Scalar loop. Outer loop was not auto-vectorized; consider using SIMD directive.			
28	No loop transformations applied.			
29	{			
30	for (int col = 0; col < COLS; ++col)			
31	{			
32	loop in main at example2.cpp:13			
33	Scalar loop. Not vectorized; vectorization possible but seems insufficient. Inner loop was unrolled by 3.			
34	}			
35	}			
36	}			
37	}			

Selected Total Time: 0s

## Barriers to Vectorization

## Example 3

- ▶ Let's look at this example:

```
#include <cstdlib>

int main()
{
    const int N = 8;
    float a[N], b[N], c[N];

    for (int i=0; i<N; ++i)
    {
        a[i] = rand() % 100;
        b[i] = rand() % 100;
    }

    for (int i = 0; i < N; ++i)
        c[i] = a[i] + b[i];
}
```

- ▶ We have 2 for loops. Will the compiler vectorize them?

- ▶ Let's compile this (O2 is default; we don't need to type it):

```
icc -qopt-report=1 example3.cpp
```

- ▶ Vectorization report:

```
LOOP BEGIN at example3.cpp(8,2)
    remark #25436: completely unrolled by 8
LOOP END
```

```
LOOP BEGIN at example3.cpp(14,2)
    remark #15300: LOOP WAS VECTORIZED
LOOP END
```

- ▶ Let's compile this again to find out why the first loop is not vectorized:

```
icc -qopt-report=2 example3.cpp
```

- ▶ Vectorization report:

```
LOOP BEGIN at example3.cpp(8,2)
```

```
    remark #15344: loop was not vectorized: vector  
    dependence prevents vectorization.
```

```
    First dependence is shown below. Use level 5 report  
    for details
```

```
LOOP BEGIN at example3.cpp(14,2)
```

```
    remark #15300: LOOP WAS VECTORIZED
```

```
LOOP END
```

- ▶ Now, the vectorization-report to guides us (and, compiling this again):

```
icc -qopt-report=5 example3.cpp
```

- ▶ Vectorization report:

```
LOOP BEGIN at example3.cpp(8,2)
    remark #15382: vectorization support: call to function
    rand() cannot be vectorized    [ example3.cpp(10,10) ]
```

- ▶ This loop is not vectorized because we are using rand() which doesn't support vectorization.

## Example 4

- ▶ Another example of a loop that's not auto-vectorized:

```
for (int i = 0; i < N; ++i)
    if(i>3) c[i] = a[i] + b[i] + c[i-1];
```

- ▶ This loop won't be auto vectorized:

```
remark #15344: loop was not vectorized: vector dependence
prevents vectorization.
```

- ▶ Why?

- ▶ Let's unroll this loop to see what's going on:

```
c[0] = a[0] + b[0];  
c[1] = a[1] + b[1];  
.....  
c[4] = a[4] + b[4] + c[3];  
c[5] = a[5] + b[5] + c[4];  
.....
```

- ▶ We cannot calculate  $c[4]$  and beyond in parallel due to dependency to other elements.
- ▶ This data dependence prevents vectorization.



## Example 5

- ▶ Let's look at this example, which is similar to Black Scholes pricer where we are passing several arrays to a function:

```
void add(float *a, float *b, float *c,  
        float *d, float *e, int N)  
{  
    for (int i=0; i<n; ++i)  
        a[i] = b[i] + c[i] + d[i] + e[i];  
  
}
```

- ▶ Having many pointers may make it difficult for the compiler to figure out any dependence.
- ▶ Compiler may not know if the pointers are pointing to aliased memory.
- ▶ We have a data dependency problem if elements are overlapped.

- ▶ You may see a vectorization report similar to what's shown below, where one entry indicates the loop is vectorized:

```
LOOP BEGIN at example4.cpp(7,5)
<Multiversiomed v1>
    remark #25228: Loop multiversiomed for Data Dependence
    remark #15300: LOOP WAS VECTORIZED
LOOP END
```

- ▶ And, another entry indicates the same loop is not vectorized:

```
LOOP BEGIN at example4.cpp(7,5)
<Multiversiomed v2>
    remark #25436: completely unrolled by 8
LOOP END
```

- ▶ We have 2 versions for the same loop. What's going on?

# Multiversions and Unrolling Loops

- ▶ Compiler may generate two versions (a vectorized version and a non-vectorized version) when it is not sure if vectorization is safe.
- ▶ Sometimes a compiler may unroll a loop instead of vectorizing it.
- ▶ Run time uses most appropriate one (i.e. vectorization is not guaranteed) so this is not ideal.

## Example 6

- ▶ Loop count should remain constant during the execution of the loop for auto vectorization.

```
while (i<N)
{
    a[i] = a[i] * b[i];

    if (a[i] < 2) break;

    ++i;
}
```

remark #15520: loop was not vectorized: loop with multiple exits cannot be vectorized

- ▶ A loop must have a single entry and a single exit (entire loop must run) for auto vectorization.

# Reading Vectorization Reports

- ▶ Examples above show some (not all) common vectorization reports.
- ▶ We can use them to learn how read and understand vectorization reports.
- ▶ You may see similar types of reports for other applications.

## Improving Vectorization

- ▶ We saw some cases where auto vectorization is not used/possible.
- ▶ Shown below are some techniques to improve vectorization in such cases:
  1. Using vectorized implementations (e.g. SVMML)
  2. Compiler directives
  3. Writing code to support vectorization



# 1. Using vectorized implementations - Short Vector Math Library (SVML)

- ▶ A loop is not vectorized if a non vectorizable function is used in a loop.
- ▶ One solution is to use vectorized implementations of such functions.
- ▶ *Intel Short Vector Math Library* library provides vectorized implementations for some functions:

```
void test(float* a, float* b, int n)
{
    for (int i=0; i<n; ++i)
    {
        a[i] = sinf(b[i]);
    }
}
```

- ▶ A loop that uses vectorized functions will be auto vectorized.

- ▶ Support for vectorized implementations in the SVML include:  
sin, cos, tan, asin, acos, atan, log, log2, log10, exp, exp2,  
sinh, cosh, tanh, asinh, acosh, atanh, erf, erfc, erfinv, sqrt,  
cbrt, trunc, round, ceil, floor, fabs, fmin, fmax, pow, atan2
- ▶ Reference:  
<https://www.intel.com/content/www/us/en/docs/cpp-compiler/developer-guide-reference/2021-8/intrinsics-for-short-vector-math-library-ops.html>

## 2. Compiler Directives

- ▶ The compiler uses a static analysis to determine if vectorization safe (i.e produce correct results).
  - ▶ Won't vectorize any code unless it can guarantee correctness.
  - ▶ May ignore vectorization even when vectorization is possible due to ambiguity.
- ▶ Compilers provides directives so the programmer can guide/force vectorization when we (the programmer) know it is safe to vectorize such code.
- ▶ A guidance usually applies to a localized area (e.g. a function, a loop).

- ▶ The Intel C++ supports following pragma directives to help vectorization:
  - ▶ simd: instructs the compiler to enforce vectorization
  - ▶ ivdep: instructs the compiler to ignore assumed vector dependencies (guidance to the compiler)
  - ▶ vector always: force vectorization when "vectorization possible but seems inefficient"
- ▶ Related:
  - ▶ novector: tells the compiler not to vectorize a loop
  - ▶ unroll: unroll a loop
  - ▶ nounroll: don't unroll a loop
- ▶ Ref: <https://www.intel.com/content/www/us/en/docs/cpp-compiler/developer-guide-reference/2021-8/pragmas.html>
- ▶ We will discuss openmp directives next week.

## Example 4 (cont..): simd Keyword

- Compiler generated two versions in this case, due to pointer aliasing (Example 4). We can force vectorization if we know pointer aliasing is not an issue in our application:

```
void add(float *a, float *b, float *c,  
        float *d, float *e, int n)  
{  
    #pragma simd  
    for (int i=0; i<n; i++)  
        a[i] = b[i] + c[i] + d[i] + e[i];  
}
```

## Example 4 (cont..): ivdep Keyword

- Or, we could use:

```
void add(float *a, float *b, float *c,  
        float *d, float *e, int n)  
{  
    #pragma ivdep  
    for (int i=0; i<n; i++)  
        a[i] = b[i] + c[i] + d[i] + e[i];  
}
```

## Example 2 (cont.): vector Keyword

- Compiler generated two versions for the second inner loop earlier (Example 2):

```
for (int row = 0; row < ROWS; ++row)
{
    for (int col = 0; col < COLS; ++col)
    {
        data[row][col] = row + col;
    }
}

for (int row = 0; row < ROWS; ++row)
{
    #pragma vector always
    for (int col = 0; col < COLS; ++col)
    {
        sum += data[row][col] + data[col][row];
    }
}
```

- Both inner loops are vectorized now.

### 3. Writing Code to Support Vectorization

► Following guidelines may improve auto vectorization:

1. Simplify loops. Avoid multiple exits and complex loop termination conditions.
2. Avoid data dependance in loops:

- E.g.: Move the first and/or the last iterations out of the loop to remove dependencies (known as loop peeling).

Before

```
for (int i=0; i<10; ++i)
{
    a[i] = b[i] + a[0];
}
```

After

```
a[0] = b[0] + a[0];
for (int i=1; i<10; ++i)
{
    a[i] = b[i] + a[0];
}
```

3. Avoid mixing types in the same loop.
4. ...



# Unrolling Loops

- ▶ We cannot vectorize every loop. Unrolling can be helpful when vectorization is not possible.
- ▶ Loops is an important control structure that allow us to write concise and readable code.
- ▶ Unrolling is a technique used to optimize a loop by minimizing the cost of loop overhead:
  - ▶ Evaluate termination condition.
  - ▶ Update loop counter/counters.
- ▶ Unroll directives allow us to write code using loops but unroll them at compile time.

- ▶ Suppose we have a loop:

```
for (int i=0; i<4; ++i)
{
    a[i] = b[i] + c[i];
}
```

- ▶ Fully unrolling it:

```
a[0] = b[0] + c[0];
a[1] = b[1] + c[1];
a[2] = b[2] + c[2];
a[3] = b[3] + c[3];
```

- ▶ Unrolling by a factor of two:

```
for (int i=0; i<4; i+=2)
{
    a[i] = b[i] + c[i];
    a[i+1] = b[i+1] + c[i+1];
}
```

- ▶ Code is executed sequentially – not as efficient as vectorization.
- ▶ Performance improvements depend on the unrolling factor and the best factor can only be determined through measurements (discussed last week).

# Vectorization: Usage

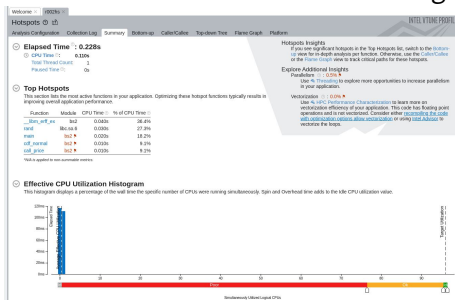
- ▶ Many popular libraries use vectorization to optimize operations:
  1. Eigen: [http://eigen.tuxfamily.org/index.php?title=Main\\_Page](http://eigen.tuxfamily.org/index.php?title=Main_Page)
  2. RapidJSON: <https://github.com/Tencent/rapidjson>
  3. NumPy: [https://www.pythonlikeyoumeanit.com/Module3\\_IntroducingNumpy/VectorizedOperations.html#](https://www.pythonlikeyoumeanit.com/Module3_IntroducingNumpy/VectorizedOperations.html#)

## Remarks

- ▶ Vectorization is important.
- ▶ We discussed 2 ways to introduce vectorization:
  1. Using processor intrinsic functions
  2. Compiler auto vectorization
- ▶ Every application is different. There are no hard and fast rules that guarantee auto-vectorization.
- ▶ Recommendations/techniques described above may increase the success rate.

## Using Multicore Nodes

- ▶ Let's go back to the report from vtune last time and focus on the *Effective CPU Utilization Histogram* section.



- ▶ We have over 90 CPU cores but we just use one.
- ▶ How do we use more than one CPU cores?

## Parallel Programming - Introduction

# Parallel Programming

- ▶ One obvious way get things done faster is to do more than one task simultaneously (in parallel):
  - ▶ This idea has been around for a long time.
  - ▶ It has become a very important topic now.
- ▶ We've seen vectorization parallelism already, and it works within one CPU core, giving us parallelism at the instruction level.
- ▶ Our next topic is parallelism using multithreading, allowing us to use many CPU cores.

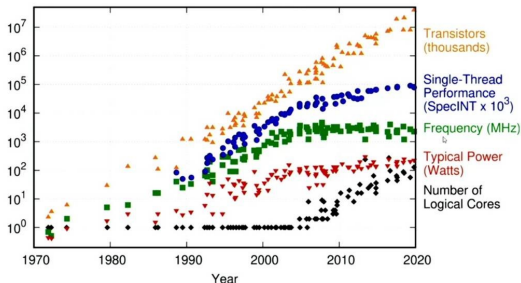


# Moore's Law

- ▶ Let's first try to understand why parallel programming using multi cores is needed.
- ▶ Moore's law says: every two years computing power doubles.
- ▶ Graphs below confirm that, but only upto about 2010. <sup>3</sup>

## 50 Years of Technology Scaling

48 Years of Microprocessor Trend Data



<sup>3</sup>source:<https://www.datacenterknowledge.com/supercomputers/after-moore-s-law-how-will-we-know-how-much-faster-computers-can-go>

- ▶ Frequency has hit a limit due to hardware limitations (due to leakage currents in transistors).
- ▶ Single thread performance is still improving mainly due to vectorization.
- ▶ Trend now is to have more and more CPU cores.
  - ▶ Achieve same performance or better.
  - ▶ Less power consumption and heat generation.

# Learning Parallel Programming

- ▶ New challenge for us (programmers):
  - ▶ We should know how to use multicores.
  - ▶ Otherwise, we are wasting a lot of computing power.
  - ▶ Learning how to write sequential code is not enough anymore.
- ▶ Parallel computing is not a highly-specialized/exotic topic anymore; it is something every programmer should know.

# Parallel Computing: Example 1

- ▶ Suppose we want to add two arrays (vectors):

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} + \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix}$$

- ▶ We can write a simple for loop:

```
for (int i=0; i<N; ++i)
    c[i] = a[i] + b[i];
```

- ▶ This loop adds two values and assign it to  $c[i]$  for each  $i$  in  $N$ .
- ▶ Usually when we think about programs (thus far), we think about doing things sequentially:
  - ▶ Use one data item from each array
  - ▶ Executing one instruction at a time
- ▶ Each addition is independent of the others (i.e.  $c[0]$  doesn't depend on  $c[1]$  and so on) – we can compute them in parallel.

## Parallel Computing: Example 2

- ▶ Matrix multiplication is another example:

$$A_{I,K} B_{K,J} = C_{I,J} \quad c_{i,j} = \sum_{k=0}^{K-1} a_{i,k} b_{k,j} \quad \text{where } 0 \leq i < I \text{ and } 0 \leq j < J$$

$$\begin{pmatrix} a_{0,0} & a_{0,1} & \dots & a_{0,k-1} \\ a_{1,0} & a_{1,1} & \dots & a_{1,k-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i-1,0} & a_{i-1,1} & \dots & a_{i-1,k-1} \end{pmatrix} \begin{pmatrix} b_{0,0} & b_{0,1} & \dots & b_{0,j-1} \\ b_{1,0} & b_{1,1} & \dots & b_{1,j-1} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k-1,0} & b_{k-1,1} & \dots & b_{k-1,j-1} \end{pmatrix} \\ = \begin{pmatrix} c_{0,0} & c_{0,1} & \dots & c_{0,j-1} \\ c_{1,0} & c_{1,1} & \dots & c_{1,j-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{i-1,0} & c_{i-1,1} & \dots & c_{i-1,j-1} \end{pmatrix}$$

- ▶ Each element  $c_{i,j}$  is independent of others – we can compute them in parallel.

# Natural Parallelism

- ▶ Many applications in real life exhibit natural parallelism - vector addition and matrix multiplication are two examples.
- ▶ Our goal in this course is to identify and use natural parallelism to speed up program executions.
- ▶ We will explore 3 *technologies*:
  1. Vectorization ✓
  2. Multicore
  3. GPGPU
- ▶ FPGA is another interesting technology but we won't have time to discuss that topic.

# Multithreading

# Threads

- ▶ To use more than one core (multi cores), we break up a program into smaller *tasks*.
- ▶ We use *threads* to execute these tasks on different cores.
- ▶ This is generally known as multithreading.
- ▶ Our next topic is to explore how to use threads to do work in parallel.
- ▶ First, let's look at some important concepts about using threads.



## Using Threads: Example 1

- ▶ Let's extend our familiar *Hello World* example to use a thread to perform a task.
- ▶ Task in this case is to write the greeting message to console.

```
#include <iostream>
#include <thread>

void Greeting()
{
    std::cout << "Hello, World" << std::endl;
}

int main()
{
    std::thread t(Greeting);

    t.join();
}
```

To build, on midway:

```
icc helloworld.cpp -o helloworld -lpthread
```

# Hello World Example

- ▶ To create a thread, we use `std::thread`.
- ▶ The `std::thread` constructor takes a function as an argument.
- ▶ Thread execution begins in this function.
- ▶ Once the new thread is started, we have two threads in the program:
  1. main thread
  2. new thread (t)
- ▶ We use `join()` to make sure the calling thread (main) waits until new thread (t) finishes its execution.
- ▶ Thread is defined in `<thread>`  
<http://www.cplusplus.com/reference/thread/thread/>

# Thread Join and Detach

- ▶ Once a thread is created:
  - ▶ calling thread waits until the new thread completes its execution: use `join()`
  - ▶ calling thread continues execution without waiting for the new thread: use `detach()`

# How Many Threads

- ▶ We can create a large number of threads in a program.
- ▶ How many threads can run in parallel depends on the number of cores/cpus.
- ▶ If we create a large number of threads, every thread may not run in parallel.
- ▶ The OS uses a scheduling algorithm to run the threads.

Detour: Lambdas (C++)

# Lambdas

- ▶ We saw the `std::thread` constructor takes a function as an argument.
- ▶ There are other ways to pass an initial function to a thread:
  - ▶ using a lambda
  - ▶ using a function object

# Lambda: Syntax

- ▶ The example below shows a very simple lambda which writes a message to console:

```
[] (string s)
{
    cout << s << endl;
}
```

- ▶ [] is called the capture clause; a lambda is always introduced by the capture clause.
- ▶ () parenthesis allows us to pass optional arguments to a lambda.
- ▶ {} lambda body is enclosed by the {} brackets.

# Creating a Thread

- ▶ We can pass a lambda to a thread:

```
std::thread t([]()  
{  
    cout << "Hello, World" << endl;  
});  
  
t.join();
```



## Lambda Syntax: Captures

- ▶ Lambdas allow us to *capture* parameters by value, or by reference.
- ▶ You can use *everything* notation to capture. In this case the compiler captures what's needed (used inside the body) by the lambda.
- ▶ [=] captures everything by value – allows reads but no write access.
- ▶ [&] captures everything by reference – allows read and write access.
- ▶ [=, &x] captures everything by value except x; x is captured by reference.
- ▶ [&, x] captures everything by reference except x; x is captured by value.

## Using Threads: Example 2

► Matrix multiplication:

$$A_{I,K} B_{K,J} = C_{I,J} \quad c_{i,j} = \sum_{k=0}^{K-1} a_{i,k} b_{k,j} \quad \text{where } 0 \leq i < I \text{ and } 0 \leq j < J$$

$$\begin{pmatrix} a_{0,0} & a_{0,1} & \dots & a_{0,k-1} \\ a_{1,0} & a_{1,1} & \dots & a_{1,k-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i-1,0} & a_{i-1,1} & \dots & a_{i-1,k-1} \end{pmatrix} \begin{pmatrix} b_{0,0} & b_{0,1} & \dots & b_{0,j-1} \\ b_{1,0} & b_{1,1} & \dots & b_{1,j-1} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k-1,0} & b_{k-1,1} & \dots & b_{k-1,j-1} \end{pmatrix} \\ = \begin{pmatrix} c_{0,0} & c_{0,1} & \dots & c_{0,j-1} \\ c_{1,0} & c_{1,1} & \dots & c_{1,j-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{i-1,0} & c_{i-1,1} & \dots & c_{i-1,j-1} \end{pmatrix}$$

- We can write a serial program:

```
void matrix_multiply(const matrix& m1, const matrix& m2,
    matrix& m3, int rows, int columns)
{
    for (int i = 0; i < rows; ++i)
    {
        for (int j = 0; j < columns; ++j)
        {
            m3[i][j] = 0;
            for (int k = 0; k < rows; ++k)
            {
                m3[i][j] += m1[i][k]*m2[k][j];
            }
        }
    }
}
```

- Inputs (m1 and m2) are passed by const reference.
- Output (m3) passed by reference.

- ▶ This is a naturally parallel program - each  $c_{i,j}$  can be computed in parallel.
- ▶ We can parallelize it in many different ways:
  - ▶ one thread to calculate each element  $c_{i,j}$  – we need numRows \* numColumn number of threads
  - ▶ one thread for one row – we need numRows number of threads
  - ▶ one thread for one column – we need numColumn number of threads
- ▶ Which choice is better?

► Suppose we use one thread for each element:

```
void multiply_matrix(const matrix& m1, const matrix& m2,
    matrix& m3, int rows, int columns)
{
    vector<thread> threads(rows*columns);

    for (int i = 0; i < rows; ++i)
    {
        for (int j = 0; j < columns; ++j)
        {
            int idx = i*columns + j;
            threads[idx] = thread(&m3[i][j], m1, m2);
            {
                m3[i][j] = 0;
                for (int k = 0; k < columns; ++k)
                {
                    m3[i][j] += m1[i][k] * m2[k][j];
                }
            }
        }
    }

    for (thread& t : threads)
    {
        t.join();
    }
}
```

- Or, we can to use one thread for one row:

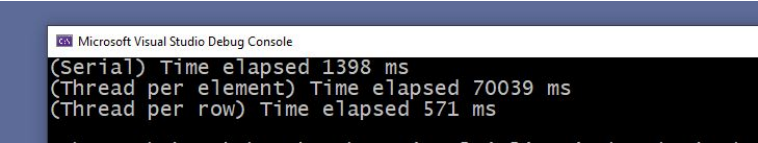
```
void multiply_matrix(const matrix& m1, const matrix& m2,
    matrix& m3, int rows, int columns)
{
    vector<thread> threads(rows);

    for (int i = 0; i < rows; ++i)
    {
        threads[i] = thread([=,&m3]()
        {
            for (int j = 0; j < columns; ++j)
            {
                m3[i][j] = 0;
                for (int k = 0; k < rows; ++k)
                {
                    m3[i][j] += m1[i][k] * m2[k][j];
                }
            }
        });
    }

    for (thread& t : threads)
    {
        t.join();
    }
}
```

- ▶ Note: This program does not use any special features of Intel compiler (i.e. you may use Visual C++ or any other compiler).
- ▶ We have 3 implementations now:
  1. sequential work – one thread (i.e. main thread) computes all elements
  2. one thread computes one element
  3. one thread computes one row
- ▶ Which program/programs will run faster?

- ▶ Let's run these programs and measure time.
- ▶ Results depend on the system and the matrix sizes etc.
- ▶ Shown below is what I saw for one case (see demo for code) on my laptop:



```
Microsoft Visual Studio Debug Console  
(Serial) Time elapsed 1398 ms  
(Thread per element) Time elapsed 70039 ms  
(Thread per row) Time elapsed 571 ms
```



# Observations

- ▶ Threads allow us to gain performance.
- ▶ More threads doesn't necessarily mean better performance.  
Why?
- ▶ When we create more threads than what we can run in parallel, we create overhead.
- ▶ When we use threads we have to pay attention to the overhead.

# Sharing Data

- ▶ All threads share same data.
- ▶ Multiple threads can read data at the same time (e.g., matrix multiplication above).
- ▶ Can more than one thread write to the same data at the the same time?
- ▶ Can one thread write while another one reads the same data?
- ▶ To answer these questions, let's look at an example.

## Threads: Example 3

- Let's look at the code snippet below:

```
unsigned long counter = 0;

int numThreads = 10;
vector<thread> threads(numThreads);

for (int j = 0; j < numThreads; ++j)
{
    threads[j] = thread([&counter]()
    {
        for (int i = 0; i < 100000; ++i)
        {
            counter++;
        }
    });
}

for (auto& t : threads) t.join();

cout << counter;
```

► To build and run (on Midway):

1. Get a compute node with 8 CPU cores

```
sinteractive --time=0:30:0 --cpus-per-task=8 --account=finm32950
```

2. Build:

```
icc counter.cpp -o counter -lpthread
```

3. Run:

```
./counter
```

► What's the value of counter?

## Counter Example: Possible Scenario 1

- ▶ Suppose we have two threads t1 and t2 running in parallel:
  - ▶ t1 reads the value of counter, counter is 0
  - ▶ t2 reads the value of counter, counter is 0
  - ▶ t1 increments it, counter is 1
  - ▶ t2 increments it, counter is 1
  - ▶ after 2 increments, the value of counter is 1
- ▶ When we use threads, we should expect threads to interleave read and modify operations as shown below:

t1	t2
-----	-----
registerA = counter	registerB = counter
counter = registerA + 1	counter = registerB + 1

v (time/clock-cycle)

- ▶ In this case, the counter will be incremented only once after two add operations.

## Counter Example: Possible Scenario 2

- ▶ Suppose we have two threads t1 and t2 running in parallel:
  - ▶ t1 reads the value of counter, counter is 0
  - ▶ t1 increments it, counter is 1
  - ▶ t2 reads the value of counter, counter is 1
  - ▶ t2 increments it, counter is 2
  - ▶ after 2 increments the value of counter is 2

t1

----

registerA = counter

counter = registerA + 1

t2

----

registerB = counter

counter = registerB + 1

- ▶ In this case, the counter will be incremented twice (correctly) after two add operations.

# Race Conditions

- ▶ If two (or more) threads write to the same shared data, the result depends on the order in which the threads ran.
- ▶ This problem (bug) is known as a *race condition*.
- ▶ How do we avoid race conditions?

## Critical Region

- ▶ The counter is a shared variable in our example.
- ▶ Incrementing (modifying) it by two or more threads at the same time leads to a race condition.
- ▶ The part where shared resource is accessed is known as the critical section/region

```
for (int j = 0; j < numThreads; ++j)
{
    threads[j] = thread([&counter]()
    {
        for (int i = 0; i < 100000; ++i)
        {
            counter++;
        }
    });
}
```

- ▶ Only one thread *should* execute the code in the critical section at a time – known as mutual exclusion.



# Using a Lock

- ▶ One way to achieve mutual exclusion is to use a lock to protect shared data.
- ▶ We can use a lock known as mutex (*mutual exclusion*).
- ▶ To protect shared data using a mutex involves:
  - ▶ lock the mutex before shared data is accessed
  - ▶ unlock the mutex after shared data is accessed
- ▶ Only one thread can lock the mutex at a time.
- ▶ Everyone else has to wait until the thread holding the mutex releases it.
- ▶ <http://en.cppreference.com/w/cpp/thread/mutex>

- ▶ We can re-write the counter example using a mutex:

```
for (int j = 0; j < numThreads; ++j)
{
    threads[j] = thread([&]()
    {
        for (int i = 0; i<100000; ++i)
        {
            count_mutex.lock();
            counter++;
            count_mutex.unlock();
        }
    });
}
```

- ▶ We are guarding the critical region using a mutex.
- ▶ Race condition is avoided.

# Deadlocks

- ▶ What happens if we lock a mutex and forget to unlock it?
- ▶ No thread will be able to access the shared resource again.
- ▶ This will lead to a problem, known as a *deadlock*.
- ▶ Deadlocks can happen due to exceptions:

```
mutex.lock();  
  
critical_region; //can throw an exception  
  
mutex.unlock();
```

## std::lock\_guard

- ▶ The `std::lock_guard` class implements the RAI technique<sup>4</sup> for a mutex:
  - ▶ locks the mutex when the `lock_guard` object is constructed (in the constructor)
  - ▶ unlocks the mutex when the `lock_guard` object is destroyed (in the destructor)
- ▶ `std::lock_guard`:
  - ▶ prevents errors due to forgetting to release a lock
  - ▶ guarantees exception safety
- ▶ Defined in `<mutex>`

---

<sup>4</sup>discussed in winter course

- ▶ The code snippet below shows how to lock a piece of shared data using a `std::mutex` using this technique.

```
unsigned long count = 0;
std::mutex count_mutex;

int numThreads = 10;
vector<thread> threads(numThreads);

for (int j = 0; j < numThreads; ++j)
{
    threads[j] = thread([&]()
    {
        for (int i = 0; i<100000; ++i)
        {
            std::lock_guard<std::mutex> guard(count_mutex);
            count++;
        }
    });
}
```

# Atomics

- ▶ Another way to handle critical regions is to use atomic operations.
- ▶ Atomic operations are performed as one (all or none) operation so the other threads see the operation as a single operation.
- ▶ Atomic operations do not require us to use locks – no need to worry about locking related issues.
- ▶ Number of atomic operations are limited – to handle complicated critical regions we still need to use locks.
- ▶ Atomic types are defined in atomic header (<http://en.cppreference.com/w/cpp/header/atomic>).

- We can write the counter example using atomics as follows:

```
atomic<unsigned long> counter;  
counter = 0;  
  
for (int j = 0; j < numThreads; ++j)  
{  
    threads[j] = thread([&]()  
    {  
        for (int i = 0; i<100000; ++i)  
        {  
            counter++;  
        }  
    }));  
}
```