

Behind the scenes perspective: Into the abyss of profiling for performance

Part II

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IT-DI WLCG-UP

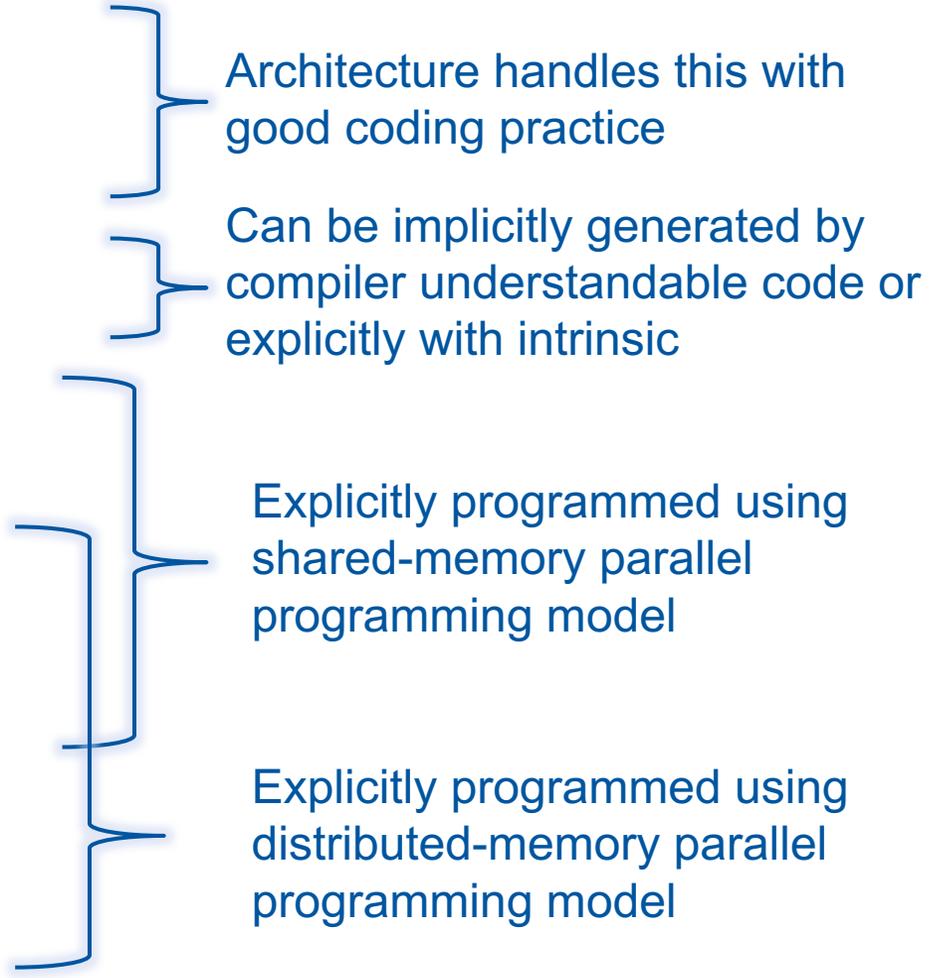
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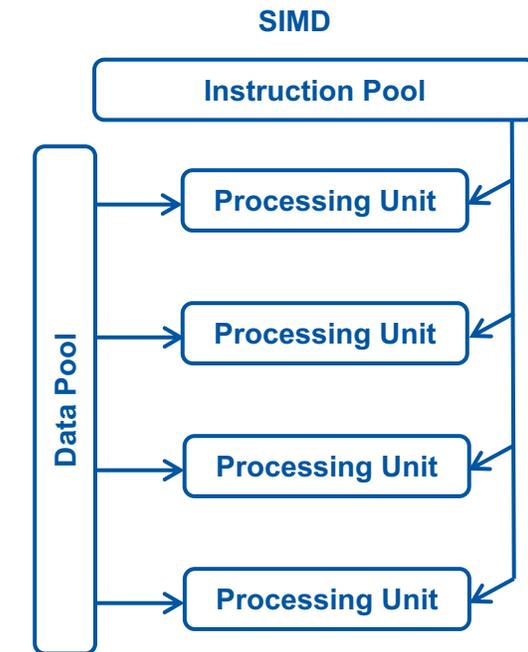
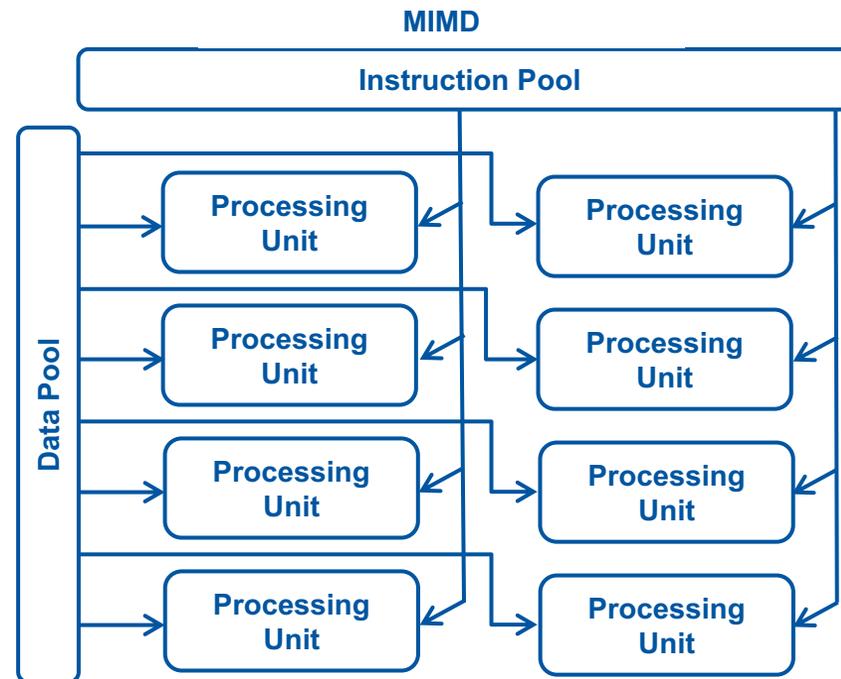
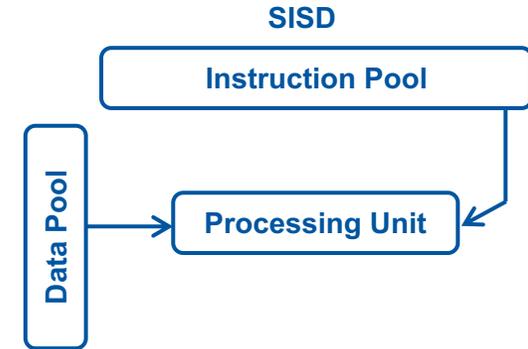
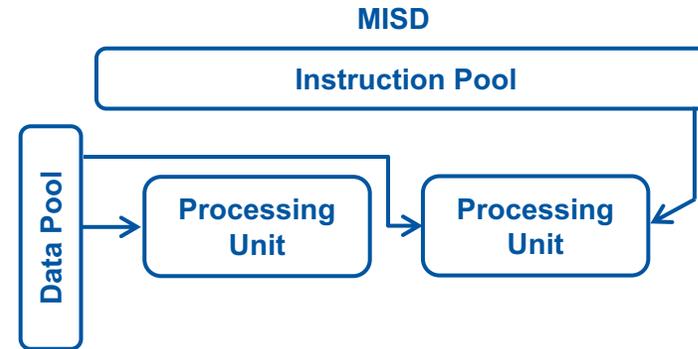
Sources of Parallelism in Modern Architectures

- 1. Instruction level parallelism (ILP)
- 2. Pipelining
- 3. Vector Operations
- 4. Hardware Threads
- 5. Multicore
- 6. Multi Socket
- 7. Cluster
- 8. Grid



Flynn's taxonomy: Can be a programmer's guideline

- ❑ Proposed in 1966
- ❑ Instruction streams
 - single (SI) or multiple (MI)
- ❑ Data streams
 - single (SD) or multiple (MD)
- ❑ Types
 - SISD
 - SIMD
 - MISD
 - MIMD



Using SIMD

- ❑ Choose between code manageability and portability and speed:
- ❑ Use different levels of abstraction
 - Assembly
 - Intrinsic
 - Wrapper functions or classes in C or C++ (using intrinsics)
 - Custom languages like Cilk/Cilk++
 - Autovectorization

SIMD: SSE, AVX & FMA

- The use of SIMD instructions in **vectorized** code can give good performance gains

(S)SSE 1,2,3

From 1999
Width 128b

SSE 4.1, 4.2

From 2007
Width 128b

AVX

From 2011
Width 256b

AVX2 + FMA

From 2013
Width 256b

AVX-512

From 2016
Width 512b

- 256b -> 8 floats or 4 doubles (possibility of 4 or 8 speedup)

Fused Multiply Add

- These are instructions which can do calculations of the form:

$$A \leftarrow A * C + B \text{ or}$$

$$A \leftarrow B * C + A$$

- Can bring gain because one instructions replaces a multiply and add instruction (reduces throughput cycles and latency)
- Is also a SIMD instruction

FMA and floating point

- ❑ FMA is specified to round only once
 - Therefore FMA is a change which can affect the result of a calculation compared to using separate multiply and add operations
- ❑ Enable with:
- ❑ GCC:
 - Will use FMA if it is compiling for an architecture that has it
 - May be explicitly set with `-mfma` or `-mno-fma`

Autovectorization

- ❑ Depends on compiler and version
- ❑ Advantages
 - Can get great speedups (x2 or more) with little change of the source code
 - Compiler can generate a report to help
 - Source code remains architecture independent
- ❑ Disadvantages
 - Can be delicate. A small change of the source can stop the compiler autovectorizing, causing a large change in performance
 - Lots of compiler options that affect the autovectorization
 - Usually you could have bigger gains using intrinsics or assembly
 - Some compiler options which help autovectorization can change the way FP operations are done: you have to be aware when that may be important

Autovectorization

- ❑ Two main places where automatic vectorization can be done
 - In loops
 - compiler tries to do several iterations of the loop at once using SIMD
 - May unroll a number of the loops so to fill pipeline and improve ILP
 - May peel loops to allow aligned access to data
 - Combining similar independent instructions into vector instructions
 - Known as SLP vectorizer

Autovectorization difficulties

```
for(i=0;i<*p;++i) {  
    A[i] = B[i] * C[i];  
    sum += A[i];  
}
```

(example from slide by Georg Zitzlsberger, Intel)

Possible to vectorize? Concerns may be:

- Is the loop range invariant during the loop
- Is A[] aliased with the other arrays or with sum, is sum aliased with B[] or C[]
- **Is the + operator associative?**
- Is the vectorized version expected to be faster?

Using autovectorization

□ GCC:

- Switch on using `-ftree-vectorize`
 - Off by default
- Information on autovecotization analysis
 - using `-ftree-vectorizer-verbose=X` (X=0-7, 7 is most information)
 - Or examine generated code with `gdb`
- May be necessary to use `-ffast-math`
 - Often with reductions (e.g. summations)
 - This will cause the compiler to relax certain some constrains, for example allow it to assume associative properties

□ ICC:

- On by default, modify with `-x` and `-ax`
 - Would switch off by using `-no-vec`
- ICC defaults to ignoring parentheses to specify floating point associativity and generally can make more aggressive optimizations on floating point calculations
 - Controlled by `-fprotect-parens` and `-fp-model`
- Information on autovectorization analysis
 - `-qopt-report=2 -qopt-report-phase=vec`
 - `-opt-report-help` and `-opt-report-phase={hpo,ipo}`
 - Or examine with `gdb...`

FP caution

- E.g. summing a number of values: One technique to reduce rounding error over long sums is Kahan summation

```
double sum = 0.0, C = 0.0, Y, T;
size_t i;
/* Kahan summation of values in A[i] */
for (i=0; i<length; i++) {
    Y = a[i] - C;
    T = sum + Y;
    C = (T-sum) - Y;
    sum = T;
}
```

- If the compiler reasons $C=0$ the correction is lost. Perhaps pairwise summation could be used instead.

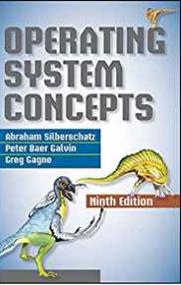
SoA vs AoS

- ❑ It is better to load the contents of a vector register from a contiguous piece of memory rather than gather the values
- ❑ Can arrange that the data layout fits this access pattern. e.g. use of **S**tructure of **A**rrays instead of **A**rray of **S**tructures. e.g.

```
struct point {  
    double x,y,z;  
} location[1000];
```

```
struct points {  
    double x[1000];  
    double y[1000];  
    double z[1000];  
} locations;
```

Software processes & threads



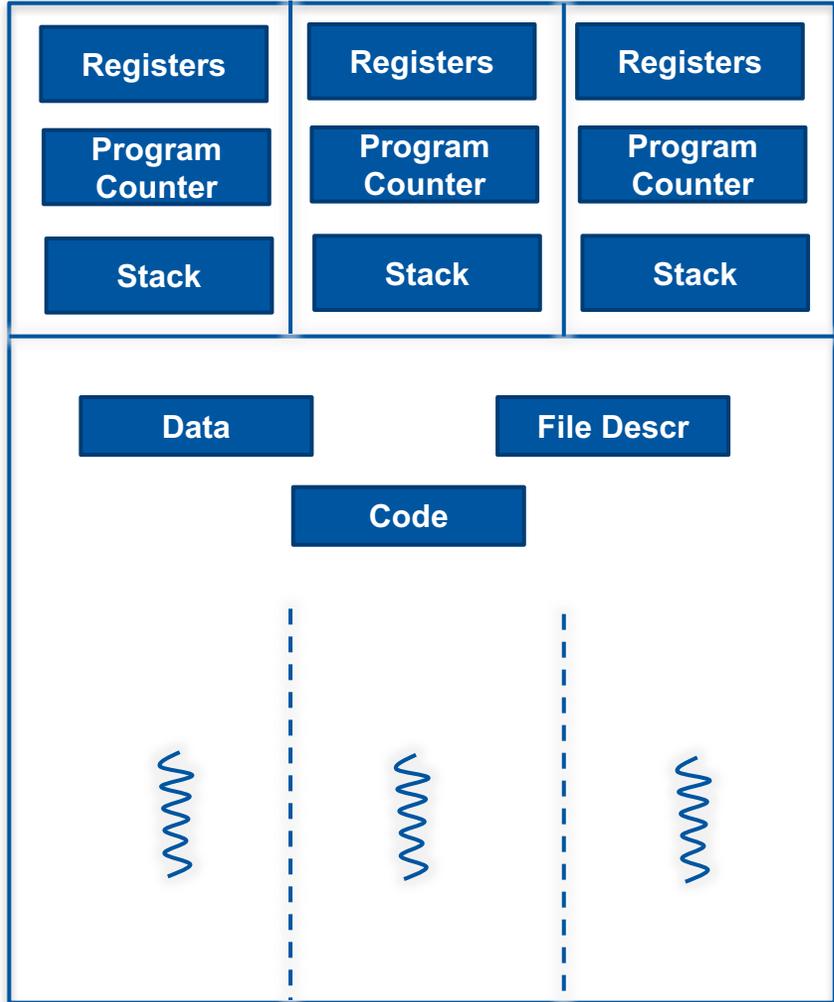
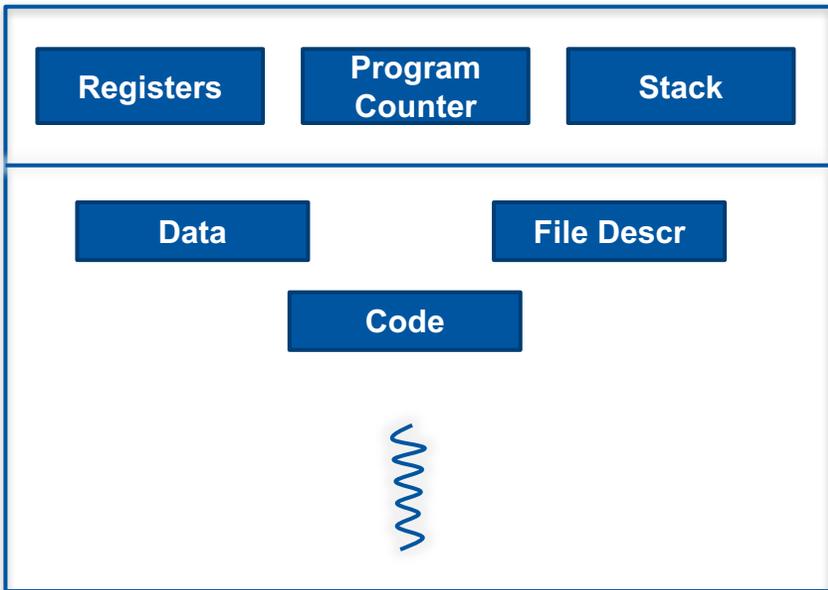
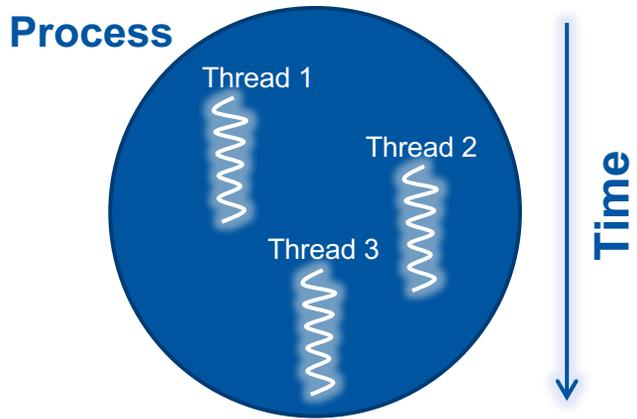
□ Process (OS process):

- Encapsulated entity of a program running in its own private address space
- It consists of a private copy of program code and data along with file descriptors and permissions
- It has a dedicated heap and stack space from which data is accessed and modified.

□ Thread

- Lightweight execution context that runs under a process
- They share address space, program code and operating system resource of their parent process
- Can be created and destroyed with low overhead in comparison to that of a process
- Consists of a small amount of thread local storage space

Processes & threads



Parallel computing

- ❑ Performing certain computations simultaneously using multiple resources
- ❑ **Amdahl's law & Gustafson's law**
 - Speedup only comes from the parallelizable part of the code
 - i.e. Serial part of the code will impact or limit the achievable performance

Amdahl's law
$$S_{\text{latency}}(s) = \frac{1}{(1 - p) + \frac{p}{s}}$$

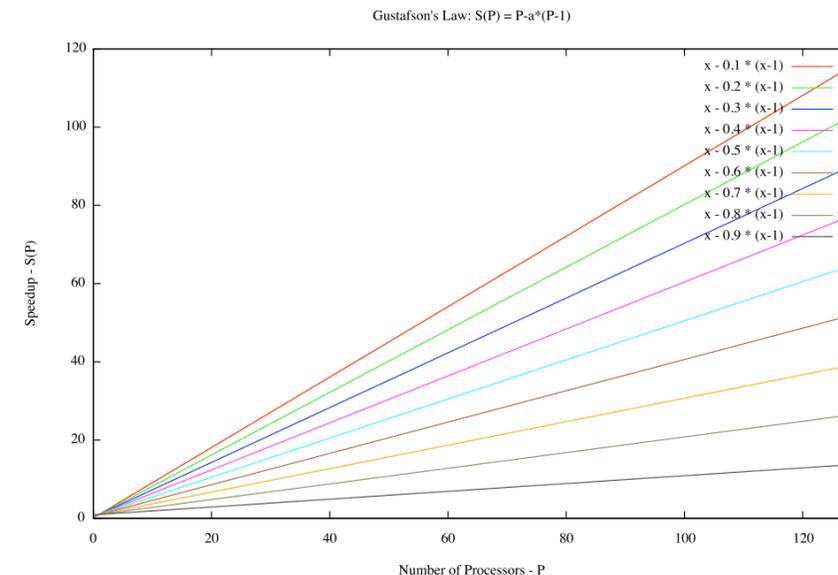
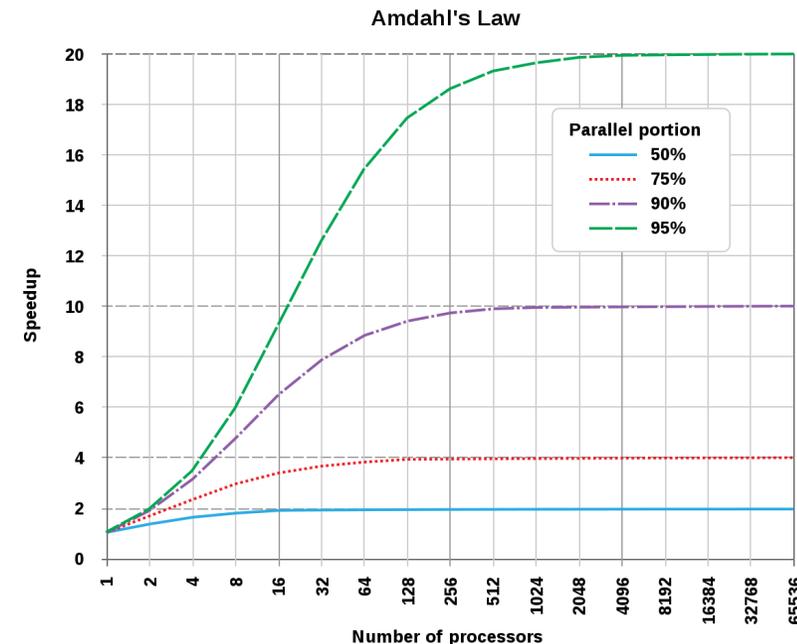
Gustafson's law
$$S_{\text{latency}}(s) = 1 - p + sp,$$

Where,

S_{latency} is the theoretical overall speedup

s is the speedup in the parallel part

p is the percentage of the execution time of serial part



Parallel Programming

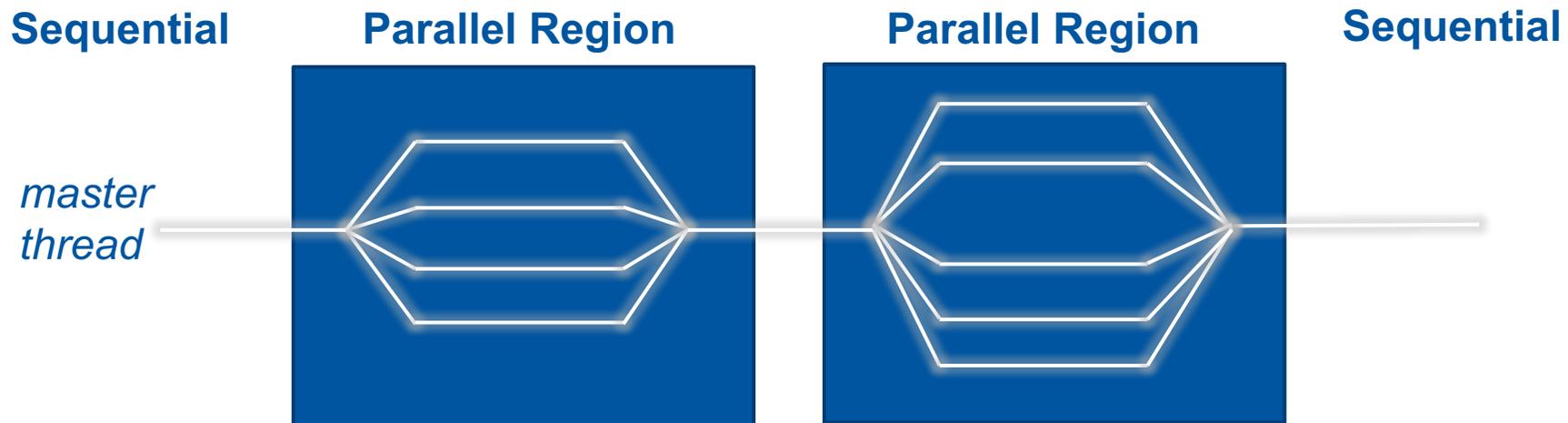
- Is a large topic. Many tools and techniques, a few:
 - pthreads is a standard API for managing threads
 - Fundamental API for threading in Linux
 - Cilk Plus
 - Language support by compiler extensions: appears as C/C++ with extensions
 - TBB (threading building blocks from Intel)
 - C++ large use of templates
 - commercial binary distribution with support or open source
 - C++11 threads
 - CUDA and OpenCL
 - GPU or CPU/GPU unified programming models
 - **OpenMP**
 - <http://concurrency.web.cern.ch/GaudiHive>
 - A framework from the HEP community

OpenMP

- ❑ A specification:
 - See <https://www.openmp.org>
 - Are compiler directives, routines and variables that can be used to specify high-level **parallelism** in C, C++ and Fortran
- ❑ GCC
 - 4.4 – OpenMP 3.0
 - 4.9 – OpenMP 4.0
 - 6.1 – OpenMP 4.5
- ❑ Clang
 - 3.7 – OpenMP 3.1
- ❑ Intel
 - 12 – OpenMP 3.1
 - 16 – OpenMP 4.0
 - 17 – OpenMP 4.5

OpenMP

- ❑ Code looks similar to a serial version
 - #pragma are used to indicate handling of parallel parts
 - Usually uses a fork-join model



OpenMP

- ❑ May need to compile with `-fopenmp` (check your compiler)
- ❑ Most OpenMP features are used through pragmas

```
#pragma omp construct [clause [clause] ... ]
```

- ❑ You can change the number of threads via environment or an API or specify it in the pragma

```
export OMP_NUM_THREADS=16
```

Parallel regions

- ❑ Threads (up to the number configured) are created, if needed, when the pragma is crossed
- ❑ Threads execute the parallel region, the sequential part continues once all the threads have come to the end of the region
- ❑ Data is shared, but stack variables declared in the parallel region are private

```
#pragma omp parallel
{
    function_called_in_parallel();
}
function_sequential();
```

Parallel for-loops

- ❑ Loop iterations become threads
- ❑ Data is shared between threads (i.e. iterations), except loop index
- ❑ Threads wait at the end of the for loop
- ❑ The pragma is specified directly before the loop

```
#pragma omp parallel
{
    #pragma omp for
    for (i=0;i < N; i++) {
        function(i);
    }
}
```

- ❑ The two pragmas above are equivalent to
`#pragma omp parallel for`

Sharing control

□ Consider

```
double x, y;  
#pragma omp parallel for  
for(i=0;i<N;i++) {  
    x = a[i]*4;  
    y = b[i] * b[i];  
    b[i] = x/y;  
}
```

- This will probably not give the intended result: x and y are shared between the threads of the parallel for loop

The private clause

- ❑ Used to give each thread a private copy of a variable which was already declared outside
- ❑ The variable is uninitialized

```
double x, y;  
#pragma omp parallel for private(x,y)  
for(i=0;i<N;i++) {  
    x = a[i]*4;  
    y = b[i] * b[i];  
    b[i] = x/y;  
}
```

Variations on sharing control

□ As well as *private*:

- *firstprivate*: initializes each private copy to the value from the master thread
- *lastprivate*: copies the value from the thread, which executed the last iteration of the loop, to the master thread
- *shared*: is the default, but for documentation or if the default is changed you can use this clause
- Plus others, e.g. those which concern `threadprivate` variables

Reductions

- ❑ Reductions will implicitly produce a local copy of the reduction variable in each thread
- ❑ Each thread updates its copy
- ❑ At the end of the construction the reduction operation merges sub-results into a single value and puts it in the reduction variable
- ❑ Operations: + * - ^ & | && || min max

```
#pragma omp for reduction(op:var)
```



Reduction example

```
double dotprod=0;
#pragma omp parallel for reduction(+:dotprod)
for(i=0;i<N;i++) {
    dotprod += a[i] * b[i];
}
```

Exercise 4 – Use SIMD in the matrix multiplication

- ❑ Starting with the blocked version of the matrix multiplication see if autovectorization has an effect
 - The Makefile already has the matrixmul-simd target.
 - Autovectorization may work or might need a small change
 - Compare the execution time to a similar multiplication not using autovectorization
 - See if you have SIMD instructions (you may use Intel SDE, see next slide)
 - Check the compiler report if it didn't work

Intel SDE

- Is the software development emulator
 - In this case we can use it to count and classify different types of instructions

```
export PATH=/home/gss2018/exercises/sde-external-8.16.0-2018-01-30-lin:$PATH
sde -iform 1 -omix test.out -top_blocks 5000 -- ./my_executable
```

- Look in test.out for lines ending in `_1`, `_2` or `_4` representing scalar or packed operations, e.g.

```
cat test.out | egrep '^\\*.*_[124]'
```

Exercise 5 - OpenMP

- Use OpenMP to make the matrix multiplication from the previous exercise use multiple threads
 - Set `OMP_NUM_THREADS=6, 12, 24, 36` and then 48
 - Run a multiplication and use `top` to look at the running process. Note that `%CPU` should be $>100\%$.
 - Compare the runtime each time and
 - Use `perf` to measure the instructions and cycles; vary the number of threads and note how each changes

