Performance Analysis and Optimization

Parallel Programming

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Outline

Motivation

- Parallel programming is used to increase application performance
  - Parallel applications use multiple cores or even machines
  - Using more resources also increases runtime costs
  - Make sure that resources are used as efficiently as possible
- Parallel computers are complex
  - Measuring performance is not always straightforward
  - Estimating potential performance is even harder

Motivation...

- There are several goals for performance optimization
  1. Minimizing runtime
     - Allows getting the results as fast as possible
     - Typically the most important factor for users
  2. Maximizing throughput
     - Executes as many jobs as possible within a given time
     - Does not necessarily say anything about performance
  3. Maximizing utilization
     - Makes the best use of investment for resources
     - Does not necessarily match the above goals
- Performance measurements are necessary to check goals
  - Measure, assess and optimize

Approaches

- When doing performance optimization, there is a loop:
  1. Conduct performance measurements
     - Running the application, measuring time etc.
  2. Check if performance is satisfactory
     - Might not have anything to do with actual utilization
     - Should also check whether performance is already optimal
  3. Speculate about the reason for the performance problems
     - Measurements can point you in the right direction
  4. Fix performance problems
     - You might actually fix something else (or nothing at all)
- This is more or less "debugging for performance"

Approaches…

- There are two major approaches for performance measurements
  1. Offline approaches
     - Record metrics at runtime, write them to storage
     - Analyze performance afterwards
  2. Online approaches
     - Record metrics at runtime, forward them to a tool
     - Analyze performance at runtime
- In practice, the approaches we use are a mix of both

Offline Approaches

- Benefits
  - Metrics are available for multiple analyses
    - You might want to look at different metrics etc.
  - Allows easily comparing multiple runs
- Drawbacks
  - Typically constant overhead for collecting metrics
  - There is often not an easy way to refine collection
    - If you notice a performance hotspot, you have to rerun the application
  - Metrics can get quite large
    - Up to gigabytes or even terabytes for large applications

Online Approaches

- Benefits
  - Allows adapting collected metrics and thus overhead
  - Easy to switch collection on and off
    - Possible to collect performance metrics in production runs
- Drawbacks
  - Typically not possible to analyze performance afterwards
    - Collected metrics are transient and lost after the application finishes
  - Requires a separate tool that can process online metrics
    - This also makes the whole approach more complex

Outline

Measurements

- It is difficult to measure performance correctly
  - There are many factors and components to consider
  - Random errors can influence results significantly
  - Systematic errors can invalidate all results
- Measuring performance is a complex process
  - Performance is influenced by caching, network, I/O etc.
  - Which components are involved and have to be measured?
  - Which performance can we expect on a given system?

Measurements. . .

- Optimization requires deep knowledge of the hardware
  - How do the different levels of caches interact?
  - Can we reach the main memory from all cores with the same speed?
  - How does our application behave with more cores?
- There are also technical issues to take into account
  - HPC applications are typically run via a batch scheduler
  - Operating system services can influence performance

Measurements…

- Our goal is to collect metrics quantitatively
    - Metrics include runtime, throughput, latency and more
    - The metrics to collect depend on the software and hardware
- Published measurements should be scientifically sound
    - Other scientists should be able to reproduce your findings
    - Measurements of metrics have errors that have to be accounted for
- Results always vary slightly even for the same configuration

Quiz

- Application A runs for 4.274 s, application B for 4.176 s. Which one is faster?
  1. Application A
  2. Application B
  3. Difference is negligible, performance is the same
  4. Not enough information

- Application A runs for 4.274 s, application B for 4.176 s. Which one is faster?
    1. Application A
    2. Application B
    3. Difference is negligible, performance is the same
    4. Not enough information ✔

- Single measurements are more or less random
    - Processor might be busy with something else
    - Some other application is currently occupying the network
    - There is a certain variability for each component
- It is never enough to do a single measurement
    - Always repeat measurements at least three times
    - If you talk to physicists, they will probably say 30 times
- Averaging the metrics is also not enough
    - There are important derived metrics, such as standard deviation etc.

Measurements…

```
Benchmark #1: ./sincos-O2
Time (mean +- sig):    4.192 s +-   0.033 s    [User: 4.181 s, System: 0.001 s]
Range (min .. max):    4.160 s ..   4.274 s    10 runs

Benchmark #2: ./sincos-O3
Time (mean +- sig):    4.191 s +-   0.016 s    [User: 4.179 s, System: 0.001 s]
Range (min .. max):    4.176 s ..   4.221 s    10 runs

Summary
'./sincos-O3' ran
    1.00 +- 0.01 times faster than './sincos-O2'
```

- Application A and B have the same performance
  - Both previous results were extreme values (minimum and maximum)

- There are two kinds of errors
    1. Random errors
        - Cancel out after infinite measurements
        - Might be caused by operating system activity in the background
        - Performance of most hardware varies a bit
        - Larger variations are also possible due to hardware defects, load balancing etc.
    2. Systematic errors
        - These errors do not cancel out with more measurements
        - They are caused by wrong methodology/implementation
        - For instance, you want to measure disk speed but measure the cache

Measurements. . .

- Always use a well-defined hardware/software environment
  - Document the setup, including version numbers etc.
- Minimize external influence to keep random errors low
  - Use resources exclusively if possible
  - For example, do not run anything in the background
- Increase measurement time and repeat measurements
  - This helps canceling out random errors
- Compare results with expected performance
  - "My application finishes in two hours. Could it finish in one?"
  - This typically involves some kind of performance modeling

Measurements…

- Twelve Ways to Fool the Masses When Giving Performance Results on Parallel Computers by David Bailey [Bailey, 1991]

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11. "Measure parallel run times on a dedicated system, but measure conventional run times in a busy environment."

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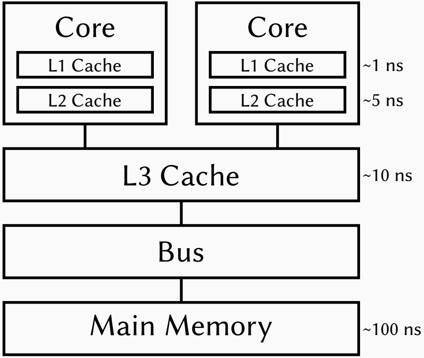
9. "Quote performance in terms of processor utilization, parallel speedups or MFLOPS per dollar."
11. "Measure parallel run times on a dedicated system, but measure conventional run times in a busy environment."
12. "If all else fails, show pretty pictures and animated videos, and don't talk about performance."

Metrics

- The simplest performance metric: Wall-clock time (or real time)
  - Measure how long the application runs
- There are different kinds of times
  - CPU time denotes the time the processor spent running the application
    - Can be lower or higher than wall-clock time
    - Lower: Two applications share a core, that is, each gets 50 % of CPU time
    - Higher: An application runs on ten cores for one hour, that is, for ten CPU hours
  - User time denotes the time spent in user mode
    - This counts normal calculations etc.
  - System time denotes the time spent in kernel mode
    - This counts system calls, such as I/O

Problems

- Numerous reasons for performance problems
- Inefficient access to resources
  - These are often caused by latencies
  - Data not available in fastest cache
  - Main memory is relatively slow
  - Indirect memory access
- Access conflicts on shared resources
  - Multiple applications want to access the bus
  - File systems are typically shared



Problems…

- Processor utilization is often not optimal
  - Sometimes only 1–10 % are used, especially for parallel applications
  - Parallel applications have communication and synchronization overhead
- Scientific software is often not well-optimized
  - Domain scientists are interested in scientific results, not optimizing software
  - Domain scientists often do not have a computer science background
  - Best case: Domain scientist + mathematician/physicist + computer scientist

Problems...

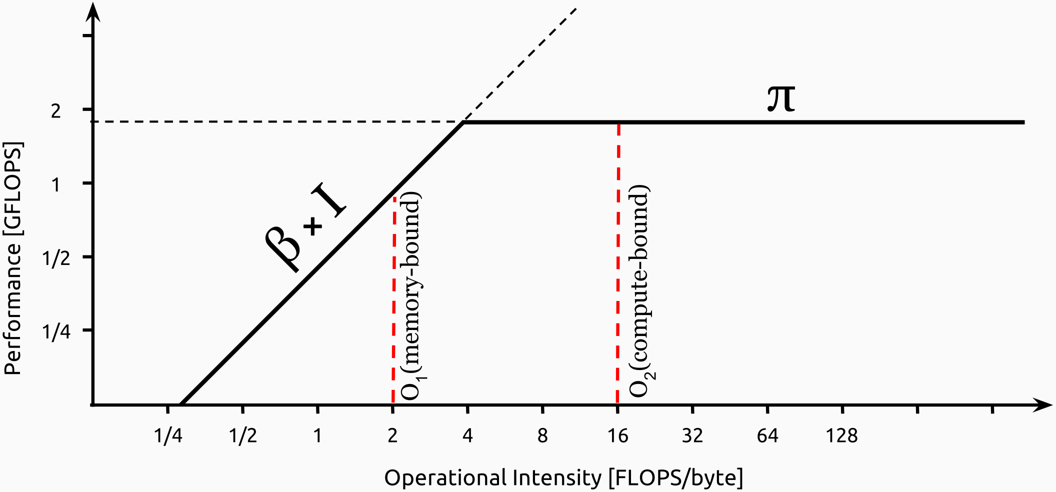
- Application-specific limitations
  - CPU-bound: Limited by processor
    - For instance, processor cannot do more floating point operations
    - Could be solved by increasing the clock rate or adding more floating point units
  - Memory-bound: Limited by memory
    - Data cannot be transferred from the main memory to the processor fast enough
    - Typically caused by not doing enough operations per transferred byte
  - I/O-bound: Limited by storage and/or network
    - Data cannot be transferred to/from storage fast enough
- Unrealistic performance gains, such as superlinear speedup
  - For instance, making the problem smaller allows it to fit into the cache

Approaches

- Theoretical
  - Determine time and memory complexity
  - Can be impractical for general applications
  - Helps to have at least a rough understanding of complexity
    - Get a feeling for potential runtime/memory consumption
- Practical
  - Measure time and memory consumption
  - Relatively easy to do with the right tools
- A combination of both approaches makes most sense

Roofline Model

- One way to assess performance is the so-called roofline model
    - Visual representation of performance limits in current architectures
    - Requires finding out peak memory throughput and computational performance
    - Application's operational intensity has to be determined
    - Can be extended using other factors important for performance
- The performance metric given most attention in HPC is FLOPS
    - FLOPS = Floating point operations per second
    - Different metrics are discussed since FLOPS are only one aspect



[Giu.natale, 2016]

Outline

Goals

- The overall goal is to optimize resource usage
  - This applies to all involved components
  - Processor, storage, network etc. require different approaches
- Resources are typically used exclusively in HPC
  - There are exceptions; for example, the file system is shared
  - Problems cannot be compensated by running additional applications
  - Users should make sure that they do not underutilize resources
- Also important for shared resources
  - Worst case: A single application can bring down performance for everyone
  - Applications should not overload the file system

Approaches

- We will focus on the computational performance for now
    - Moreover, we will mainly look at numerical applications

1. Optimize the mathematics and algorithms
    - Requires the most knowledge about the problem
    - Should rather be done by a domain scientist and/or mathematician
2. Optimize the code manually
    - Determine which data structures and algorithms are best suited
        - Vectorization can be a huge performance benefit
    - Take software and hardware characteristics into account
        - How much main memory is available? How does the compiler align/order data?
3. Optimize the code automatically
    - The compiler can take care of a lot of optimizations for us

Programming Languages

- The programming language can also have a huge influence on performance
  - In the end, use the language you are most comfortable with
  - Using a new language will not automatically make your application faster
- There is a wide range of programming languages to choose from
  - C, C++, Fortran, Python, Java, MATLAB etc.
- Some languages are better suited for specific problems
  - For example, good data science and machine learning support for Python

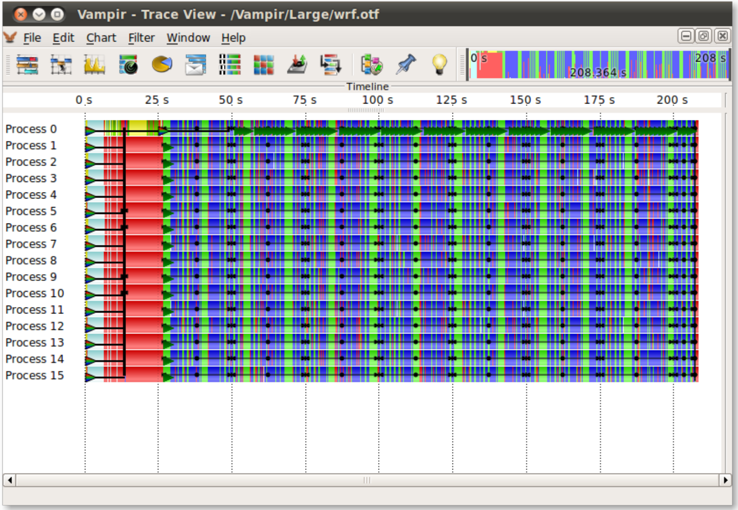
- C (which we will use in the lecture and exercises)
  - Allows low-level programming and direct access to the hardware
  - Requires you to take care of memory management yourself
  - Compilers are mature and produce efficient code
  - Most functionality like threading is supported
  - A lot of performance-critical libraries and framework are written in C
- C++
  - More or less the same benefits and drawbacks as C with a nicer syntax
  - More convenient memory management than C
- Fortran (from Formula Translation)
  - Easier to handle for non-computer scientists
  - Has a long history and is still updated frequently

Programming Languages...

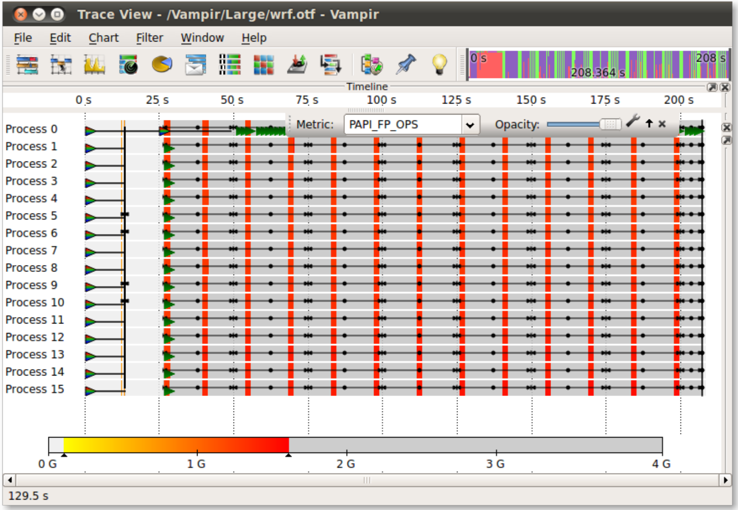
- Python
  - Very popular right now and has a huge community
  - Many modules are available, providing a lot of features
  - Standard version is interpreted and thus slow
    - There are a number of modules written in C for high performance
  - There is no easily usable threading support
- Java
  - Popular in industry, large community and many features
  - Byte code can be optimized at runtime

Tools

- Time measurement
  - `time` and `/usr/bin/time` are available everywhere
  - Can also be done manually using, for example, `clock_gettime`
- Profiling
  - `gprof` can be used to display application profiles
- Dedicated performance analysis
  - `perf` is part of the Linux kernel and features many dedicated metrics
- Graphical applications
  - Vampir is a commercial tool to display traces and profiles



[GWT-TUD GmbH, 2020]



[GWT-TUD GmbH, 2020]

- Simple numerical application
  - Nested loop with calculations
- Two complex operations
  - Plus two simple operations
- Performance expectations
  - sin and cos are expensive
  - Maximum is hard to judge

```c
int main (void) {
    double result = 0.0;
    for (int i = 0; i < 20000; i++) {
        for (int j = 0; j < 20000; j++) {
            result += sin(i) + cos(j);
        }
    }
    printf("result=%f\n", result);
    return 0;
}
```

```
$ time ./sincos
result=10120.671812
./sincos  8.88s user 0.00s system 99% cpu 8.896 total

$ /usr/bin/time ./sincos
result=10120.671812
8.88user 0.00system 0:08.89elapsed 99%CPU (... 2132maxresident)k
0inputs+0outputs (0major+78minor)pagefaults 0swaps
```

- `time` is a shell built-in
  - `/usr/bin/time` is a regular system tool
- Both show user, system and total time as well as processor utilization
  - `/usr/bin/time` also provides memory consumption etc.

- Profiling using gprof does not help in this case
  - Everything is contained in the `main` function
- Compile the application with the -pg flag
  - Running it will automatically produce a profile called `gmon.out`
- Most of the time is probably spent in `sin` and `cos`

```
$ gprof ./sincos
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  Ts/call  Ts/call  name
101.86      0.81     0.81                             main
```

```
$ perf stat ./sincos
result=10120.671812
 Performance counter stats for './sincos':
          9,016.15 msec task-clock:u              #    0.998 CPUs utilized
                 0      context-switches:u        #    0.000 K/sec
                 0      cpu-migrations:u          #    0.000 K/sec
                68      page-faults:u             #    0.008 K/sec
    37,667,245,120      cycles:u                  #    4.178 GHz
        46,473,927      stalled-cycles-frontend:u #    0.12% frontend cycles idle
    23,374,754,930      stalled-cycles-backend:u  #   62.06% backend cycles idle
    89,573,942,974      instructions:u            #    2.38  insn per cycle
                                                  #    0.26  stalled cycles per insn
    11,597,942,217      branches:u                # 1286.352 M/sec
        45,071,449      branch-misses:u           #    0.39% of all branches
       9.035267264 seconds time elapsed
       9.013823000 seconds user
       0.000000000 seconds sys
```

- `perf` shows a number of different performance metrics
  - Runtime is just one of them
- Context switches occur when talking to the kernel
  - They are relatively fast but should be taken into account
- CPU migrations can have negative influence on caching
  - Moving the application to another core or processor will invalidate caches
- Cycles and instructions show how much the processor had to do
  - Modern processors can do multiple instructions per cycle
- Branches can be bad for performance if there are many misses

Compilers

- Compilers can do a lot of optimizations for us
  - Can also be tuned for specific architectures
    - Takes instruction sets, number of registers etc. into account
- `-O0`
  - Default, no optimizations are performed
- `-O1`
  - Basic optimizations, compilation requires more time and memory
- `-O2`
  - More optimizations, often used as the “default” optimization
- `-O3`
  - Even more optimizations, including vectorization

- `-Og`
  - Optimize for debugging, some important passes are disabled at `-O0`
- `-Os`
  - Optimize for size, good for embedded systems with little storage
- `-Ofast`
  - Optimize by disregarding standards compliance, might influence results

- Inlining allows avoiding function calls (starting from -O1)
  - Function calls require putting arguments onto the stack
  - Afterwards, there are jumps into the function and back to the original location
- Loop unrolling (-O3)
  - Loops also require jumps, which can be negative for performance

```c
for (int i = 0; i < 3; i++) {
    a[i] += b[i];
}
```

→

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

- Vectorization can perform multiple operations at once (-O3)
  - Especially useful in combination with loop unrolling

- Which speedup can we get for our application with compiler optimizations alone?
    1. None
    2. Factor 10
    3. Factor 100
    4. Factor 1,000

```
$ perf stat ./sincos
result=10120.671812
 Performance counter stats for './sincos':
          9,016.15 msec task-clock:u
                 0      context-switches:u
                 0      cpu-migrations:u
                68      page-faults:u
    37,667,245,120      cycles:u
        46,473,927      stalled-frontend:u
    23,374,754,930      stalled-backend:u
    89,573,942,974      instructions:u

    11,597,942,217      branches:u
        45,071,449      branch-misses:u
       9.035267264 seconds time elapsed
       9.013823000 seconds user
       0.000000000 seconds sys
```

```
$ perf stat ./sincos-O3
result=10120.671812
 Performance counter stats for './sincos':
         4,278.80 msec task-clock:u
                0      context-switches:u
                0      cpu-migrations:u
               67      page-faults:u
   17,886,687,516      cycles:u
       19,370,964      stalled-frontend:u
   11,376,027,366      stalled-backend:u
   45,200,173,879      instructions:u

    6,000,368,555      branches:u
       19,211,736      branch-misses:u
      4.288728446 seconds time elapsed
      4.278149000 seconds user
      0.000000000 seconds sys
```

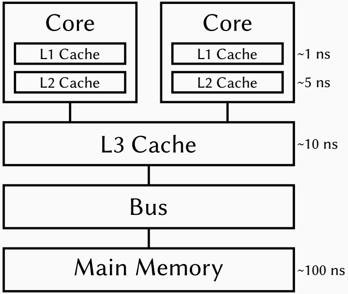
```
$ perf stat ./sincos
result=10120.671812
 Performance counter stats for './sincos':
         9,016.15 msec task-clock:u
                0      context-switches:u
                0      cpu-migrations:u
               68      page-faults:u
   37,667,245,120      cycles:u
       46,473,927      stalled-frontend:u
   23,374,754,930      stalled-backend:u
   89,573,942,974      instructions:u

   11,597,942,217      branches:u
       45,071,449      branch-misses:u
      9.035267264 seconds time elapsed
      9.013823000 seconds user
      0.000000000 seconds sys
```

Compilers...

- This time, `sincos` was compiled with `-O3`
  - Runtime was more than halved from 9 s to 4.3 s
  - Cycles, instructions and branches were roughly halved
  - Instructions per cycle went up slightly
- Teaser: `-Ofast` achieves a runtime of only 1.5 s
  - `-Ofast` also requires linking with `libmvec`, that is, uses vectorization
  - Optimizing for the architecture with `-march=native` gets it down to 0.5 s

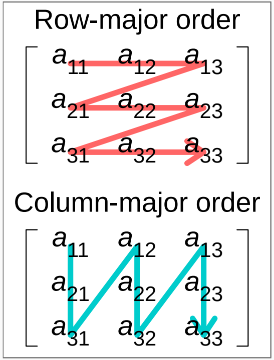
Memory Access

- Memory access and caches important for performance
  - Access to main memory takes approximately 100 ns
  - At 3 GHz (at least) 300 instructions in 100 ns
- Caches can help get data to the processor fast enough
  - Processors will speculatively load data into the cache
  - Typically assume spatial locality, that is, nearby memory will be accessed in the future
- Caches work well if you access data the right way
  - Jumping around randomly will destroy locality



Memory Access...

- Memory access depends on the programming language
  - C stores memory in row-major order
  - Fortran stores memory in column-major order
- Access in the wrong order will reduce performance
  - Has to be considered when porting code
- Combining programming languages can be problematic
  - For instance, using a C library from Fortran



[Cmglee, 2017]

Memory Access…

- C application with row-major matrix
  - Still potential performance problems
- Gray cells contain calculation values
  - Blue cells are loaded into cache
  - CPU-bound given enough math

1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50
51	52	53	54	55	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70
71	72	73	74	75	76	77	78	79	80
81	82	83	84	85	86	87	88	89	90
91	92	93	94	95	96	97	98	99	100

- C application with row-major matrix
  - Still potential performance problems
- Gray cells contain calculation values
  - Blue cells are loaded into cache
  - CPU-bound given enough math
- White cells are empty
  - Values are still loaded into cache
  - Memory-bound due to unused values
- Special data structures for efficient access to sparse matrices

1	2								
11	12	13							
	22	23	24						
		33	34	35					
			44	45	46				
				55	56	57			
					66	67	68		
						77	78	79	
							88	89	90
							99	100	

- Memory interleaving
  - Important for performance
- Array of structures
  - Intuitive representation
  - Potentially bad cache utilization

```c
struct coordinate
{
    double x;
    double y;
    double z;
};

int main (void) {
    struct coordinate e[N] = { 0 };
    double result = 0.0;
    for (int i = 0; i < N; i++)
    {
        result += e[i].x * e[i].y;
    }
    return 0;
}
```

Memory Access…

- Memory interleaving
  - Important for performance
- Array of structures
  - Intuitive representation
  - Potentially bad cache utilization
- Structure of arrays
  - Potentially better for vectorization

```
struct coordinates
{
    double x[N];
    double y[N];
    double z[N];
};

int main (void) {
    struct coordinates e = { 0 };
    double result = 0.0;
    for (int i = 0; i < N; i++)
    {
        result += e.x[i] * e.y[i];
    }
    return 0;
}
```

Outline

Summary

- There is a range of approaches and tools to find performance problems
  - Parallel computers and applications are complex
- Performance measurements require a thought-out approach
  - Single measurements can be more or less random
- Performance optimizations can be done on several levels
  - Code optimizations can be done manually or automatically
- Compilers often can take care of sophisticated optimizations
  - It is important to understand the compiler's capabilities

References

[Bailey, 1991] Bailey, D. (1991). **Twelve ways to fool the masses when giving performance results on parallel computers.** *Supercomputing Review*, pages 54–55.

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[GWT-TUD GmbH, 2020] GWT-TUD GmbH (2020). **Vampir.** `https://vampir.eu/`.

Approaches

- O(1)
  - Constant runtime/memory consumption
  - Example: Array access, hash tables
- O(n)
  - Linear runtime/memory consumption
  - Touch every data point once (or a few times)
  - Example: Calculating the sum of a list
- O(n^2)
  - Quadratic runtime/memory consumption
  - Example: (Bad) sorting algorithms

```
for (int i = 0; i < n; i++) {
    for (int j = 0; j < n; j++) {
        result += sin(i) + cos(j);
    }
}
```