

Performance Analysis and Optimization

Parallel Programming for Engineers

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Performance Analysis and Optimization

Introduction

Performance Analysis

Performance Optimization

Summary

- 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

- 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

- 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”

- 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

- 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

- 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

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- 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?

- 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

- 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

- 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.

```
1 Benchmark #1: ./sincos-02
2 Time (mean +- sig): 4.192 s +- 0.033 s [User: 4.181 s, System: 0.001 s]
3 Range (min .. max): 4.160 s .. 4.274 s 10 runs
4
5 Benchmark #2: ./sincos-03
6 Time (mean +- sig): 4.191 s +- 0.016 s [User: 4.179 s, System: 0.001 s]
7 Range (min .. max): 4.176 s .. 4.221 s 10 runs
8
9 Summary
10 './sincos-03' ran
11 1.00 +- 0.01 times faster than './sincos-02'
```

- 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

- 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

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

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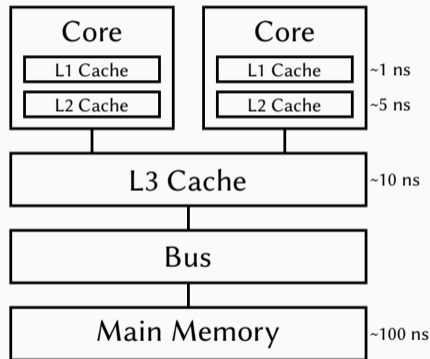
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 9. “Quote performance in terms of processor utilization, parallel speedups or MFLOPS per dollar.”
 11. “Measure parallel run times on a dedicated system, but measure conventional run times in a busy environment.”
 12. “If all else fails, show pretty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

- 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

- 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

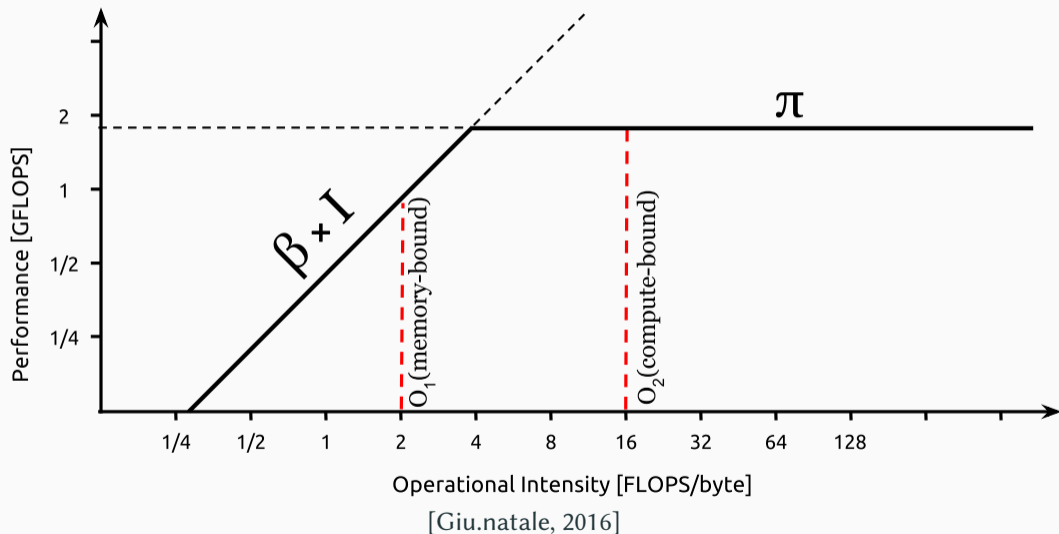


- Processor utilization is often not optimal
 - Sometimes only 1–10 % are used, especially for parallel applications
 - Parallel applications have communication and synchronization overhead
- Scientific software is often not well-optimized
 - Domain scientists are interested in scientific results, not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

- 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

- 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

- 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



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- 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

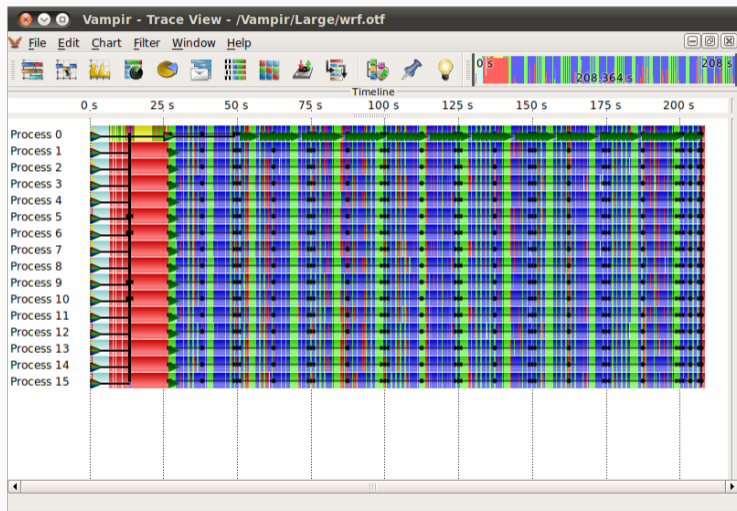
- We will focus on the computational performance for now
 - Moreover, we will mainly look at numerical applications
- 1. Optimize the mathematics and algorithms
 - Requires the most knowledge about the problem
 - Should rather be done by a domain scientist and/or mathematician
- 2. Optimize the code 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

- 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

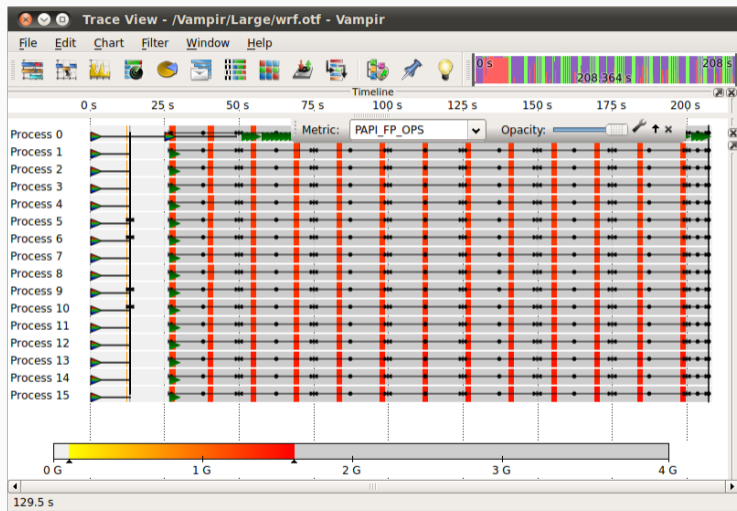
- C (which we will use in the lecture and exercises)
 - Allows low-level programming and direct access to the hardware
 - Requires you to take care of memory management yourself
 - Compilers are mature and produce efficient code
 - Most functionality like threading is supported
 - A lot of performance-critical 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

- 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

- 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

```
1 int main (void) {
2     double result = 0.0;
3     for (int i = 0; i < 20000; i++) {
4         for (int j = 0; j < 20000; j++) {
5             result += sin(i) + cos(j);
6         }
7     }
8     printf("result=%f\n", result);
9     return 0;
10 }
```

```
1 $ time ./sincos
2 result=10120.671812
3 ./sincos  8.88s user 0.00s system 99% cpu 8.896 total
4
5 $ /usr/bin/time ./sincos
6 result=10120.671812
7 8.88user 0.00system 0:08.89elapsed 99%CPU (... 2132maxresident)k
8 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`

```
1 $ gprof ./sincos
2 Flat profile:
3
4 Each sample counts as 0.01 seconds.
5 %   cumulative   self           self       total
6 time  seconds  seconds    calls  Ts/call  Ts/call  name
7 101.86      0.81      0.81
```

```
1 $ perf stat ./sincos
2 result=10120.671812
3 Performance counter stats for './sincos':
4      9,016.15 msec task-clock:u          #    0.998 CPUs utilized
5              0      context-switches:u    #    0.000 K/sec
6              0      cpu-migrations:u      #    0.000 K/sec
7              68     page-faults:u         #    0.008 K/sec
8      37,667,245,120 cycles:u             #    4.178 GHz
9      46,473,927     stalled-cycles-frontend:u #    0.12% frontend cycles idle
10     23,374,754,930 stalled-cycles-backend:u #   62.06% backend cycles idle
11     89,573,942,974 instructions:u        #    2.38 insn per cycle
12                                     #    0.26 stalled cycles per insn
13     11,597,942,217 branches:u            # 1286.352 M/sec
14     45,071,449     branch-misses:u       #    0.39% of all branches
15     9.035267264 seconds time elapsed
16     9.013823000 seconds user
17     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 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 -01)
 - Function calls require putting arguments onto the stack
 - Afterwards, there are jumps into the function and back to the original location
- Loop unrolling (-03)
 - Loops also require jumps, which can be negative for performance

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

→

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

- Vectorization can perform multiple operations at once (-03)
 - 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

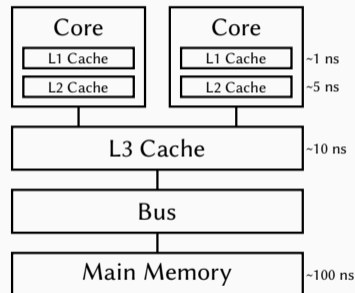
 11,597,942,217 branches:u
   45,071,449 branch-misses:u
   9.035267264 seconds time elapsed
   9.013823000 seconds user
   0.000000000 seconds sys
```

```
1 $ perf stat ./sincos-03
2 result=10120.671812
3 Performance counter stats for './sincos':
4      4,278.80 msec task-clock:u
5          0 context-switches:u
6          0 cpu-migrations:u
7          67 page-faults:u
8 17,886,687,516 cycles:u
9  19,370,964 stalled-frontend:u
10 11,376,027,366 stalled-backend:u
11 45,200,173,879 instructions:u
12
13 6,000,368,555 branches:u
14  19,211,736 branch-misses:u
15 4.288728446 seconds time elapsed
16 4.278149000 seconds user
17 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
12
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
```

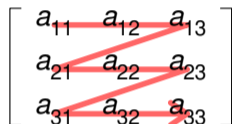
- This time, sincos was compiled with `-O3`
 - Runtime was more than halved from 9 s to 4.3 s
 - Cycles, instructions and branches were roughly halved
 - Instructions per cycle went up slightly
- Teaser: `-Ofast` achieves a runtime of only 1.5 s
 - `-Ofast` also requires linking with `libmvec`, that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

- Memory access 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

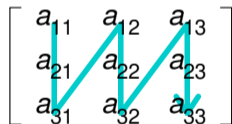


- Memory access depends on the programming language
 - C stores memory in row-major order
 - Fortran stores memory in column-major order
- Access in the wrong order will reduce performance
 - Has to be considered when porting code
- Combining programming languages can be problematic
 - For instance,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

Row-major order



Column-major order



[Cmglee, 2017]

- 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

```
1  struct coordinate
2  {
3      double x;
4      double y;
5      double z;
6  };
7
8  int main (void) {
9      struct coordinate e[N] = { 0 };
10     double result = 0.0;
11     for (int i = 0; i < N; i++)
12     {
13         result += e[i].x * e[i].y;
14     }
15     return 0;
16 }
```

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

```
1  struct coordinates
2  {
3      double x[N];
4      double y[N];
5      double z[N];
6  };
7
8  int main (void) {
9      struct coordinates e = { 0 };
10     double result = 0.0;
11     for (int i = 0; i < N; i++)
12     {
13         result += e.x[i] * e.y[i];
14     }
15     return 0;
16 }
```

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- 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

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- [Giu.natale, 2016] Giu.natale (2016). **Example of a naive Roofline model.**
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- [GWT-TUD GmbH, 2020] GWT-TUD GmbH (2020). **Vampir.** <https://vampir.eu/>.

- $O(1)$
 - 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

```
1 for (int i = 0; i < n; i++) {  
2     for (int j = 0; j < n; j++) {  
3         result += sin(i) + cos(j);  
4     }  
5 }
```