Performance Analysis and Optimization

Parallel Programming

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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
Motivation...

Introduction

• 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
Offline Approaches

Introduction

- 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

Introduction

• 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

Performance Analysis and Optimization

Introduction

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Performance Optimization

Summary
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
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
• 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...

Benchmarks:

1. **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)

2. **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-03' ran 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
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.”
• 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...

Performance Analysis

- 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
Approaches

Performance Analysis

• 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
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

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

Performance Analysis

\[ \pi \]

[Giulianale, 2016]
Outline

Performance Analysis and Optimization

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Performance Analysis

Performance Optimization

Summary
• 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

Performance Optimization

- 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
Programming Languages...

Performace Optimization

- 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
Tools...

Performance Optimization

[Image of a tool interface with a timeline and processes]

[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

```
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
1 101.86  0.81  0.81
```
$ 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
9.013823000 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
Compilers...

Performance Optimization

- `-0g`
  - Optimize for debugging, some important passes are disabled at `-00`
- `-0s`
  - Optimize for size, good for embedded systems with little storage
- `-0fast`
  - 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
• 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

[Row-major order]

\[
\begin{bmatrix}
  a_{11} & a_{12} & a_{13} \\
  a_{21} & a_{22} & a_{23} \\
  a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

[Column-major order]

\[
\begin{bmatrix}
  a_{11} & a_{12} & a_{13} \\
  a_{21} & a_{22} & a_{23} \\
  a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

[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

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• 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
Performance Analysis and Optimization

Introduction
Performance Analysis
Performance Optimization
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

