Hardware Specific Optimizations

or

What to do if there is no bigger hammer?

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Workshop on Advanced Techniques
in Scientific Computing

A Bit of History or:
How Did We Get Where We Are Now?

- The need for doing (numerical) calculations faster is as old as the underlying math

- There are multiple approaches to address this:
  - Use approximations, when possible
  - Develop more efficient algorithms
  - Get faster hardware
  - Use/write optimized software for your hardware
  - Parallelize

- The focus on each of these changes over time

Improving Hardware Performance

Optimizations:

- Type faster, read faster (Faster I/O)

- Turn handle faster, use faster motor (Higher Clock)

- Build better mechanics, use better technology (Better CPU)

A Bit of History or: How Did We Get Where We Are Now?

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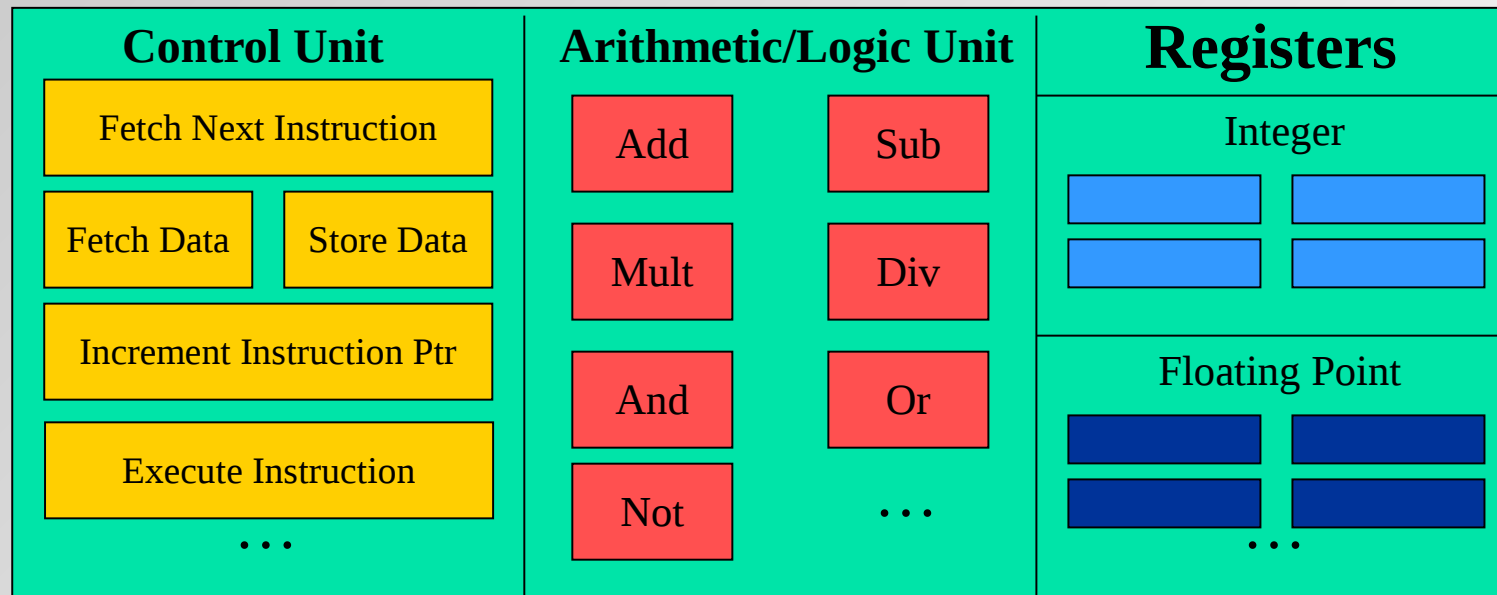- The focus on each of these changes over time

Where Are The Problems?

- Increasing clock rates is technologically difficult => multi-core architectures => parallelization

- Compilers <u>can</u> optimize for vector units and superscalar, pipelined CPUs, but <u>only</u> if the original code (and its language) allows it => many codes underutilize current CPUs

- With multi-core and non-uniform memory access, performance is often limited by I/O => data structures and access patterns matter

- We are not used to "think like a CPU"

A Simple CPU

- The basic CPU design is not much different from the mechanical calculator.

- Data still needs to be fetched into <u>registers</u> for the CPU to be able to operate on it.

Control Unit	Arithmetic/Logic Unit		Registers
Fetch Next Instruction	Add	Sub	Integer
Fetch Data	Store Data	Mult	Div	
Increment Instruction Ptr	And	Or	Floating Point
Execute Instruction	Not	…	
…			…

CPU Pipeline

- One CPU "operation" has multiple steps/stages: fetch instr, decode instr, execute instr, memory lookup, write back => multiple functional units

- Using a pipeline allows for a faster CPU clock => like assembly line

- Dependencies and branches may force CPU to stall pipeline

- Complex operations usually not pipelined

Instr. No.	Pipeline Stage						
1	IF	ID	EX	MEM	WB		
2		IF	ID	EX	MEM	WB	
3			IF	ID	EX	MEM	WB
4				IF	ID	EX	MEM
5					IF	ID	EX
Clock Cycle	1	2	3	4	5	6	7

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How Would This Statement Be Executed?

$z = a * b + c * d;$

Actual steps:

$z1 = a * b;$

> Data load can start while multiplying

$z2 = c * d;$

> Start data load for next command

$z = z1 + z2;$

1. Load **a** into register **R0**
2. Load **b** into **R1**
3. Multiply **R2** = **R0** * **R1**
4. Load **c** into **R3**
5. Load **d** into **R4**
6. Multiply **R5** = **R3** * **R4**
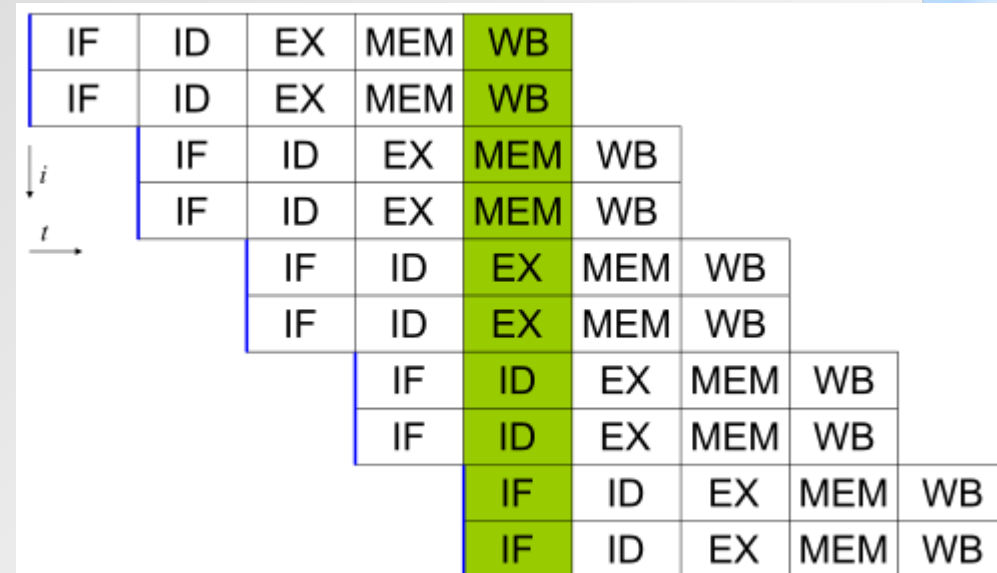7. Add **R6** = **R2** + **R5**
8. Store **R6** into **z**

Pipeline savings:
1 step out of 8, plus 3 more if next operation independent

Superscalar CPU design

- Superscalar CPU => <u>instruction level parallelism</u>

- Redundant functional units in single CPU core
  => multiple instructions executed at same time
  => typically combined with pipelined CPU design

- This is **not** SIMD!

- How to program for this:
  - write simple code
  - no data dependencies
  - avoid branches
  - compiler optimization

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Superscalar & Pipelined CPU Execution

Actual steps:

z1 = a * b;

z2 = c * d;

z= z1 + z2;

Start data load for next command

$$z = a * b + c * d;$$

1. Load **a** into register **R0**
   and load **b** into **R1**
2. Multiply **R2** = **R0** * **R1**
   and load **c** into **R3**
   and load **d** into **R4**
3. Multiply **R5** = **R3** * **R4**
4. Add **R6** = **R2** + **R5**
5. Store **R6** into **z**

Superscalar pipeline savings:
3 out of 8 steps, plus 3 if next operation independent

Superscalar & Pipelined Loop

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

1. Load **a[0]** into **R0**
   <u>and</u> load **b[0]** into **R1**
2. Multiply **R2 = R0 * R1**
   <u>and</u> load **c[0]** into **R3**
   <u>and</u> load **d[0]** into **R4**
3. Multiply **R5 = R3 * R4**
   <u>and</u> load **a[1]** into **R0**
   <u>and</u> load **b[1]** into **R1**

4. Add **R6 = R2 + R5**
   <u>and</u> load **c[1]** into **R3** <u>and</u>
   load **d[1]** into **R4**
5. Store **R6** into **z[0]**
   <u>and</u> multiply **R2 = R0 * R1**
   <u>and</u> multiply **R5 = R3 * R4**
   <u>and</u> load **a[2]** into **R0**
   <u>and</u> load **b[2]** into **R1**

Repeat steps 4. and 5. with increasing index until done

Vectorized Loop

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

Vector registers on a CPU can hold multiple numbers and load, store or process them in parallel (**SIMD**):

```
for (i = 0; i < length; i +=2) {
 z[i] = a[i]  *b[i]   + c[i]  *d[i];
 z[i+1]=a[i+1]*b[i+1] + c[i+1]*d[i+1];
}
```

Executed together

This is **in addition** to superscalar pipelining and with using special vector instructions (SSE,AVX,etc.)

Fast and Slow Operations

- Fast (0.5x-1x): add, subtract, multiply

- Medium (5-10x): divide, modulus, sqrt()

- Slow (20-50x): most transcendental functions

- Very slow (>100x): power (x^y for real x and y)

  Often **<u>only</u>** the fastest operations are pipelined, so code will be the fastest when using only add and multiply => linear algebra
  => BLAS (= Basic Linear Algebra Subroutines)
     plus LAPACK (Linear Algebra Package)

Simple Optimization Techniques
(so easy a ~~caveman~~ compiler can do it)

Copy Propagation

Before

$$x = y$$
$$z = 1 + x$$

Has data dependency

Compile

After

$$x = y$$
$$z = 1 + y$$

No data dependency

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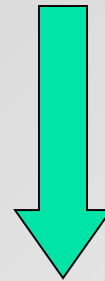
Constant Folding

Before   **After**

```
add = 100;                    sum = 300;
aug = 200;
sum = add + aug;
```

sum is the sum of two constants. The compiler can precalculate the result (once) at compile time and eliminate code that would otherwise need to be executed at (every) run time.

Strength Reduction

Before	**After**
`x = pow(y, 2.0);`	`x = y * y;`
`a = c / 2.0;`	`a = c * 0.5;`

Raising one value to the power of another, or dividing, is more expensive than multiplying.

If the compiler can tell that the power is a small integer, or that the denominator is a constant, it will use multiplication instead.

Easier to do with intrinsic functions (cf. Fortran).

Common Subexpression Elimination

Before	After

```
         Before                     After

d = c * (a / b);        adivb = a / b;
e = (a / b) * 2.0;      d = c * adivb;
                        e = adivb * 2.0;
```

The subexpression **(a / b)** occurs in both assignment statements, so there's no point in calculating it twice.

This is typically only worth doing if the common subexpression is expensive to calculate, or the resulting code requires the use of less registers.

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Variable Renaming

Before

```
x = y * z;
q = r + x * 2;
x = a + b;
```

After

```
x0 = y * z;
q = r + x0 * 2;
x = a + b;
```
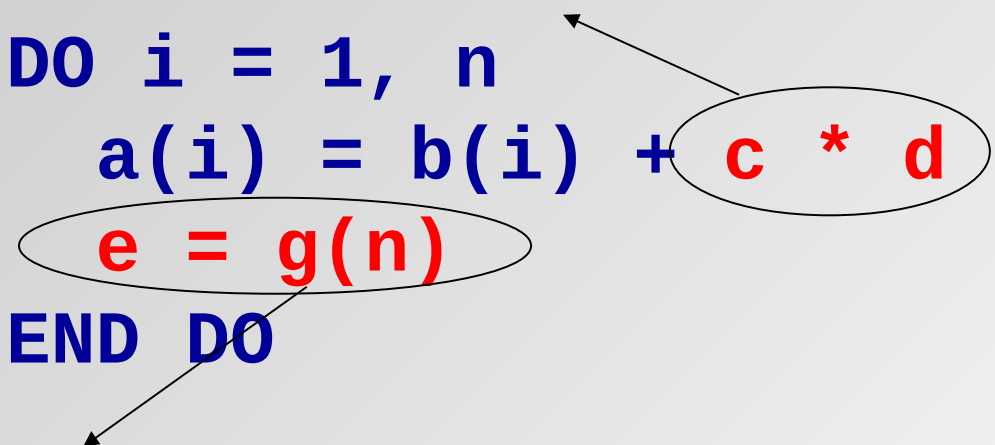
The original code has an **output dependency**, while the new code **doesn't** – but the final value of **x** is still correct.

Hoisting Loop Invariant Code

Code that doesn't change inside the loop is known as *loop invariant*. It doesn't need to be calculated over and over.

Before

```
DO i = 1, n
   a(i) = b(i) + c * d
   e = g(n)
END DO
```

After

```
temp = c * d
DO i = 1, n
   a(i) = b(i) + temp
END DO
e = g(n)
```

Loop Unrolling

Before

```fortran
DO i = 1, n
  a(i) = a(i)+b(i)
END DO
```

After

```fortran
DO i = 1, n, 4
   a(i)   = a(i)  +b(i)
   a(i+1) = a(i+1)+b(i+1)
   a(i+2) = a(i+2)+b(i+2)
   a(i+3) = a(i+3)+b(i+3)
END DO
```

You generally **shouldn't** unroll by hand.
Compilers are much more reliable.

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Loop Interchange

Before

```
DO i = 1, ni
  DO j = 1, nj
    a(i,j) = b(i,j)
  END DO
END DO
```

After

```
DO j = 1, nj
  DO i = 1, ni
    a(i,j) = b(i,j)
  END DO
END DO
```

Array elements **a(i,j)** and **a(i+1,j)** are near each other in memory, while **a(i,j+1)** may be far, so it makes sense to make the **i** loop be the inner loop. (This is reversed in C, C++)

Loop Fusion / Fission

```
DO i = 1, n
  a(i) = b(i) + 1
END DO
DO i = 1, n
  c(i) = a(i) / 2
END DO
DO i = 1, n
  d(i) = 1 / c(i)
END DO
```

Separate

```
DO i = 1, n
  a(i) = b(i) + 1
  c(i) = a(i) / 2
  d(i) = 1 / c(i)
END DO
```

Together
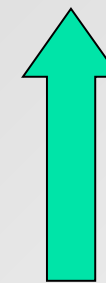
Fusion

Fission

Fusion: fewer branches (combine with unrolling).
        fewer total memory references.
Fission: smaller cache footprint

Inlining

Before

```
DO i = 1, n
  a(i) = func(i)
END DO
…
REAL FUNCTION func (x)
  …
  func = x * 3
END FUNCTION func
```

After

```
DO i = 1, n
  a(i) = i * 3
END DO
```

When a function or subroutine is *inlined*, its contents are transferred directly into the calling routine, and thus eliminating the overhead of making the call.
=> compilers use an inline library at high optimization
=> math is instrinsic in Fortran => better for compiler

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Quick 'n' Dirty Optimization or: How Much Can You Optimize a Code Over the Weekend?

- Example from the "HPC Helpdesk" @ TempleU

- User requests access to HPC resource because his self-written program needs to much memory and runs too slow

- Next the users asks for parallel programming courses to handle large matrices

- Application is one file with ~1000 lines C code => could be perfect showcase for a "minimum effort" optimization and parallelization study

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Structure of the Application

- <u>Input data</u>: a network, a list of nodes (names) and a list of connections between those nodes (e.g. "friends" in a social network)

- <u>Objective</u>: find a subset where the ratio of internal vs. external connections is maximal

    1) <u>Clustering</u>: pick a sample of connected nodes around a seed, pick the most connected nodes as new seed, repeat until converged

    2) <u>Pruning</u>: Take connection matrix from 1), remove most unfavorable entry, record target function value and subset, repeat until empty

Optimization 1: Reduce Memory

- The by far most time consuming step is the calculation of a "connection matrix" of the selected nodes

- The matrix elements are either 1 if two nodes are connected or 0, if not.

- Storage element was **`unsigned long int`**

  => use **`char`** instead

  => 4x (32-bit) to 8x (64-bit) memory savings

  => 1.5-2x performance increase

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Optimization 2: Compiler

- The reference executable was compiled with gcc using default settings, i.e. <u>no</u> optimization

- Using compiler optimizations leads to significant performance increase

- Compiler optimization can be improved through using `const` qualifiers in the code wherever possible and local code changes

- Hide complex data types with `typedef`

  => 2.5 – 3.5x speedup

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Optimization 3: Parallelization

- The construction of the connection matrix has no data dependencies => multi-threading

- Using OpenMP requires only adding one directive and a little bit of code reorganization

- Speedup going from serial to 2 threads: 1.5x

- Speedup levels out at 6-8 threads: 2.5x total

  => very little computation, mostly data access
  => performance limited by memory contention

- Total improvement: 8x-12x with 8 threads

2x Intel Xeon X5677, 3.5GHz
96 GB 1333MHz DDR3 RAM
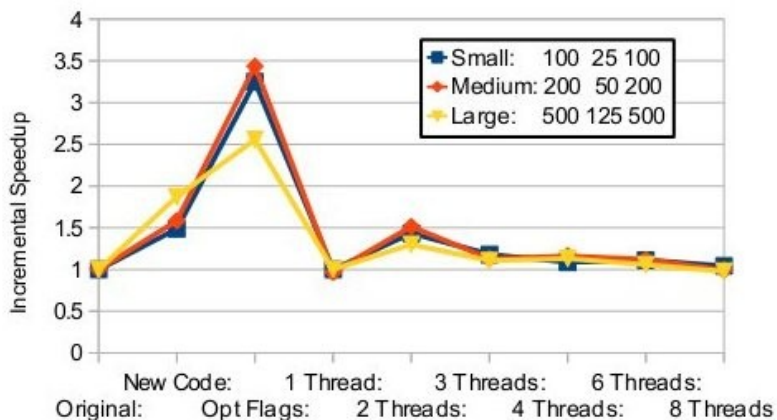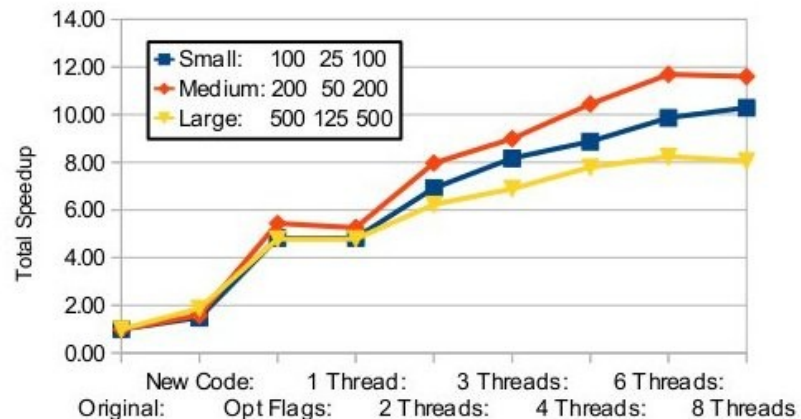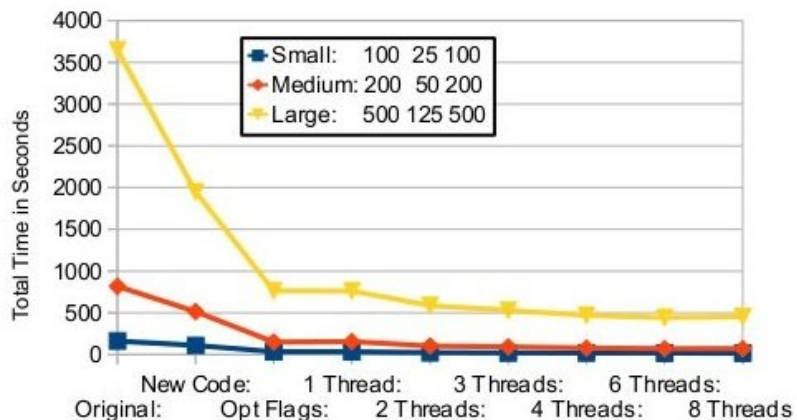
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4 GB 800MHz DDR2 RAM
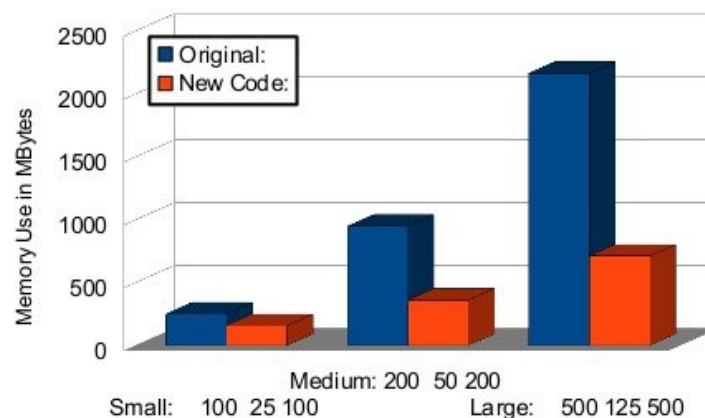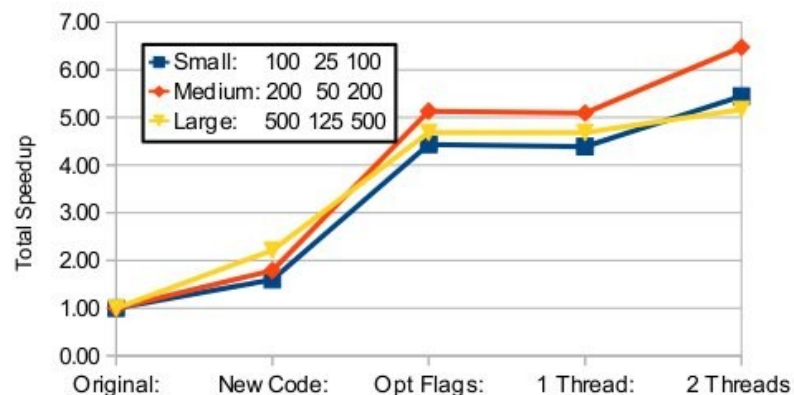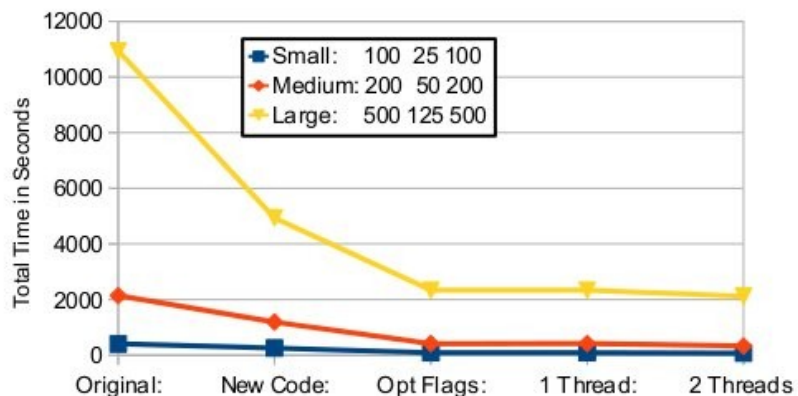
Proper Optimization or:
# The Power of the Rewrite

- Quick'n'dirty optimizations of T-CLAP resulted in significant improvements in a short time

- More optimization potential with a full rewrite:

  - Connection matrix information requires only 1 bit
    => reduce storage need by factor of 8 (vs. `char`)

  - Network represented by structs and lists of pointers
    => multiple pointers refer to the same data
    => pointers require more storage in 64-bit mode

  - Pruning implementation uses memmove() to compact matrix rows
    => performance bottleneck for large data ($O(N^2)$)

The Rewrite

- Rewrite in C++ (more optimization hints than C)

- Use STL container classes

- std::vector<bool> uses single bit per entry

- Single list of structs for all network nodes, all references via index lists (std::vector<int>)

- Leave data in place during pruning, maintain lists of valid rows and columns instead

- Avoid some redundant operations
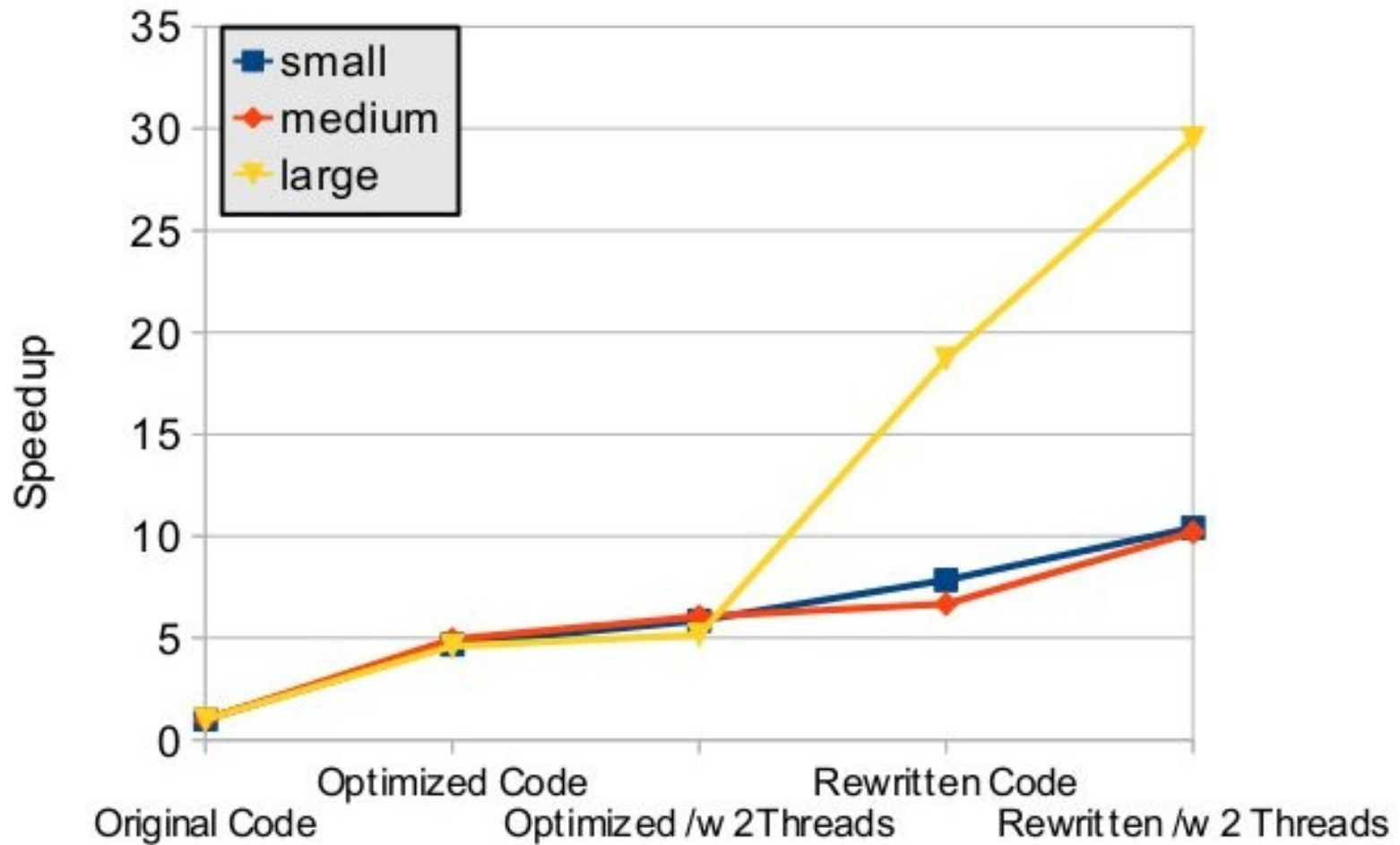
- Rewrite piece-by-piece to reproduce original
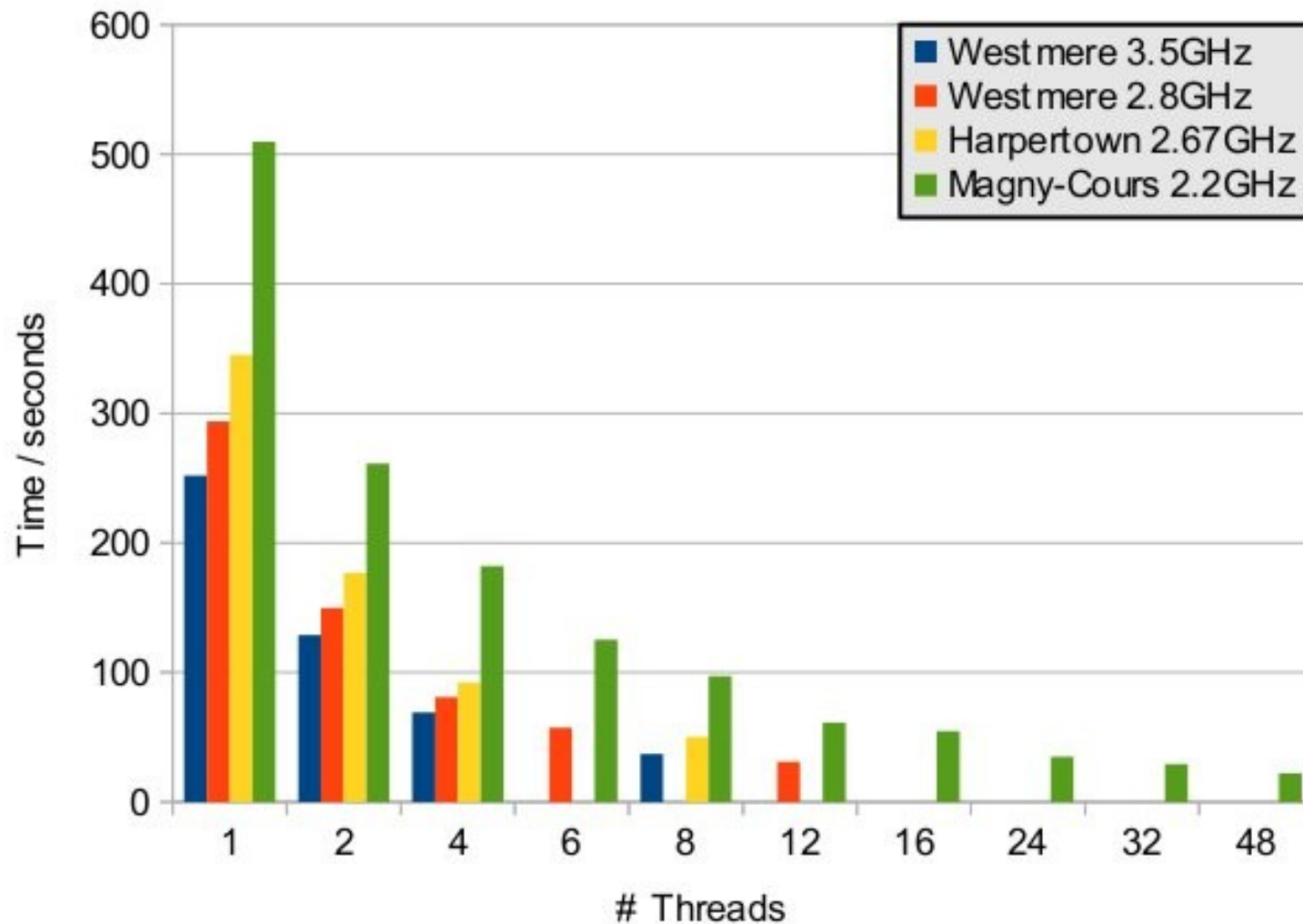
Memory Usage After Rewrite
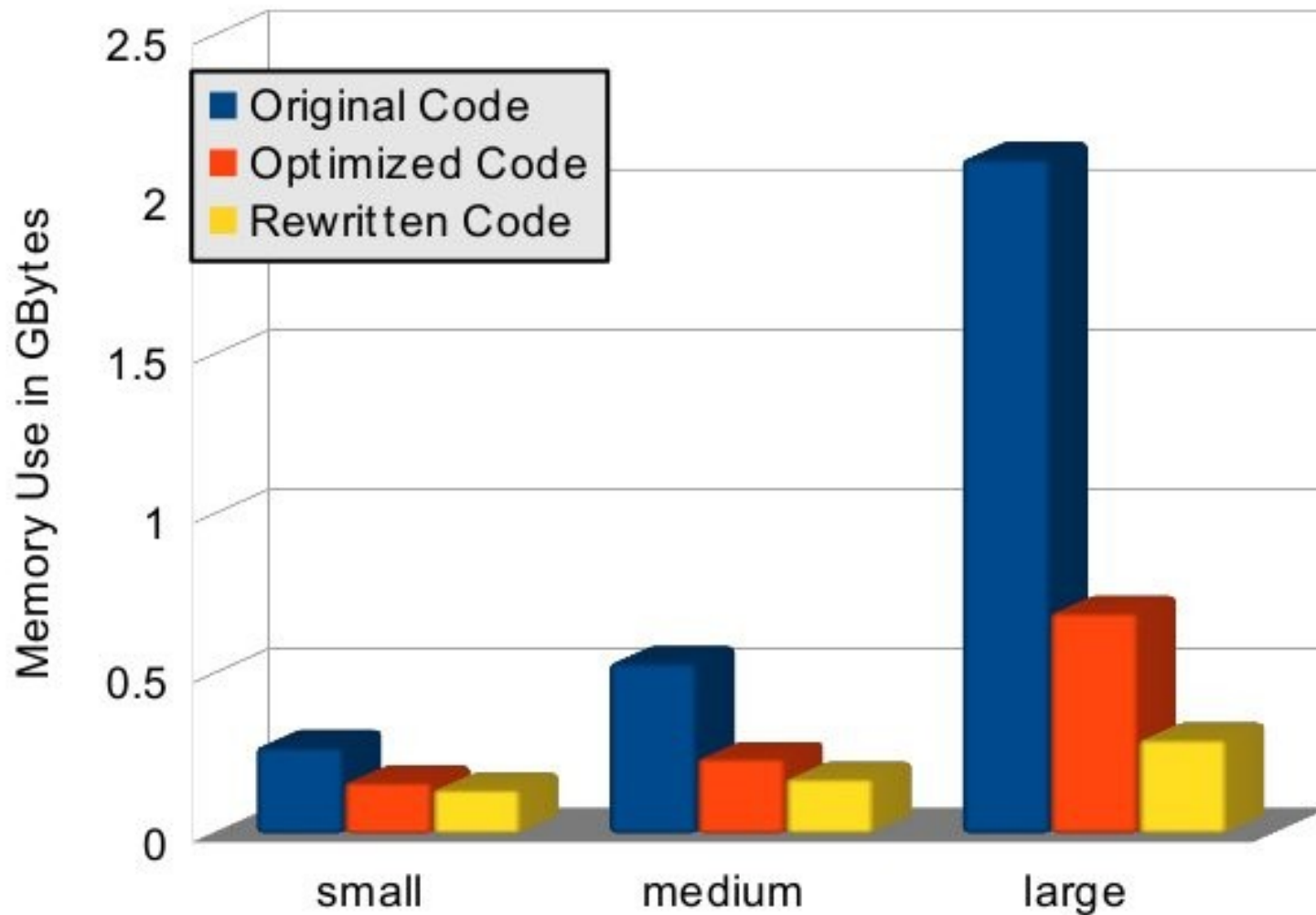
Performance After Rewrite

Parallel Performance After Rewrite

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