How to Write Fast Numerical Code

Spring 2011

Lecture 2

Instructor: Markus Püschel

TA: Georg Ofenbeck

ETH

Eidgenössische Technische Hochschule Zürich

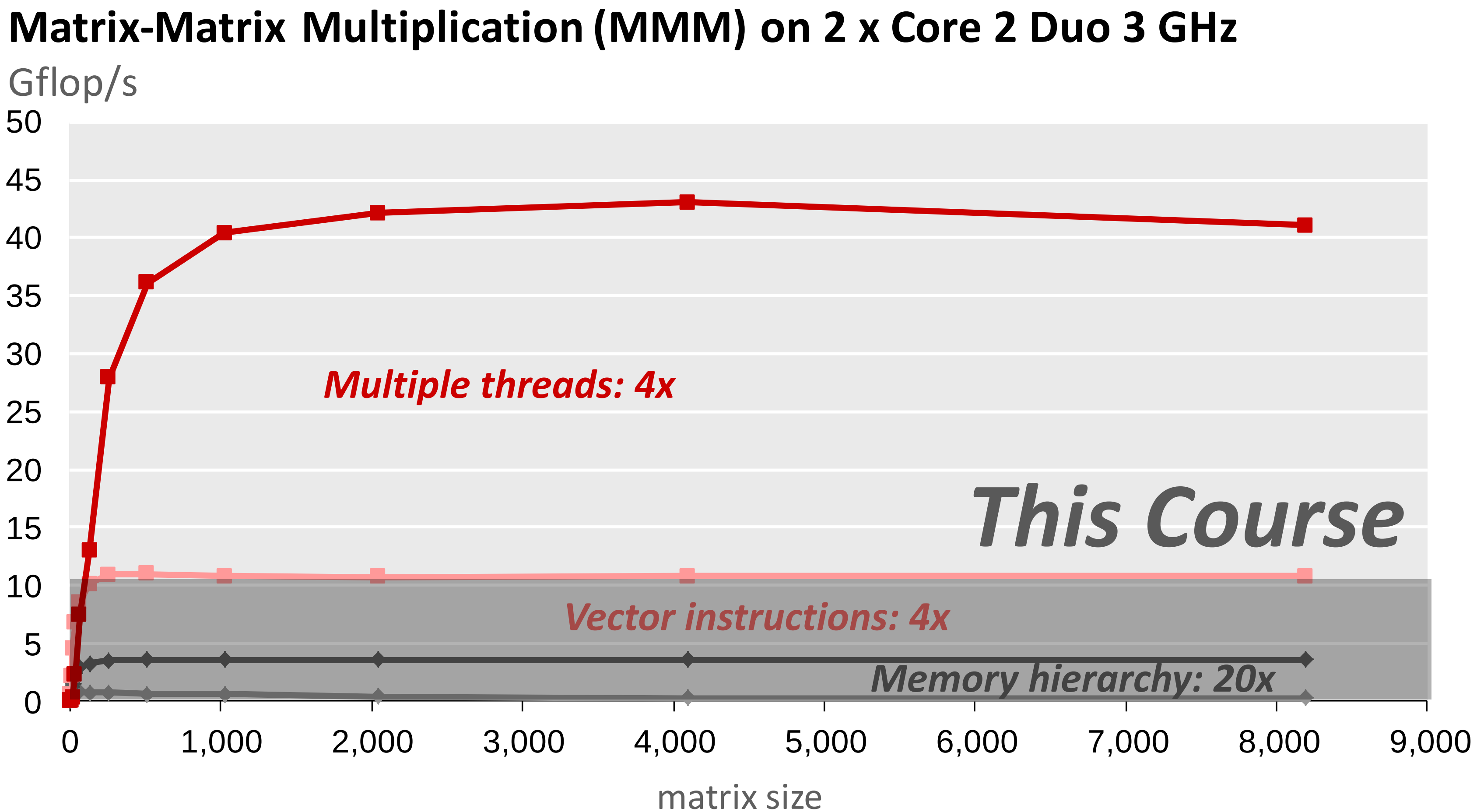
Swiss Federal Institute of Technology Zurich

Technicalities

- **Research project: Let me know**
  - if you know with whom you will work
  - if you have already a project idea

- **Deadline: March 9th**

Last Time


Matrix-Matrix Multiplication (MMM) on 2 x Core 2 Duo 3 GHz
Gflop/s
50
45
40
35
30
25
20
15
10
5
0
Multiple threads: 4x
This Course
Vector instructions: 4x
Memory hierarchy: 20x
0
1,000
2,000
3,000
4,000
5,000
6,000
7,000
8,000
9,000
matrix size

Today

- Problem and Algorithm
- Asymptotic analysis: Do you know the O?
- Cost analysis

- *Standard book:* Introduction to Algorithms (2nd edition), Corman, Leiserson, Rivest, Stein, McGraw Hill 2001)

Problem

- ***Problem:*** **Specification of the relationship between a given input and a desired output**

- **Numerical problems: In- and Output are numbers**
  (or lists, vectors, arrays, … of numbers)

- **Examples**
  - Compute the discrete Fourier transform of a given vector x of length n
  - Matrix-matrix multiplication (MMM)
  - Compress an n x n image with a ratio …
  - Sort a given list of integers
  - Multiply by 5, $y = 5x$, using only additions and shifts

Algorithm

- *Algorithm:* **A precise description of a sequence of steps to solve a given problem.**

- **Numerical algorithms: These steps involve arithmetic computation (addition, multiplication, …)**

- **Examples:**
  - Cooley-Tukey fast Fourier transform
  - A description of MMM by definition
  - JPEG encoding
  - Mergesort
  - y = x<<2 + x

Tips for Presenting and Publishing

- **If your topic is an algorithm, *you must:***
  - Give a formal problem specification, like:
    Given *.....;* ***We want to compute****......*
    or
    Input: ......; Output: .....

- **Analyze the algorithm, at least asymptotic runtime in O-notation**

Origin of the Word "Algorithm"

- Mathematician, astronomer and geographer; founder of Algebra (his book: Al'Jabr wa'al'Muqabilah)
- Al'Khowârizmî → ***Algorithm***
  Al'Jabr → ***Algebra***
- Khowârizm is today the small Soviet city of Khiva
- Earlier word Algorism: The process of doing arithmetic using Arabic numerals
- Algorithm: since 1957 in Webster Dictionary

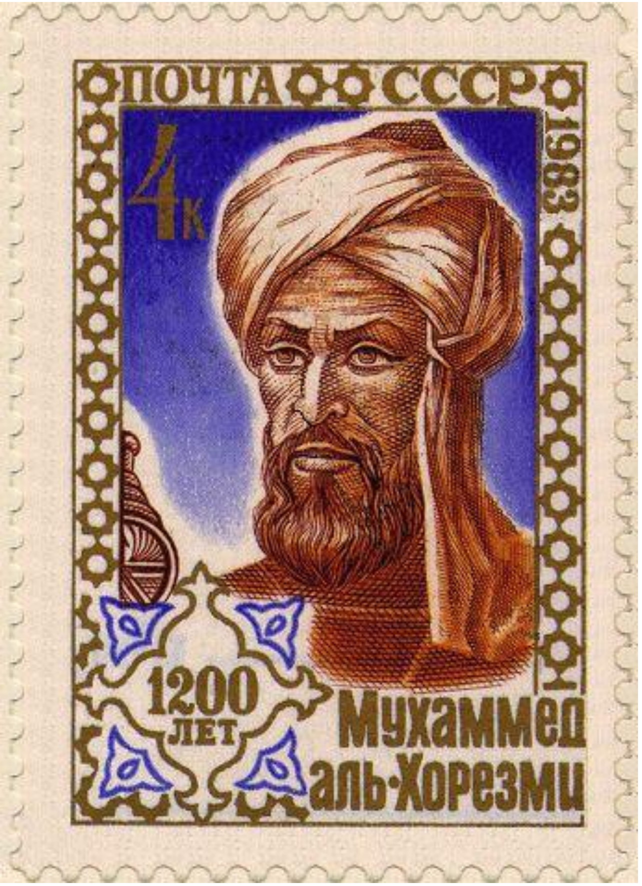


image from http://jeff560.tripod.com/

Abu Ja'far Mohammed ibn Mûsâ al'Khowârizmî (c. 825)

source:
http://www.disc-conference.org/disc2000/mirror/khorezmi/

Asymptotic Analysis of Algorithms & Problems

- **Analysis of Algorithms for**
  - Runtime
  - Space = memory requirement (or footprint)

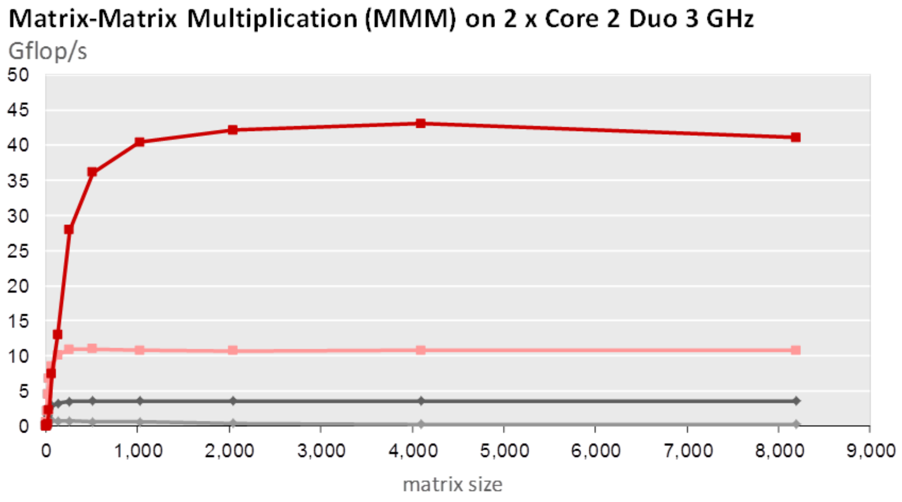
- **Runtime of an algorithm:**
  - Count “elementary” steps
    (for numerical algorithms: usually floating point operations)
    dependent on the input size n (more parameters may be necessary)
  - State result in O-notation
  - Example MMM (square and rectangular): C = A*B + C

- **Runtime complexity of a problem =**
  Minimum of the runtimes of all possible algorithms
  - Result also stated in asymptotic O-notation

Complexity is a property of a problem, not of an algorithm

Valid?

- **Is asymptotic analysis still valid given this?**



- **Yes: if the algorithm is O(f(n)), all memory effects are O(f(n))**
- **Vectorization, parallelization may introduce additional parameters**
  - Vector length v
  - Number of processors p
  - Example: MMM

Do You Know The O?

- $O(f(n))$ is a … ? set
- How are these related? $\Theta(f(n) = \Omega(f(n)) \cap O(f(n))$
  - $O(f(n))$
  - $\Theta(f(n))$
  - $\Omega((f(n))$
- $O(2^n) = O(3^n)$? no
- $O(\log_2(n)) = O(\log_3(n))$ yes
- $O(n^2 + m) = O(n^2)$? no

Always Use Canonical Expressions

- **Example:**
  - ***not*** $O(2n + \log(n))$, ***but*** $O(n)$
- **Canonical? If not replace:**

$O(100)$	$O(1)$
$O(\log_2(n))$	$O(\log(n))$
$\Theta(n^{1.1} + n \log(n))$	$O(n^{1.1})$
$2n + O(\log(n))$	yes
$O(2n) + \log(n)$	$O(n)$
$\Omega(n \log(m) + m \log(n))$	yes

Master Theorem: Divide-And Conquer Algorithms

Recurrence

Runtime for problem size *n* — **Cost of conquer step**

$$T(n) = aT(n/b) + f(n), \quad a \geq 1, b > 1$$

a **subproblems of size *n/b***

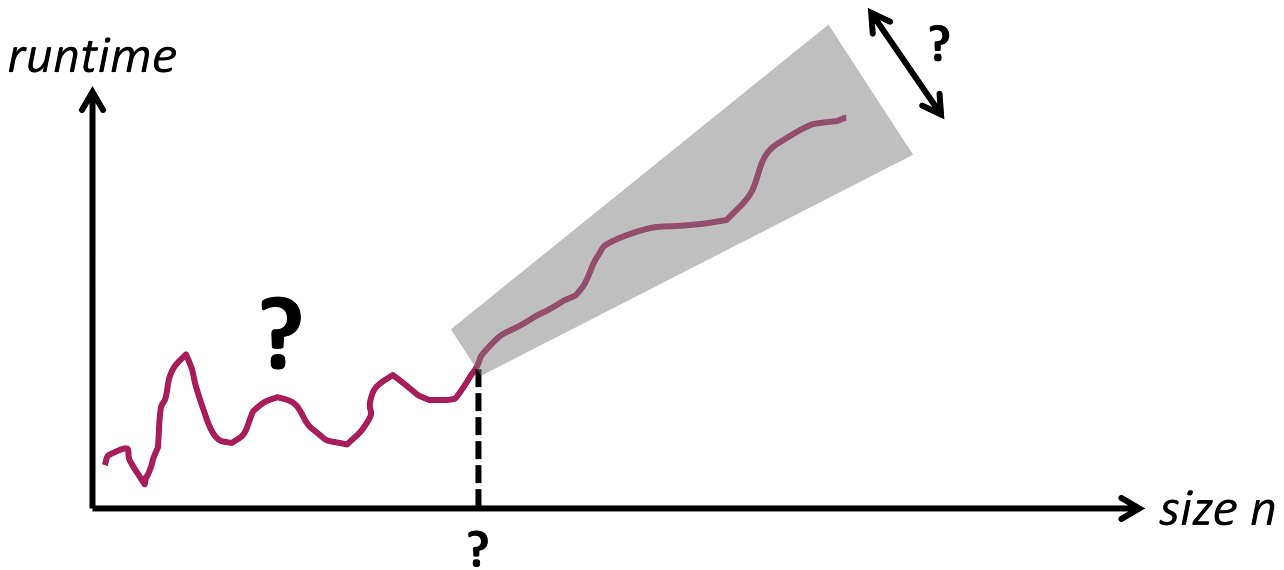
Solution

$$T(n) = \begin{cases} \Theta(n^{\log_b a}), & f(n) = O(n^{\log_b a - \epsilon}),\ \text{for some } \epsilon > 0 \\ \Theta(n^{\log_b a} \log(n)), & f(n) = \Theta(n^{\log_b(a)}) \\ \Theta(f(n)), & f(n) = \Omega(n^{\log_b a + \epsilon}),\ \text{for some } \epsilon > 0 \end{cases}$$

Stays valid if *n/b* is replaced by its floor or ceiling

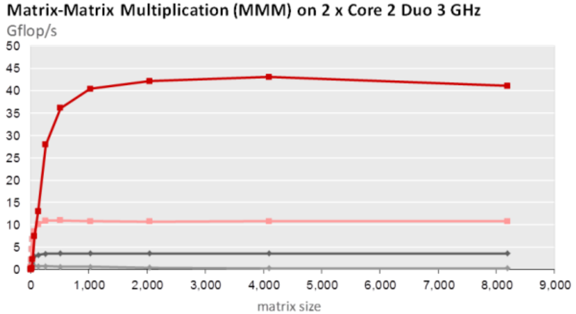
Asymptotic Analysis: Limitations

- **Θ(f(n)) describes only the *eventual shape* of the runtime**



- **Constants matter**
  - n^2 is likely better than $1000n^2$
  - 10000000000n is likely worse than n^2

- **But remember: exact op count ≠ runtime**



Refined Analysis for Numerical Problems

- ***Goal:*** **determine exact "cost" of an algorithm**
- **Approach (use MMM as running example):**
  - Fix an appropriate cost measure C: "what do I count"
  - For numerical problems typically floating point operations
  - Determine cost of algorithm as function C(n) of input size n, or, more generally, of all relevant input parameters:

$$C(n_1,..,n_k)$$

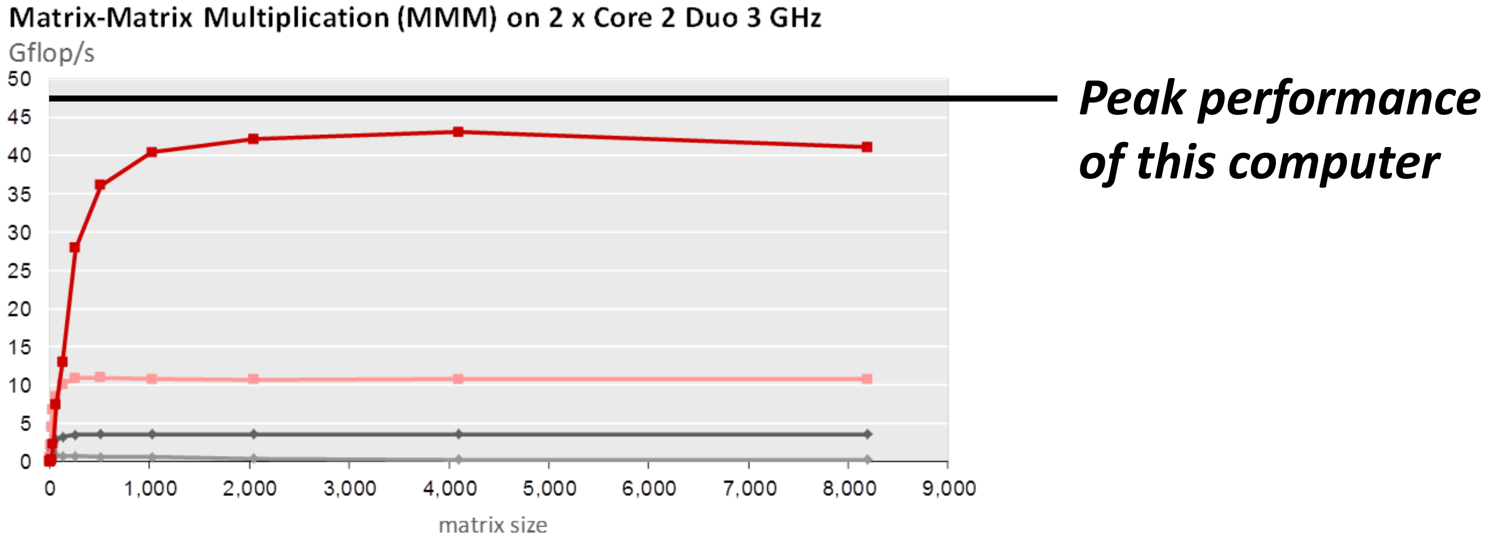
  - Cost can be multi-dimensional

$$C(n_1,..,n_k) = (c_1,..,c_m)$$

- **Exact cost is:**
  - More precise than asymptotic runtime
  - Absolutely not the exact runtime

For Publications and Presentations

- **Formally state the problem that you solve (as said before)**
- **State what is known about its complexity**
- **Analyze your algorithm (Example MMM):**
  - Define your cost measure
  - Give cost as precisely as possible/meaningful
  - Enables performance analysis



Cost Analysis

- **Cost analysis of divide-and-conquer algorithms =**
  Solving recurrences
  - Great book: Graham, Knuth, Patashnik, “Concrete Mathematics,” 2nd edition, Addison Wesley 1994
  - Blackboard