A Taste of Scientific Computing

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2022

What is Scientific Computing about?

You know the science; what more is there?

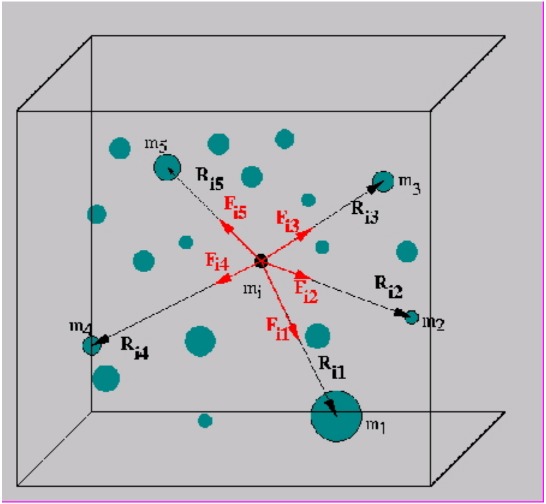
- Science often gives an implicit description.
  How do you turn it into something computational.
- Algorithms are not unique:
  There are many ways to solve a linear system

  $$\underset{x}{?}\colon\ Ax = b$$

  What are pros and cons of the choices?
- Algorithms can be implemented multiple ways, depending on your processor.

Algorithmic choices

Summing forces



Particle interactions

for each particle i

for each particle j

let $\bar{r}_{ij}$ be the vector between i and j;

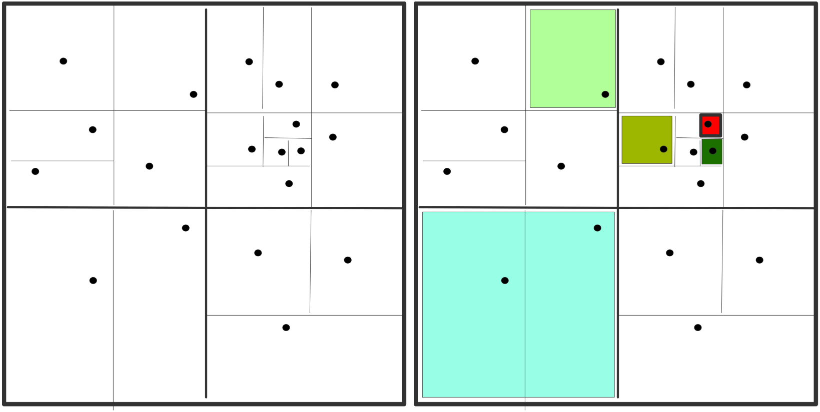
then the force on i because of j is

$f_{ij} = -\bar{r}_{ij}\frac{m_i m_j}{|r_{ij}|}$

(where m_i, m_j are the masses or charges) and

$f_{ji} = -f_{ij}$.

Naive all-pairs algorithm: $O(N^2)$



Clever algorithms: $O(N \log N)$, sometimes even $O(N)$

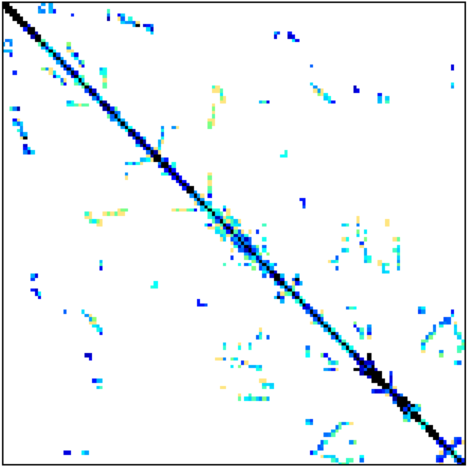
Algorithm aspects

Linear algebra

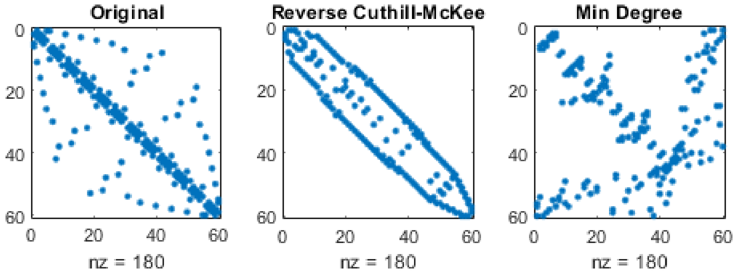
$$\underset{x}{?} : Ax = b$$

- Inversion: N^3 operations, unstable
- Gaussian elimination: N^3 but lower constant, stable
- Sparse Gaussian elimination: $N^{3/2}$, hard to program
- Iterative methods: $N \cdot \kappa^{1/2}$, not always successful
- Multigrid: $O(N)$, very limited applicability.

Sparse matrices



Permuting the matrix



The influence of your architecture

Fitting data to cache

```
for (j=0; j<size; j++)
  array[j] = 2.3*array[j]+1.2;
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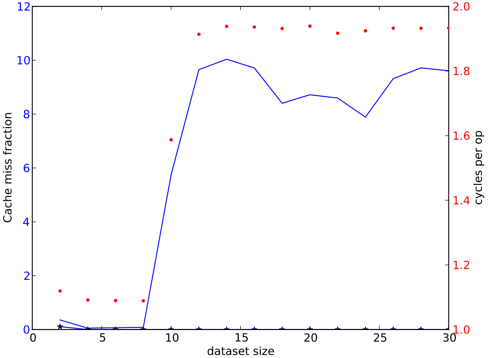
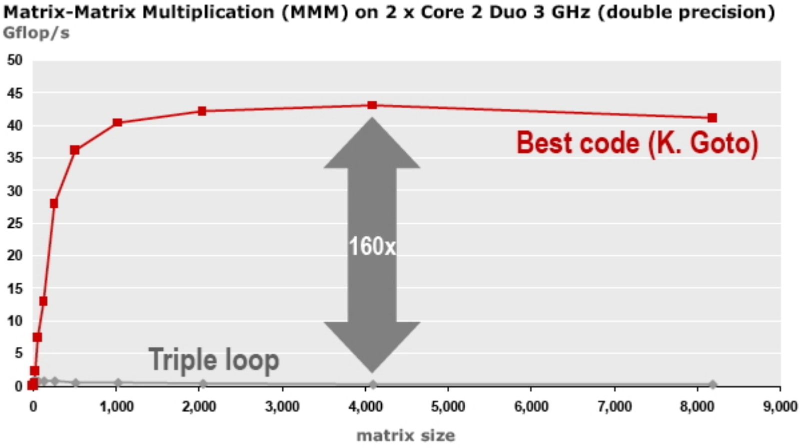


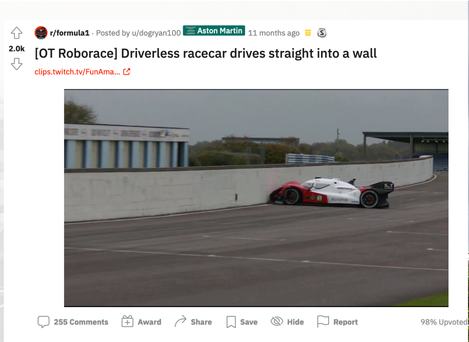
Matrix-matrix product

Lots of small optimizations add up:



Computer arithmetic

Computer numbers are not real numbers. If you don't pay attention to this you may lose you a race car, or a rocket



So what is scientific computing about?

Between science and computing

- Modeling
- Numerical analysis
- Linear algebra
- Computer architecture
- … and the interaction between any and all of these.