Memory models in a computer

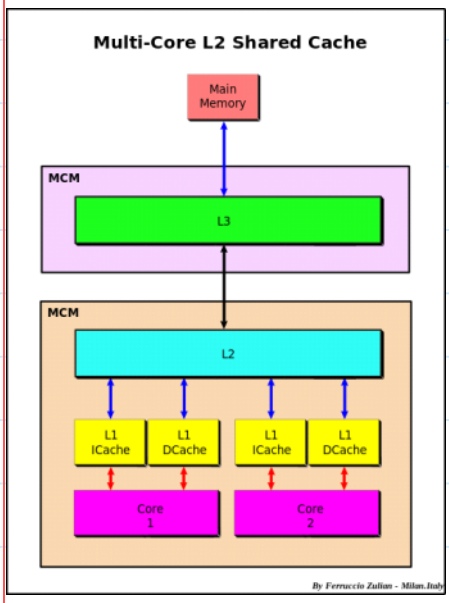
(Simplified for mathematicians)

Friday, August 23, 2024 4:51 PM

- What scientists must know about hardware to write fast code, see https://viralinstruction.com/posts/hardware/
- https://book.sciml.ai/lectures/#optional_extra_resources

Memory Hierarchy

Learning Objectives: Memory, not flops, often determines speed of an algorithm



Slow (but large)

↕ transferring memory is a major slowdown

Fast (but small)

Transferring memory to another computer or to a GPU is also slow

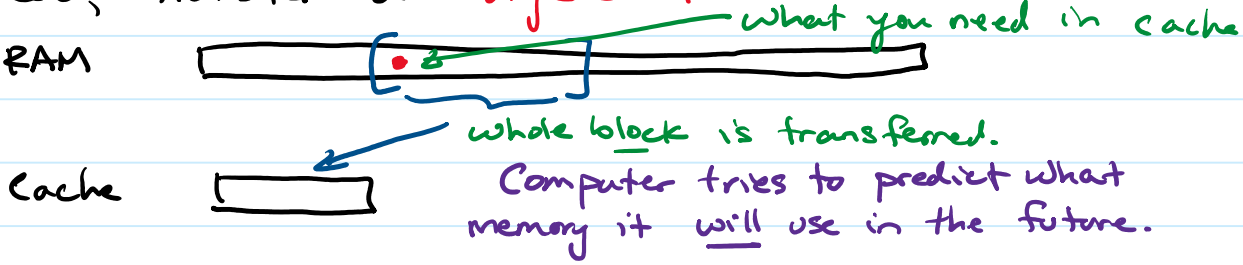
Cache misses

Transferring data is slow, has both a latency and bandwidth restrictions.

i.e. cost to move "x" bytes is $b \cdot x + l$ (in time or clock cycles)

So... due to latency, we don't like to transfer small amounts of data (since it's wasteful)

Instead, transfer a large block



Computer tries to predict what memory it will use in the future.

Memory (page 2)

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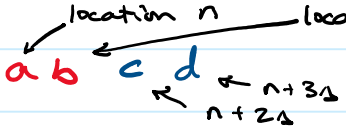
whenever you need to move memory into cache (because it wasn't there already) it's a cache miss and really slows things down.

Effect

Ex: Storing a large matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$

What's this look like in memory?

Python does row-major order



(Δ = size of float)

Matlab/fortran does column-major order $[a\ c\ b\ d]$

(RAM is linear, so must make the 2D array linear)

Let's say our cache can fit 2 numbers at once.

We compute $\|A\|_F^2 = \sum_{i=1}^{2} \sum_{j=1}^{2} A_{ij}^2$ i = row, j = column

we can choose the order

Say we're in Python

$\sum_i \left(\sum_j A_{ij}^2 \right)$

$i=1$	$j=1$	a	cache miss (Request "a", get [a,b])
	$j=2$	b	
$i=2$	$j=1$	c	cache miss (Request "c", get [c,d])
	$j=2$	d	

2 cache misses... good!

vs.

$\sum_j \left(\sum_i A_{ij}^2 \right)$

$j=1$	$i=1$	a	cache miss	get [a,b]
	$i=2$	c	cache miss	get [c,d]
$j=2$	$i=1$	b	cache miss	get [b,c]
	$i=2$	d	cache miss	get [d,?]

4 cache misses, bad!

Even more important (and complicated) for sparse matrices

Related to idea of blocked algorithms (= works on contiguous chunks of data) and exploiting fast BLAS for vector and matrix operations (multiplies)

Intel MKL, very optimized, already parallelized

and to cache oblivious algorithms (Frigo et al. '99) where you don't need to explicitly know cache size in order to get efficient performance

Memory and GPUs (page 3)

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In main memory (aka RAM), one physical location split into two (virtual) types: **stack** (includes call stack, and small amount of room for variables)

heap = the rest, used for large data

ex. in C, any `malloc` `calloc` calls

SIMD = Single Instruction Multiple Data

In most modern CPU processors (mmx, sse, sse2, avx ...)

If you want to apply $f(x) = x^2$ (or anything else simple enough) to multiple data $\{x_i\}_{i=1}^{256}$

a SIMD CPU does it efficiently, much less than 256× cost of doing it once. It's a hardware thing, less overhead

They excel at matrix multiplies... the core of much Science and ML

GPU = Graphical Processing Unit, aka video/graphics card

Like CPU but can only do simpler things, slower clock speed, but huge number (eg. 1000's) of parallel cores.

Like extreme SIMD, though at a higher level (it's "SPMD", Single Program M.D.)

- NVIDIA's **CUDA** is dominant driver/language

  Not all GPUs (even NVIDIA ones) are CUDA-compatible

- **OpenCL** and AMD's **ROCm** and Mac **MPS** (Metal Performance Shaders) are alternatives though not as widespread

amc `a100` on CURC Alpine are NVIDIA A100's

gaming GPUs often don't have much memory, or only support low-precision

`amd100` on CURC Alpine are AMD MI100's

- Data transfer from CPU to GPU is costly
- GPUs have small RAM compared to GPUs
- GPUs usually work in single (32bit) floating point precision, or less (vs. CPU/Numpy standard is double precision, 64 bit)

TPUs

Monday, September 16, 2024 10:10 AM

ref. book.sciml.ai

Tensor Processing Unit (ASIC: application specific integrated circuit) (like those for bitcoin mining)

Google's hardware specialized for linear algebra

Uses 16 bit floating point numbers for speed,

with tiny mantissa... lots of catastrophic cancellation

but... implements a FMA (fused multiply add)

which does tricks so as to not loose much precision

$a \leftarrow a + (b \times c)$

I don't know how, but could be similar to Kahan summation aka Compensated Summation

Uses an extra variable to get extra accuracy

Goal: $s = \sum_{i=1}^{n} x_i$

Algo:

```
sum = 0
c = 0
for i = 1, ..., n
    y = x_i - c
    t = sum + y
    c = (t - sum) - y   // = 0 in exact arithmetic
    sum = t
Return sum
```

Since ~2015, meant to work w/ TensorFlow mostly.

Sparse matrices

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Mathematically, a **sparse matrix** is one with "a lot" of zeros.

"nnz" = number of nonzeros, so if $nnz(A) \ll m \cdot n$, we say A is sparse.

This is vague of course!

On a computer, if your matrix is sparse but you don't do anything special, the computer treats those zeros like any other number. If you want to exploit sparsity, you must explicitly use a sparse data structure.

⚠ You need a matrix to be very sparse before it's worth it to exploit!

Sparse matrix data structures

- Baseline: Store $m \cdot n \cdot$ sizeof(float) bits (in bits) (+ $2 \cdot$ sizeof(int) for metadata)
  Location is implicit via order. row-major: A=[o co a do oef boo]
- Naive Format: "COO", Coordinate, 1-based indexing

$$A = \begin{bmatrix} 0 & c & 0 \\ a & d & 0 \\ 0 & e & f \\ b & 0 & 0 \end{bmatrix}$$

  Store (i, j, A_{ij}) triplets

  eg. (2,1,a), (4,1,b), (1,2,c), (2,2,d), (3,2,e), (3,3,f). (order unimportant)

  Cost: $nnz(A) \cdot (2 \cdot$ sizeof(int) + sizeof(float)$)$

- Compressed Sparse Column (CSC) (synonyms) = Compressed Column Storage (CCS)

[CRS is similar, just switch rows + cols] (= Compressed row storage, or CSR, Compressed Sparse Row)

Store

value A_{ij}	row i
a	2
b	4
c	1
d	2
e	3
f	3

col j

1	1
1	2
2	3
2	4
2	5
3	6

column-pointr

1
3
6

implicitly store columns via ordering.

not explicitly stored, it's implicit in

See Demo

Cost: $nnz(A) \cdot (1 \cdot$ sizeof(int) + sizeof(float)$)$ + $n \cdot$ sizeof(int) (+ metadata)

Since usually $nnz(A) > n$, this is less storage.

Implication (due to data locality + structure)

Accessing a column of a CCS matrix is way faster than accessing a row.

In Python's scipy.sparse package, easy to convert formats

Ex. of Storage

m = n = 10,000, double precision dense storage is 760 MB

if 10% sparse, CCS storage is 145 MB

(if 100% sparse, i.e. not sparse at all, it'd be 1450 MB... worse than dense!)

HDF5 (Hierarchical Data Format 5)

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Saving a dataset to disk.

Considerations:

- **documentation, metadata** (variable names...)
  Often nice to store several variables in 1 file
- **reusable by others** Use a standardized format, not homegrown, not proprietary
- **allow compression**
  exploits redundancies. Almost all data can be compressed.
  Compression can be lossless, though lossy compression obviously gives even greater savings
- **be quick to read/write** binary (not text) files, and allow you to load the data starting in the middle!
  i.e. `x = np.ones(10**9)` stored in your file.
  If you just want `x[1000:1001]` you don't want to have to load in all the data (may even not fit in RAM!)

HDF5 is an example of a well-known, standardized data format that addresses the above considerations. There are python libraries that make it easy to use (better than "pickle")

Matlab has its own format which is a variation of HDF5, and is generally interoperable w/ HDF5