Supercomputing and Science

An Introduction to High Performance Computing

Part II: The Tyranny of the Storage Hierarchy: From Registers to the Internet

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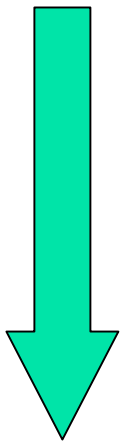
Outline

- What is the storage hierarchy?
- Registers
- Cache
- Main Memory (RAM)
- The Relationship Between RAM and Cache
- The Importance of Being Local
- Hard Disk
- Virtual Memory
- The Net

What is the Storage Hierarchy?

Small, fast, expensive



Big, slow, cheap

- Registers
- Cache memory
- Main memory (RAM)
- Hard disk
- Removable media (e.g., CDROM)
- Internet

Henry's Laptop

Dell Inspiron 4000[1]

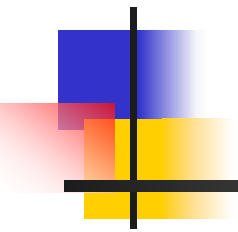
- Pentium III 700 MHz w/256 KB L2 Cache
- 256 MB RAM
- 30 GB Hard Drive
- DVD/CD-RW Drive
- 10/100 Mbps Ethernet
- 56 Kbps Phone Modem

Storage Speed, Size, Cost

On Henry's laptop

	Registers (Pentium III 700 MHz)	Cache Memory (L2)	Main Memory (100 MHz RAM)	Hard Drive	Ethernet (100 Mbps)	CD-RW	Phone Modem (56 Kbps)
Speed (MB/sec) [peak]	5340[2] (700 MFLOPS*)	11,200[3]	800[4]	100[5]	12	3.6[6]	0.007
Size (MB)	112 bytes** [7]	0.25	256	30,000	unlimited	unlimited	unlimited
Cost ($/MB)	???	$400[8]	$1.17[8]	$0.009[8]	charged per month (typically)	$0.0015[9]	free (local call)

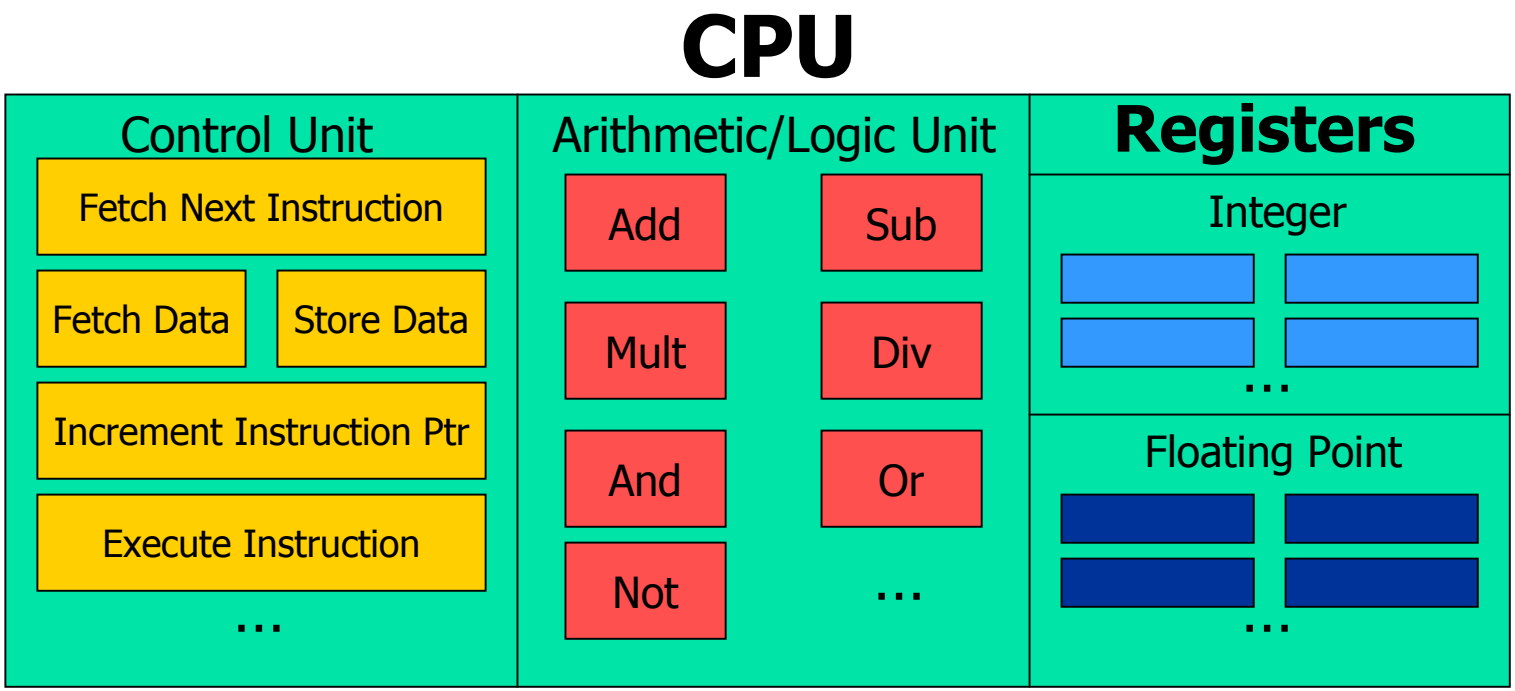
* MFLOPS: millions of floating point operations per second
** 8 32-bit integer registers, 8 80-bit floating point registers



Registers

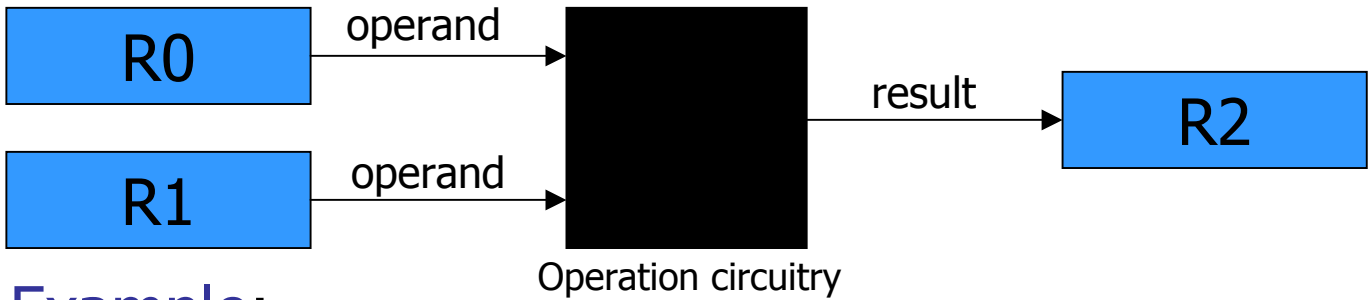
What Are Registers?

Registers are memory-like locations inside the Central Processing Unit that hold data that are **being used right now** in operations.

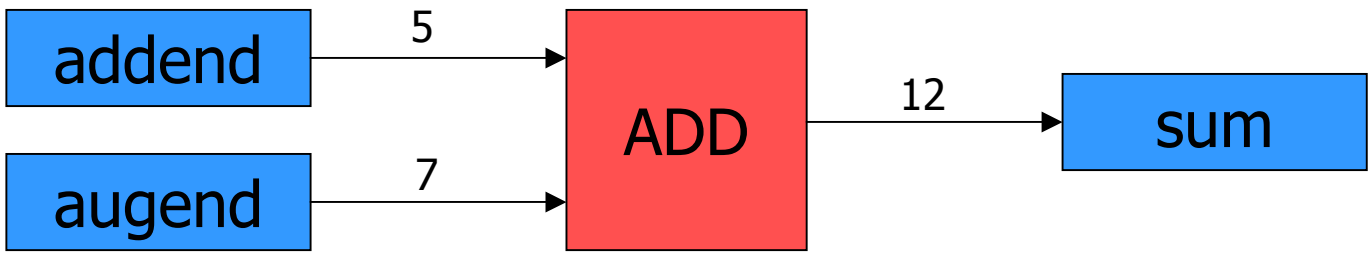


How Registers Are Used

- Every arithmetic operation has one or more source operands and one destination operand.
- Operands are contained in source registers.
- A "black box" of circuits performs the operation.
- The result goes into the destination register.

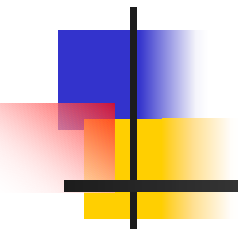


Example:



How Many Registers?

- Typically, a CPU has less than 1 KB (1024 bytes) of registers, usually split into registers for holding integer values and registers for holding floating point (real) values.
- For example, the Motorola PowerPC3 (found in IBM SP supercomputers) has 16 integer and 24 floating point registers (160 bytes).[10]

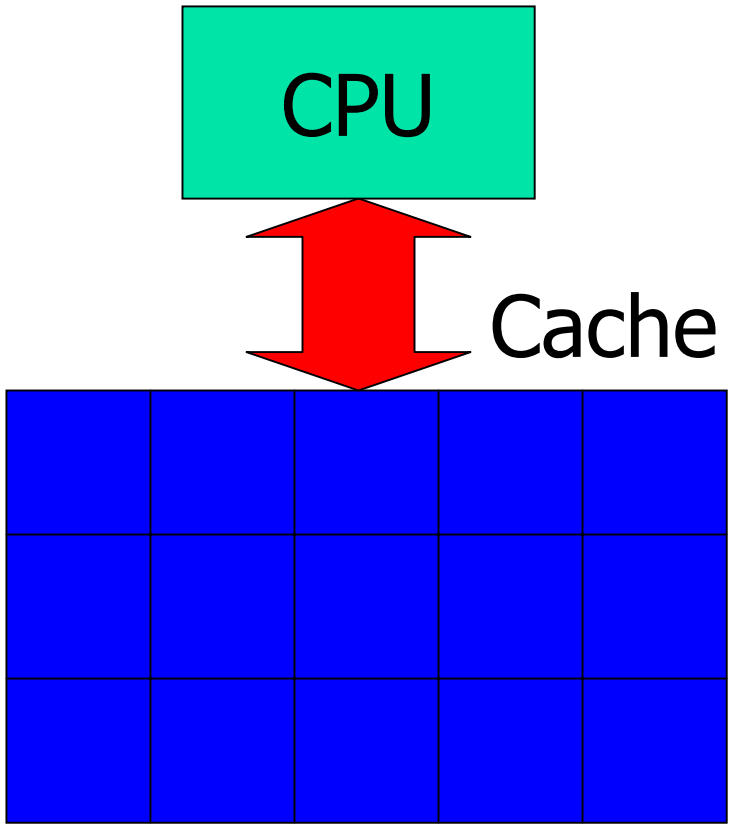


Cache

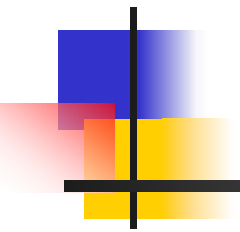
What is Cache?

- A very special kind of memory where data reside that are **about to be used** or have **just been used**
- Very fast, very expensive => very small (typically 100-1000 times more expensive per byte than RAM)
- Data in cache can be loaded into registers at speeds comparable to the speed of performing computations.
- Data that is not in cache (but is in Main Memory) takes **much** longer to load.

From Cache to the CPU



Typically, data can move between cache and the CPU at speeds comparable to that of the CPU performing calculations.

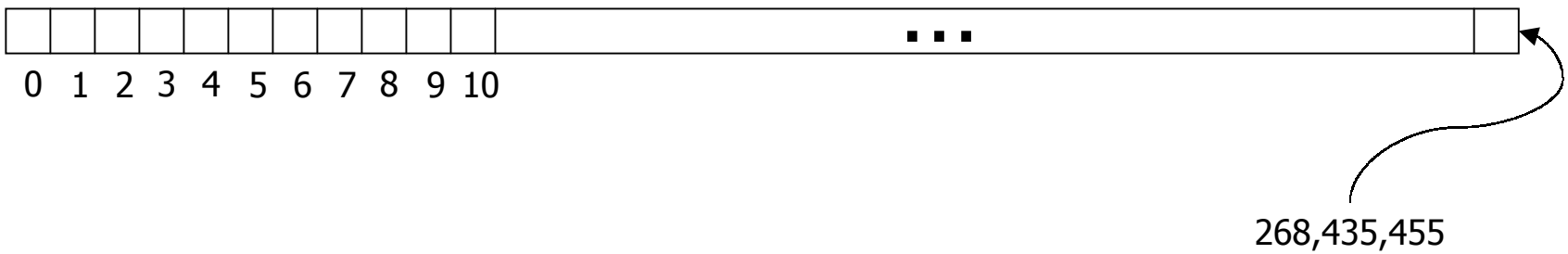


Main Memory

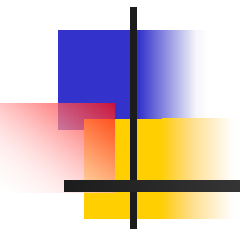
What is Main Memory?

- Where data reside for a program that is **currently running**
- Sometimes called RAM (Random Access Memory): you can load from or store into any main memory location at any time
- Sometimes called core (from magnetic "cores" that some memories used, many years ago)
- Much slower and much cheaper than cache => much bigger

What Main Memory Looks Like



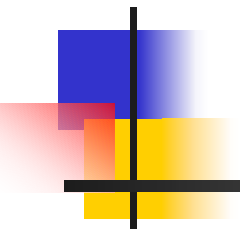
You can think of main memory as a big long 1D array of bytes.



The Relationship Between Main Memory and Cache

Cache Lines

- A cache line is a small region in cache that is loaded all in a bunch.
- Typical size: 64 to 1024 bytes.
- Main memory typically maps to cache in one of three ways:
  - Direct mapped
  - Fully associative
  - Set associative

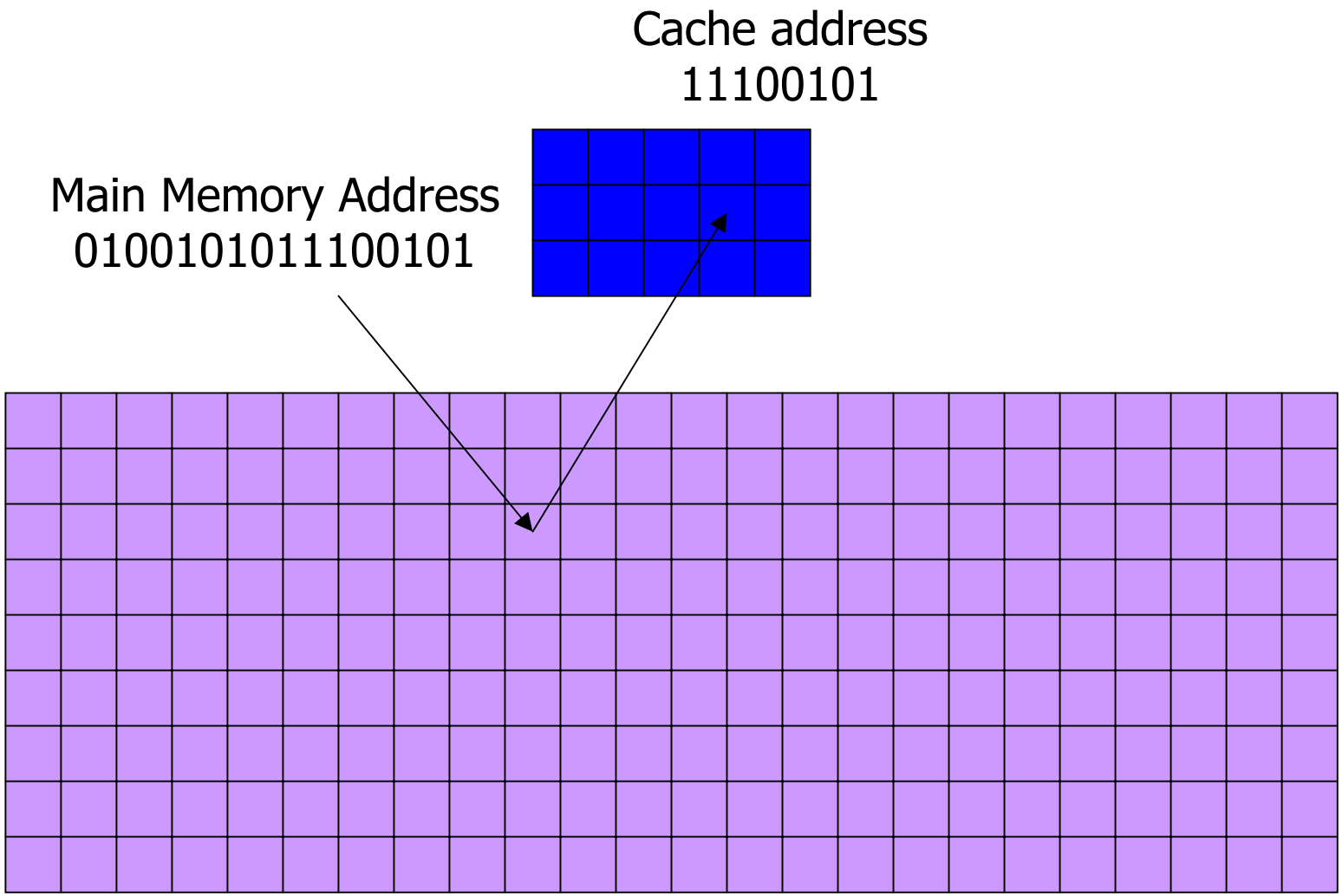


DON’T PANIC!

Direct Mapped Cache

Direct Mapped Cache is a scheme in which each location in memory corresponds to exactly one location in cache. Typically, if a cache address is represented by **c** bits, and a memory address is represented by **m** bits, then the cache location associated with address **A** is **MOD(A,2^c);** that is, the lowest **c** bits of **A**.

Direct Mapped Cache Example



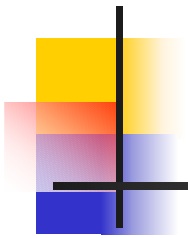
Problem with Direct Mapped

If you have two arrays that start in the same place relative to cache, then they can clobber each other– no cache hits!

```
REAL,DIMENSION(multiple_of_cache_size) :: a, b, c
INTEGER index

DO index = 1, multiple_of_cache_size
  a(index) = b(index) + c(index)
END DO !! Index = 1, multiple_of_cache_size
```

In this example, **`b(index)`** and **`c(index)`** map to the same cache line, so loading **`c(index)`** clobbers **`b(index)`**!

Fully Associative Cache



Fully Associative Cache can put any line of main memory into any cache line.

Typically, the cache management system will put the newly loaded data into the Least Recently Used cache line, though other strategies are possible.

Fully associative cache tends to be **expensive**, so it isn't common.

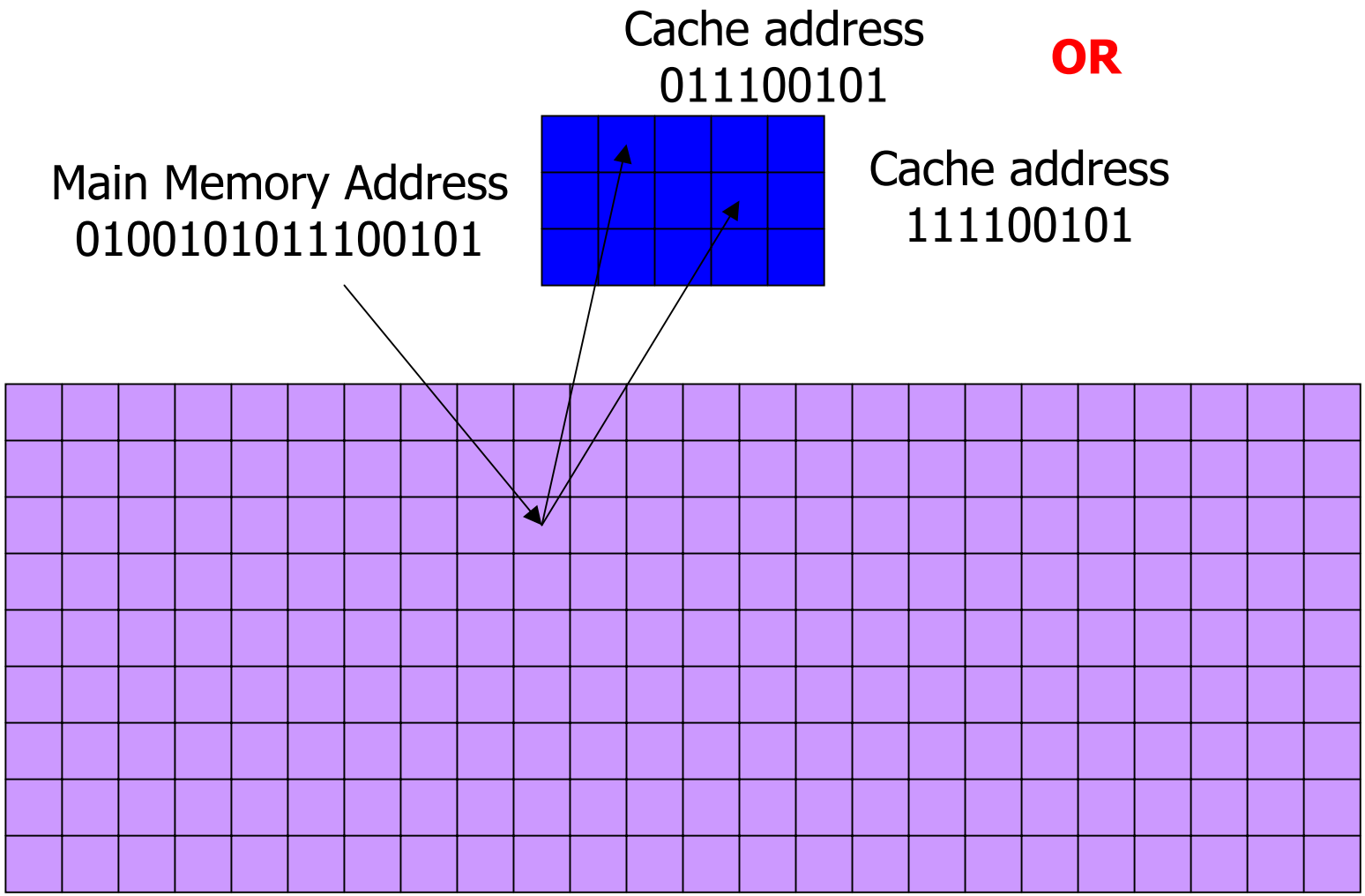
Set Associative Cache

Set Associative Cache is a compromise between direct mapped and fully associative. A line in memory can map to any of a fixed number of cache lines.

For example, 2-way Set Associative Cache maps each memory line to either of 2 cache lines (typically the least recently used), 3-way maps to any of 3 cache lines, 4-way to 4 lines, and so on.

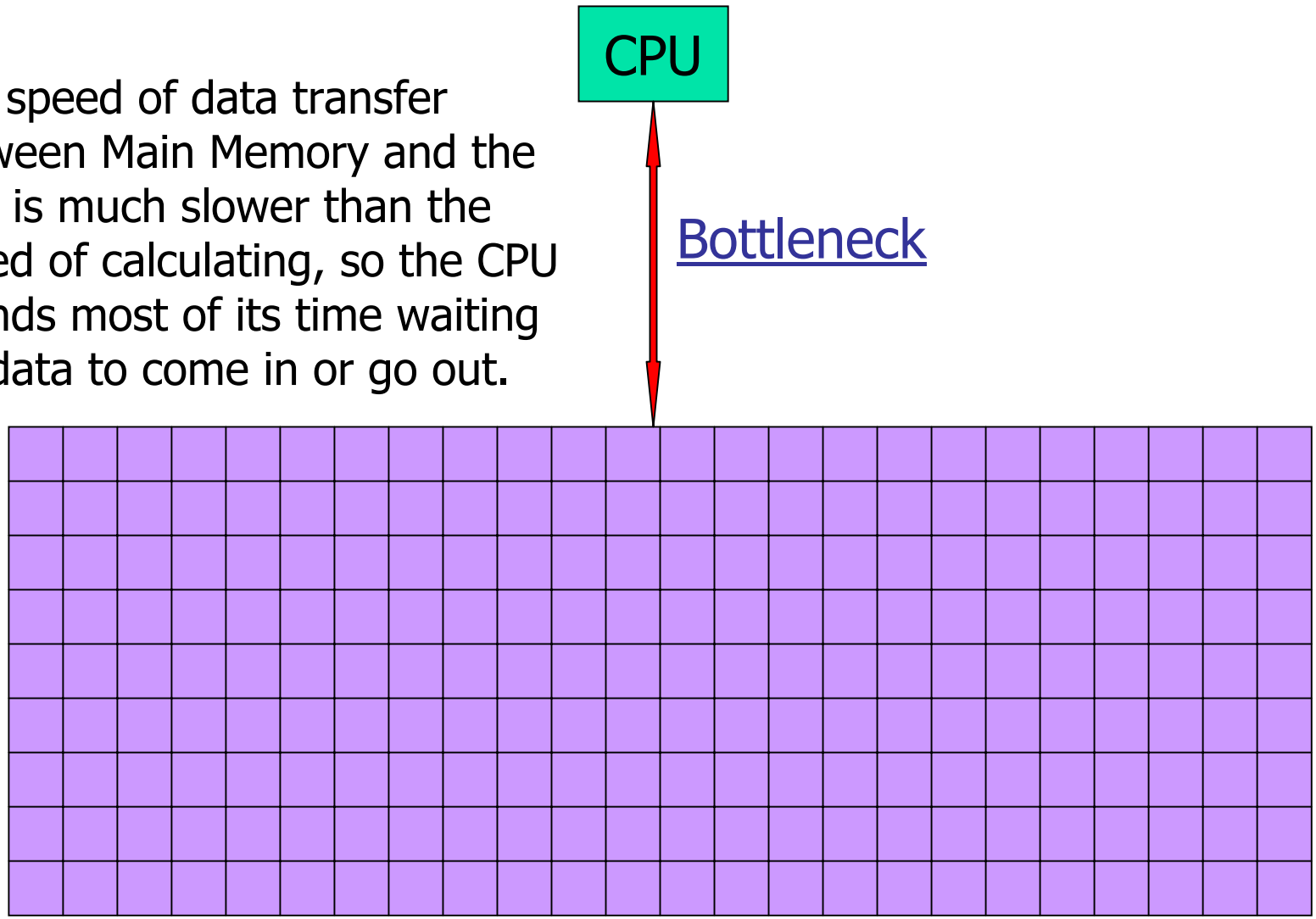
Set Associative cache is cheaper than fully associative but more robust than direct mapped.

2-way Set Associative Example



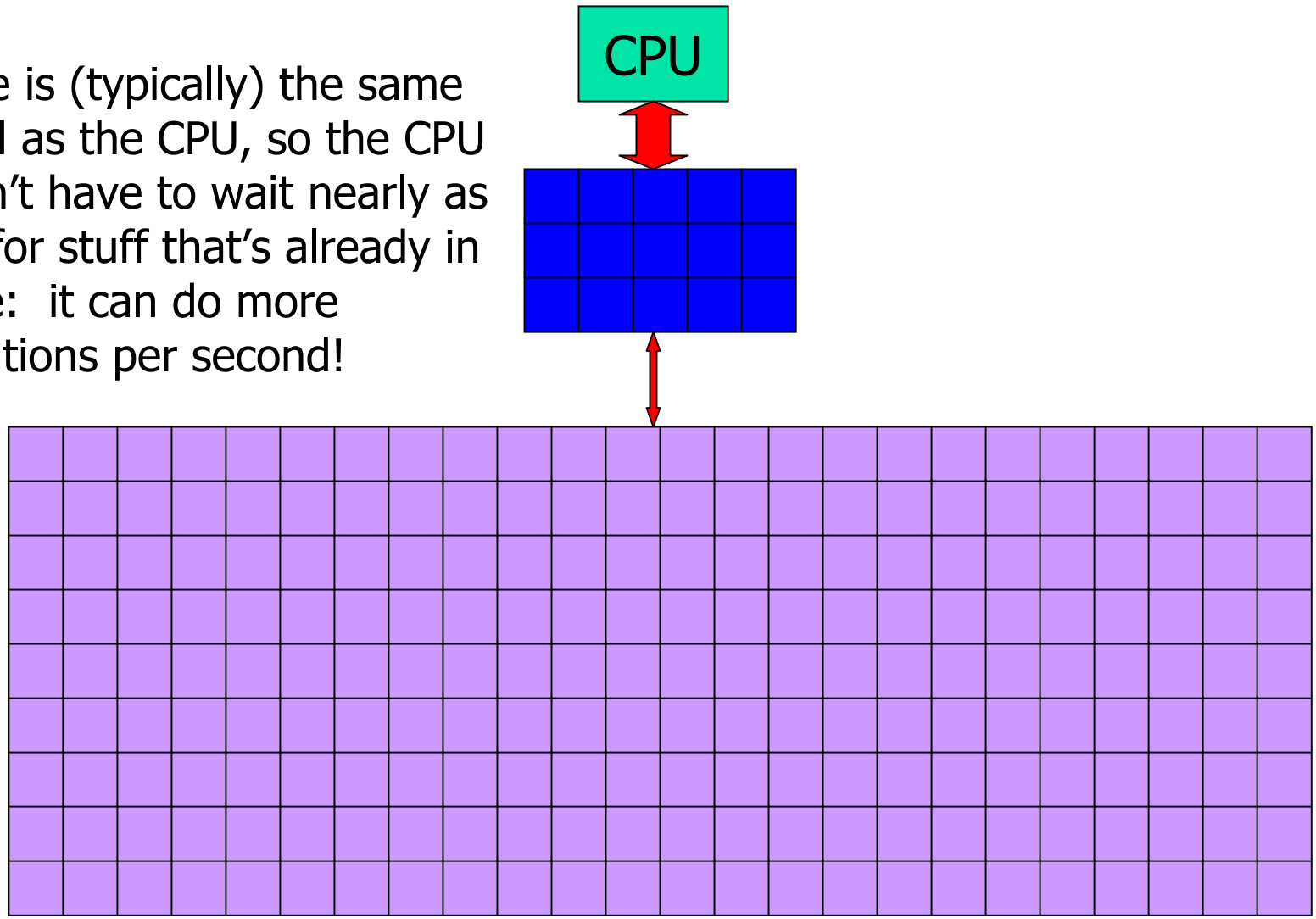
Why Does Cache Matter?

The speed of data transfer between Main Memory and the CPU is much slower than the speed of calculating, so the CPU spends most of its time waiting for data to come in or go out.

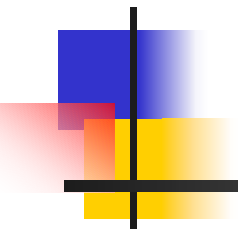


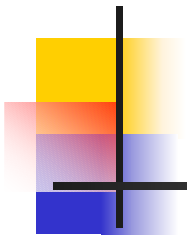
Why Have Cache?

Cache is (typically) the same speed as the CPU, so the CPU doesn't have to wait nearly as long for stuff that's already in cache: it can do more operations per second!



The Importance of Being Local





More Data Than Cache

Let's say that you have 1000 times more data than cache. Then won't most of your data be outside the cache?

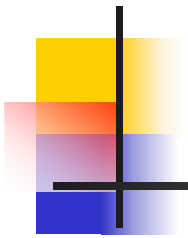
YES!

Okay, so how does cache help?

Cache Use Jargon

- Cache Hit: the data that the CPU needs right now is **already in cache**.
- Cache Miss: the data the the CPU needs right now is **not yet in cache**.
- If all of your data is small enough to fit in cache, then when you run your program, you'll get almost all cache hits (except at the very beginning), which means that your performance might be excellent!

Improving Your Hit Rate



Many scientific codes use a lot more data than can fit in cache all at once.

So, how can you improve your cache hit rate?

Use the same solution as in Real Estate:

Location, Location, Location!

Data Locality

- Data locality is the principle that, if you use data in a particular memory address, then very soon you'll use either the same address or a nearby address.
- Temporal locality: if you're using address **`A`** now, then you'll probably use address **`A`** again very soon.
- Spatial locality: if you're using address **`A`** now, then you'll probably next use addresses between **`A-k`** and **`A+k`**, where **`k`** is small.

Data Locality Is Empirical

Data locality has been observed empirically in many, many programs.

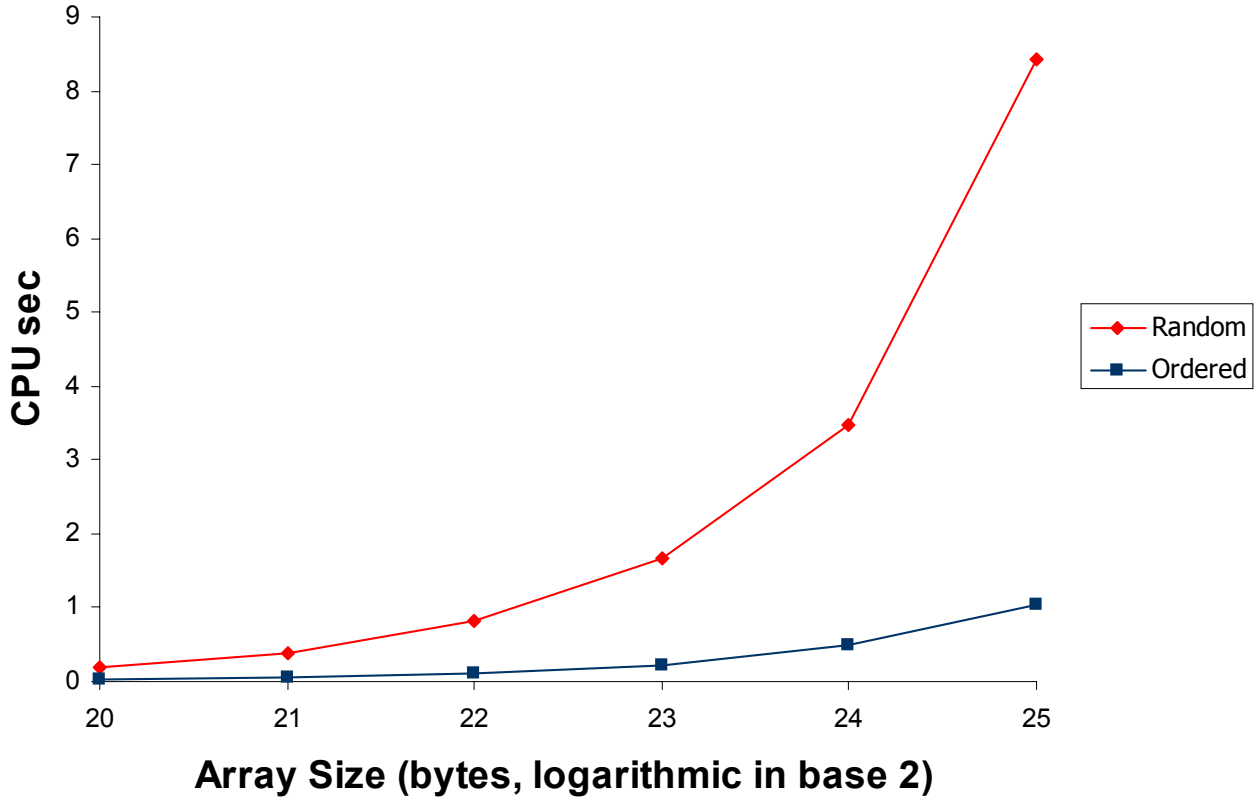
```
void ordered_fill (int* array, int array_length)
{ /* ordered_fill */
  int index;

  for (index = 0; index < array_length; index++) {
    array[index] = index;
  } /* for index */
} /* ordered_fill */
```

No Locality Example

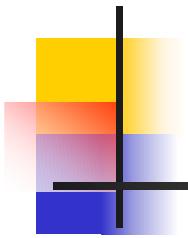
In principle, you could write a program that exhibited absolutely no data locality at all:

```
void random_fill (int* array,
                  int* random_permutation_index,
                  int array_length)
{ /* random_fill */
  int index;

  for (index = 0; index < array_length; index++) {
    array[random_permutation_index[index]] = index;
  } /* for index */
} /* random_fill */
```

Permuted vs. Ordered



In a simple array fill, locality provides a factor of 6 to 8 speedup over a randomly ordered fill on a Pentium III.



Exploiting Data Locality

If you know that your code is going to exhibit a decent amount of data locality, then you can get speedup by focusing your energy on improving the locality of the code's behavior.

A Sample Application

Matrix-Matrix Multiply

Let A, B and C be matrices of sizes $nr \times nc$, $nr \times nk$ and $nk \times nc$, respectively:

$$\mathbf{A} = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,nc} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,nc} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,nc} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{nr,1} & a_{nr,2} & a_{nr,3} & \cdots & a_{nr,nc} \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & \cdots & b_{1,nk} \\ b_{2,1} & b_{2,2} & b_{2,3} & \cdots & b_{2,nk} \\ b_{3,1} & b_{3,2} & b_{3,3} & \cdots & b_{3,nk} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{nr,1} & b_{nr,2} & b_{nr,3} & \cdots & b_{nr,nk} \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & \cdots & c_{1,nc} \\ c_{2,1} & c_{2,2} & c_{2,3} & \cdots & c_{2,nc} \\ c_{3,1} & c_{3,2} & c_{3,3} & \cdots & c_{3,nc} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_{nk,1} & c_{nk,2} & c_{nk,3} & \cdots & c_{nk,nc} \end{bmatrix}$$

The definition of $A = B\ C$ is

$$a_{r,c} = \sum_{k=1}^{nk} b_{r,k} \cdot c_{k,c} = b_{r,1} \cdot c_{1,c} + b_{r,2} \cdot c_{2,c} + b_{r,3} \cdot c_{3,c} + \ldots + b_{r,nk} \cdot c_{nk,c}$$

for $r \quad \{1, nr\}$, $c \quad \{1, nc\}$.

Matrix Multiply: Naïve Version

```
SUBROUTINE matrix_matrix_mult_by_naive (dst, src1, src2, &
 &                                      nr, nc, nq)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2

  INTEGER :: r, c, q

  CALL matrix_set_to_scalar(dst, nr, nc, 1, nr, 1, nc, 0.0)
  DO c = 1, nc
    DO r = 1, nr
      DO q = 1, nq
        dst(r,c) = dst(r,c) + src1(r,q) * src2(q,c)
      END DO !! q = 1, nq
    END DO !! r = 1, nr
  END DO !! c = 1, nc
END SUBROUTINE matrix_matrix_mult_by_naive
```

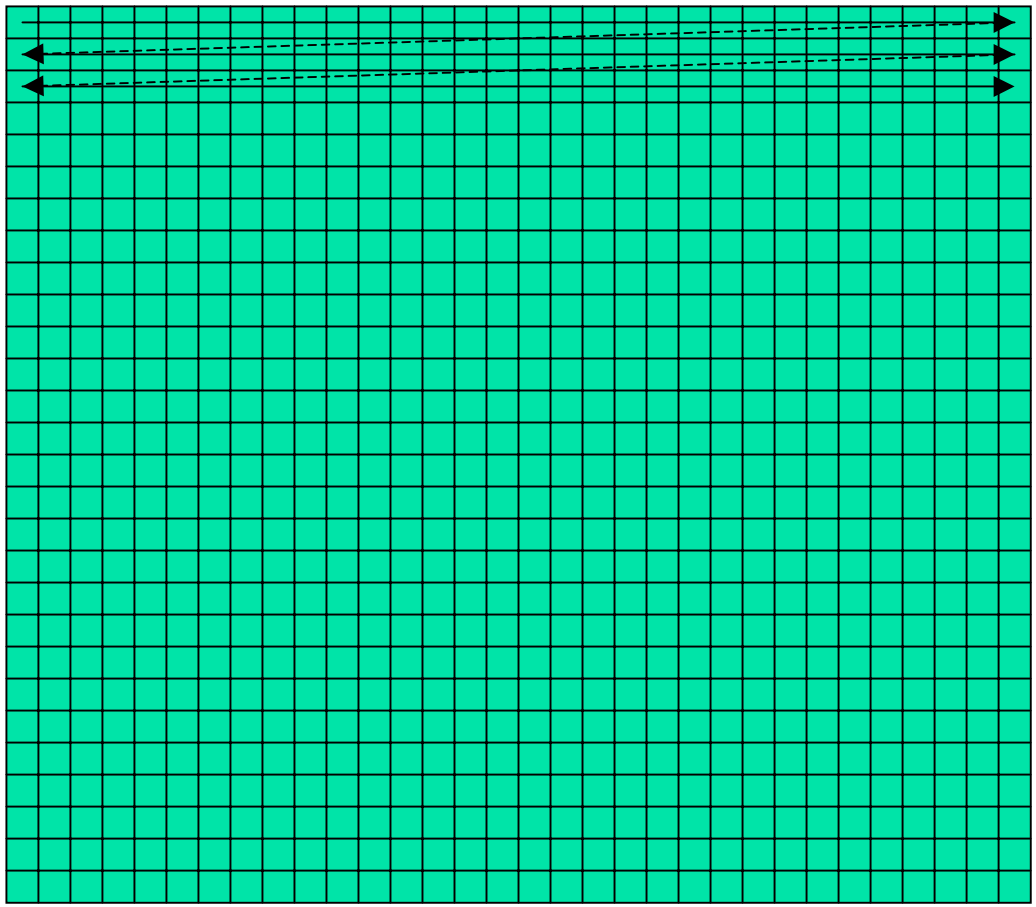
Matrix Multiply w/Initialization

```
SUBROUTINE matrix_matrix_mult_by_init (dst, src1, src2, &
 &                                     nr, nc, nq)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2

  INTEGER :: r, c, q

  DO c = 1, nc
    DO r = 1, nr
      dst(r,c) = 0.0
      DO q = 1, nq
        dst(r,c) = dst(r,c) + src1(r,q) * src2(q,c)
      END DO !! q = 1, nq
    END DO !! r = 1, nr
  END DO !! c = 1, nc
END SUBROUTINE matrix_matrix_mult_by_init
```

Matrix Multiply Via Intrinsic

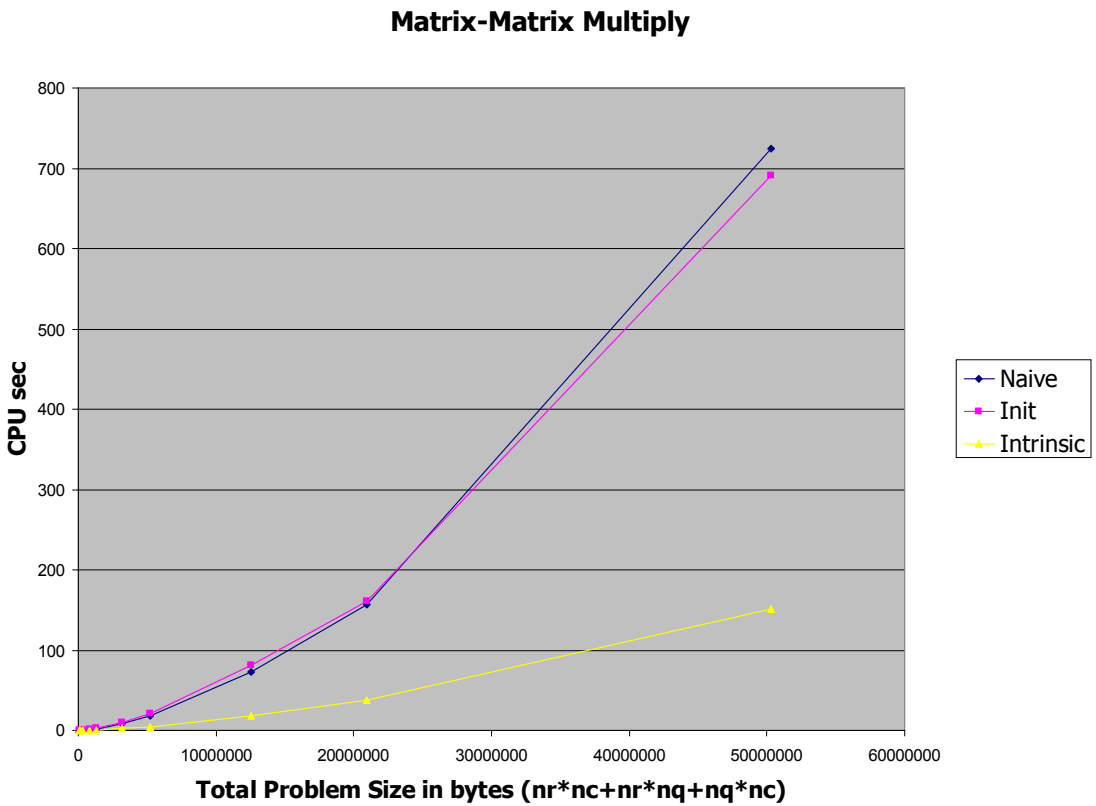
```
SUBROUTINE matrix_matrix_mult_by_intrinsic (dst, src1, src2,
   nr, nc, nq)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2

  dst = MATMUL(src1, src2)
END SUBROUTINE matrix_matrix_mult_by_intrinsic
```

Matrix Multiply Behavior

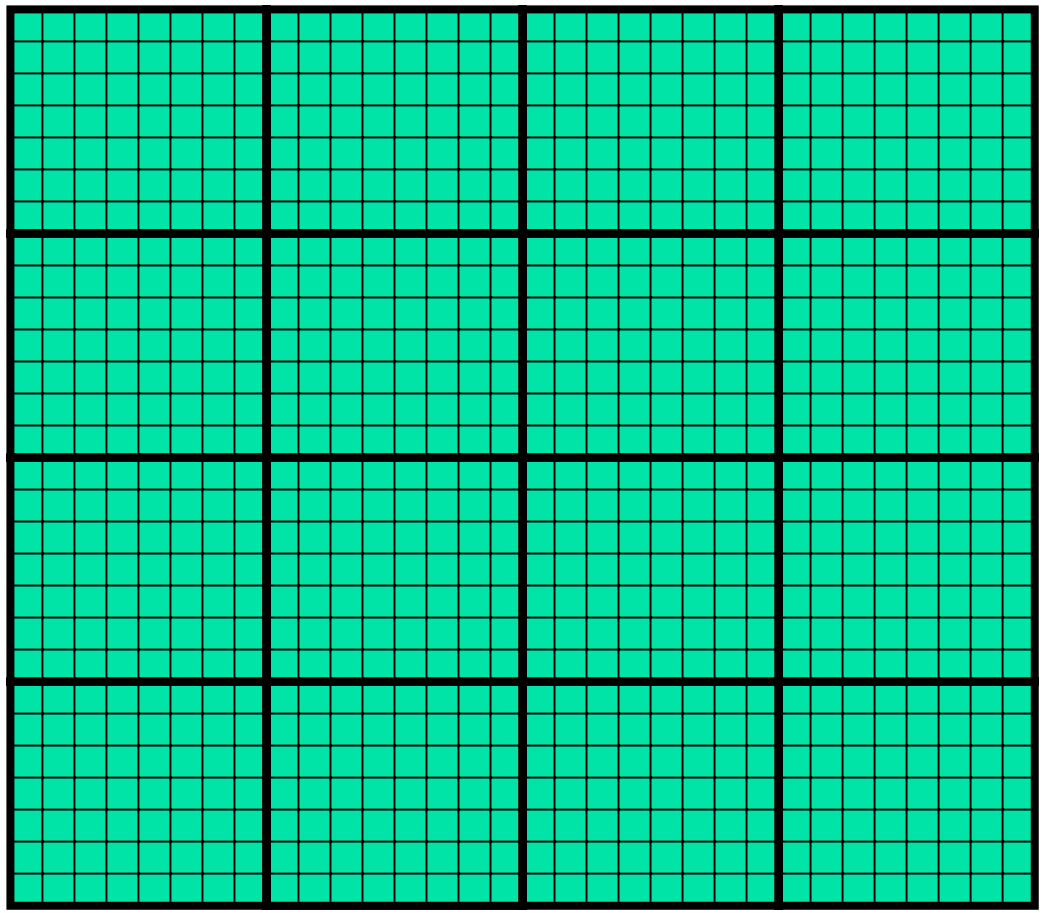


If the matrix is big, then each sweep of a row will clobber nearby values in cache.

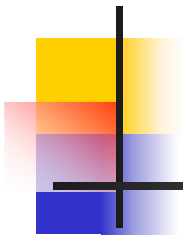
Performance of Matrix Multiply



Tiling



Tiling



- Tile: a small rectangular subdomain (chunk) of a problem domain. Sometimes called a block.
- Tiling: breaking the domain into tiles.
- Operate on each block to completion, then move to the next block.
- Tile size can be set at runtime, according to what's best for the machine that you're running on.

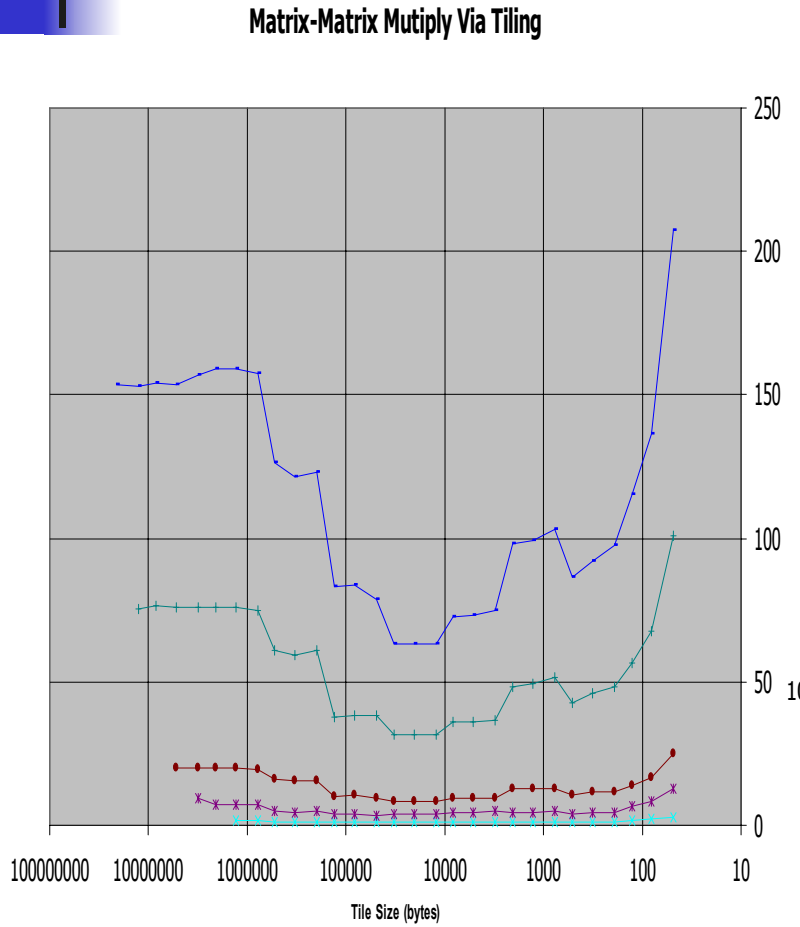
Tiling Code

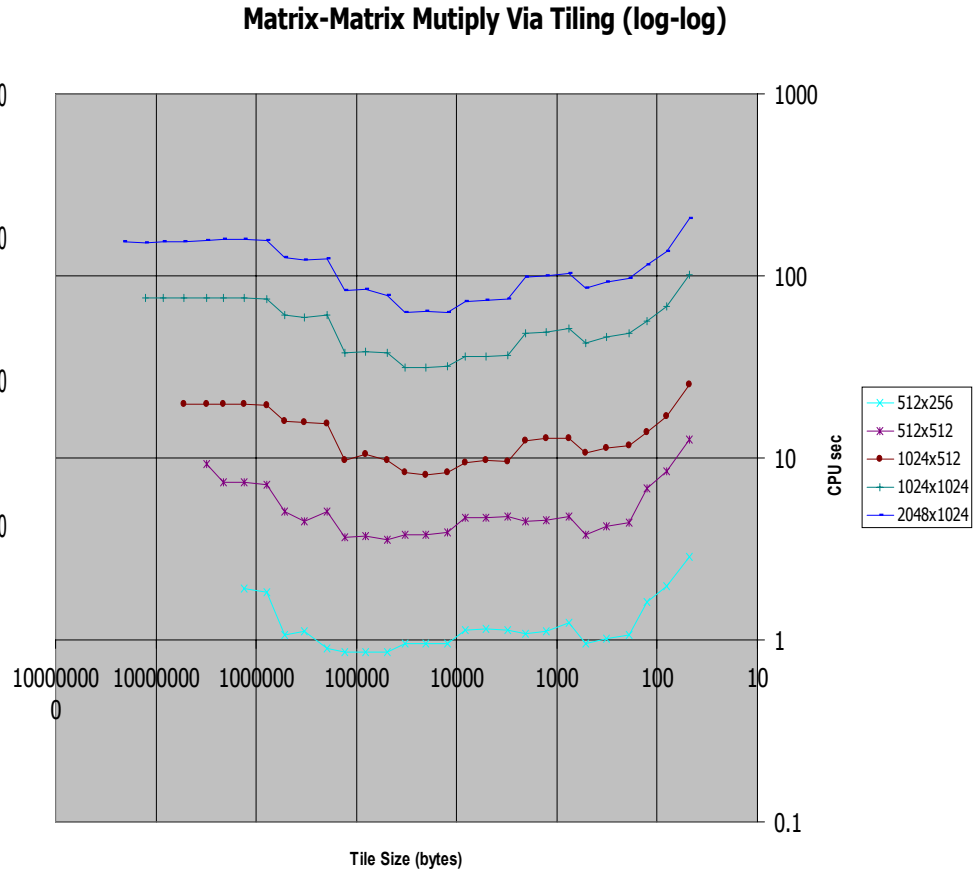
```
SUBROUTINE matrix_matrix_mult_by_tiling (dst, src1, src2, nr, nc, nq, &
 &           rtilesize, ctilesize, qtilesize)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2
  INTEGER,INTENT(IN) :: rtilesize, ctilesize, qtilesize

  INTEGER :: rstart, rend, cstart, cend, qstart, qend

  DO cstart = 1, nc, ctilesize
    cend = cstart + ctilesize - 1
    IF (cend > nc) cend = nc
    DO rstart = 1, nr, rtilesize
      rend = rstart + rtilesize - 1
      IF (rend > nr) rend = nr
      DO qstart = 1, nq, qtilesize
        qend = qstart + qtilesize - 1
        IF (qend > nq) qend = nq
        CALL matrix_matrix_mult_tile(dst, src1, src2, nr, nc, nq, &
 &                                   rstart, rend, cstart, cend, qstart, qend)
      END DO !! qstart = 1, nq, qtilesize
    END DO !! rstart = 1, nr, rtilesize
  END DO !! cstart = 1, nc, ctilesize
END SUBROUTINE matrix_matrix_mult_by_tiling
```

Multiplying Within a Tile

```
SUBROUTINE matrix_matrix_mult_tile (dst, src1, src2, nr, nc, nq, &
 &              rstart, rend, cstart, cend, qstart, qend)
  IMPLICIT NONE
  INTEGER,INTENT(IN) :: nr, nc, nq
  REAL,DIMENSION(nr,nc),INTENT(OUT) :: dst
  REAL,DIMENSION(nr,nq),INTENT(IN)  :: src1
  REAL,DIMENSION(nq,nc),INTENT(IN)  :: src2
  INTEGER,INTENT(IN) :: rstart, rend, cstart, cend, qstart, qend

  INTEGER :: r, c, q

  DO c = cstart, cend
    DO r = rstart, rend
      if (qstart == 1) dst(r,c) = 0.0
      DO q = qstart, qend
        dst(r,c) = dst(r,c) + src1(r,q) * src2(q,c)
      END DO !! q = qstart, qend
    END DO !! r = rstart, rend
  END DO !! c = cstart, cend
END SUBROUTINE matrix_matrix_mult_tile
```

Performance with Tiling

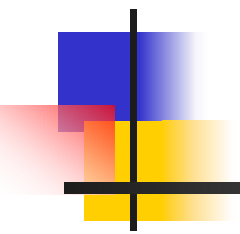




The Advantages of Tiling

- It lets your code to use more data locality.
- It's a relatively modest amount of extra coding (typically a few wrapper functions and some changes to loop bounds).
- If you don't need tiling – because of the hardware, the compiler or the problem size – then you can turn it off by simply setting the tile size equal to the problem size.

Hard Disk



Why Is Hard Disk Slow?

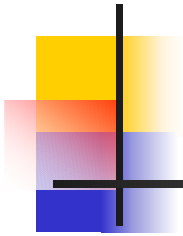
Your hard disk is **much much** slower than main memory (factor of 10-1000). **Why?**

Well, accessing data on the hard disk involves physically moving:

- the disk platter
- the read/write head

In other words, hard disk is slow because **objects** move much slower than **electrons**.

I/O Strategies



- Read and write the absolute minimum amount.
  - Don’t reread the same data if you can keep it in memory.
  - Write binary instead of characters.
  - Use optimized I/O libraries like NetCDF and HDF.

Avoid Redundant I/O

An actual piece of code recently seen:

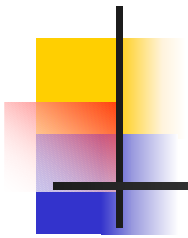
```
for (thing = 0; thing < number_of_things; thing++) {
  for (time = 0; time < number_of_timesteps; time++) {
    read(file[time]);
    do_stuff(thing, time);
  } /* for time */
} /* for thing */
```

Improved version:

```
for (time = 0; time < number_of_timesteps; time++) {
  read(file[time]);
  for (thing = 0; thing < number_of_things; thing++) {
    do_stuff(thing, time);
  } /* for thing */
} /* for time */
```

Savings (in real life): factor of 500!

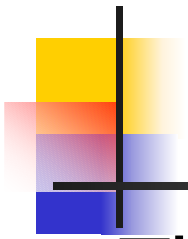
Write Binary, Not ASCII



When you write binary data to a file, you're writing (typically) 4 bytes per value.

When you write ASCII (character) data, you're writing (typically) 8-16 bytes per value.

So binary saves a factor of 2 to 4 (typically).



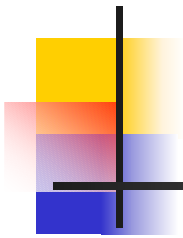
Problem with Binary I/O

There are many ways to represent data inside a computer, especially floating point data.

Often, the way that one kind of computer (e.g., a Pentium) saves binary data is different from another kind of computer (e.g., a Cray).

So, a file written on a Pentium machine may not be readable on a Cray.

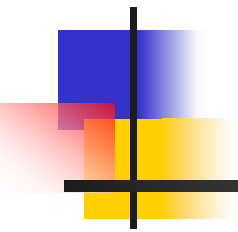
Portable I/O Libraries



NetCDF and HDF are the two most commonly used I/O libraries for scientific computing.

Each has its own internal way of representing numerical data. When you write a file using, say, HDF, it can be read by a HDF on **any** kind of computer.

Plus, these libraries are optimized to make the I/O **very fast**.



Virtual Memory

Virtual Memory

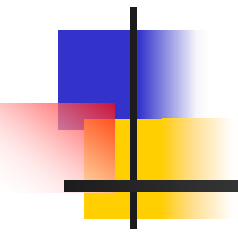
- Typically, the amount of memory that a CPU can address is larger than the amount of data physically present in the computer.
- For example, Henry's laptop can address over a GB of memory (roughly a billion bytes), but only contains 256 MB (roughly 256 million bytes).

Virtual Memory (cont'd)

- Locality: most programs don't jump all over the memory that they use; instead, they work in a particular area of memory for a while, then move to another area.
- So, you can offload onto hard disk much of the memory image of a program that's running.

Virtual Memory (cont'd)

- Memory is chopped up into many pages of modest size (e.g., 1 KB – 32 KB).
- Only pages that have been recently used actually reside in memory; the rest are stored on hard disk.
- Hard disk is 10 to 1000 times slower than main memory, so you get better performance if you rarely get a page fault, which forces a read from (and maybe a write to) hard disk: **exploit data locality!**



The Net

The Net Is Very Slow

The Internet is very slow, much much slower than your local hard disk. Why?

- The net is very busy.
- Typically data has to take several "hops" to get from one place to another.
- Sometimes parts of the net go down.

Therefore: **avoid the net!**

Storage Use Strategies

- Register reuse: do a lot of work on the same data before working on new data.
- Cache reuse: the program is much more efficient if all of the data and instructions fit in cache; if not, try to use what's in cache a lot before using anything that isn't in cache.
- Data locality: try to access data that are near each other in memory before data that are far.
- I/O efficiency: do a bunch of I/O all at once rather than a little bit at a time; don't mix calculations and I/O.
- The Net: **avoid it!**

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