



Scientific and Technical Computing

Hardware and Code Optimization

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UT Austin, 9/22/20 & 9/27/20 & 10/6/20

Our Computer: CPU, Cache, Memory, 'Connection'

CPU

1. Pipelined operation

System designed to get 1 opc

Memory

1. Data streams

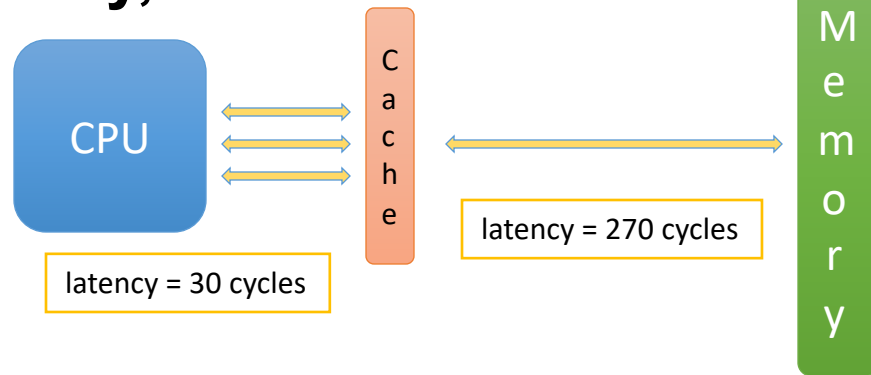
System designed to support 1 wpc (for one row)

Caches

1. Managed by run-time
2. Cache size (for stencil update)

System designed for 'enough' bandwidth to support 2 rows

Size: at least $3 \times n$ words



Our computer has been somewhat 'hypothetical' so far
We have designed the specs so that we get 'optimal' performance for a stencil update

Concurrency!

Our Computer: CPU, Cache, Memory, 'Connection'

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1. Pipelined operation

System designed to get 1 opc

Memory

1. Data streams

System designed to support 1 wpc (for one row)

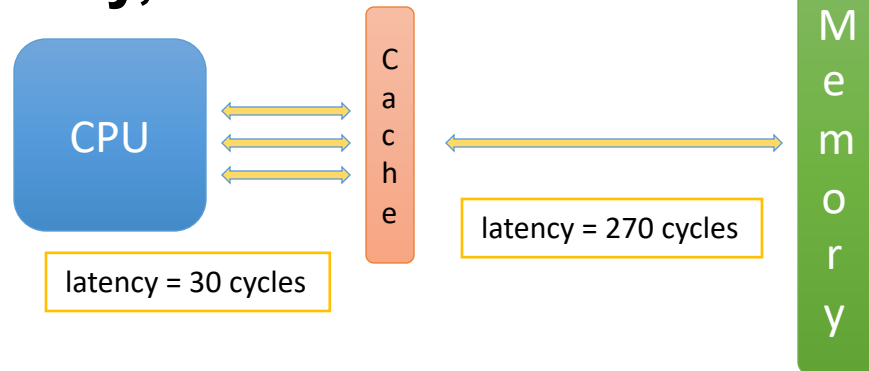
Caches

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2. Cache size (for stencil update)

System designed for 'enough' bandwidth to support 2 rows

Size: at least $3 \times n$ words

Our computer has been somewhat 'hypothetical' so far
We have designed the specs so that we get 'optimal' performance for a stencil update



Requirement: Size of the cache = $3 \times n$

n could be any number, any large number

Size of cache in hardware certainly not adjustable
Also differences between chip generations

Outline

CPU & Memory, latency, bandwidth, wpc,
opc ...

Data streaming, pipelining, caches (part 1)

Caches: software (short)

Caches (working principles)

There are at least 4 ‘working principles’
that we have to cover

My ‘big’ plan

Cover many hardware fundamentals as they guide code design

- loosely in decreasing order of importance

For each hardware feature:

Add details as necessary to describe a simplified, yet functional
‘working model’

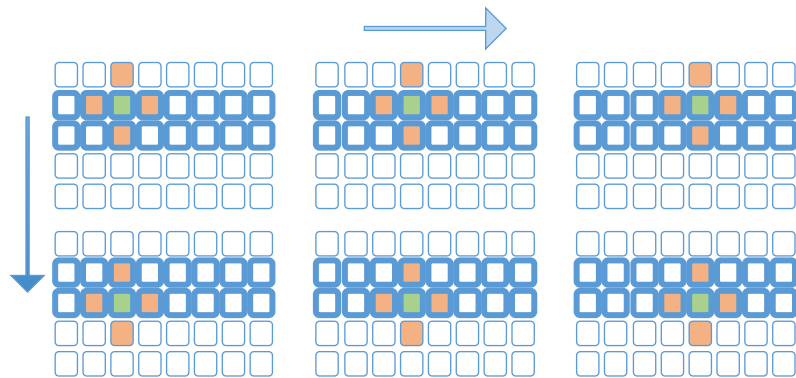
Discussion: Working around the size limitation

Example:

$n=500$, cache size=300 words

At what iteration ' i ' do we (approximately) start to replace data in the cache?

- ' i ' is inner loop



```
do j=1, n
  do i=1, n
    y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
  enddo
enddo
```

Discussion: Working around the size limitation

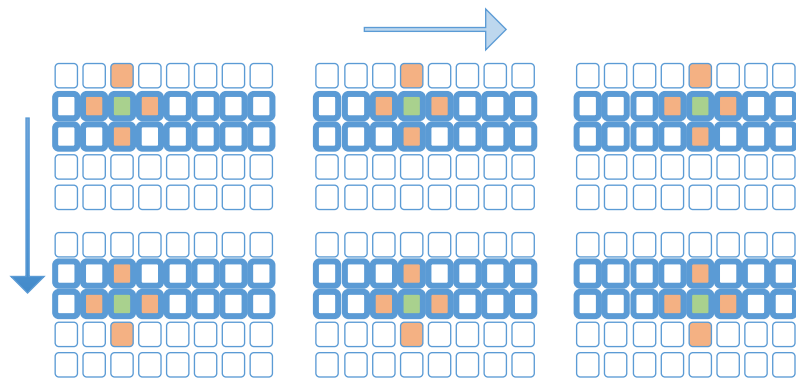
Example:

$n=500$, cache size=300 words

At what iteration ' i ' do we (approximately) start to replace data in the cache? $i \sim 100$

So what do we do when we reach ' $i=100$ '

- Hint: going further to the right is a 'dead end'



```
do j=1, n
  do i=1, n
    y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
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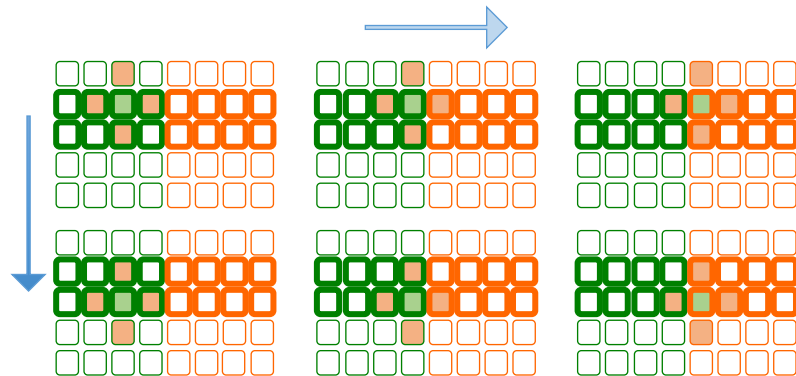
$n=500$, cache size=300 words

At what iteration 'i' do we (approximately) start to replace data in the cache? $i \sim 100$

What do we do when we reach 'i=100'?

- Hint: going further to the right is a 'dead end'
- So we go one row down
- The green area first, then the orange area

How do we do this in code?



```
do j=1, n
  do i=1, n
    y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
  enddo
enddo
```

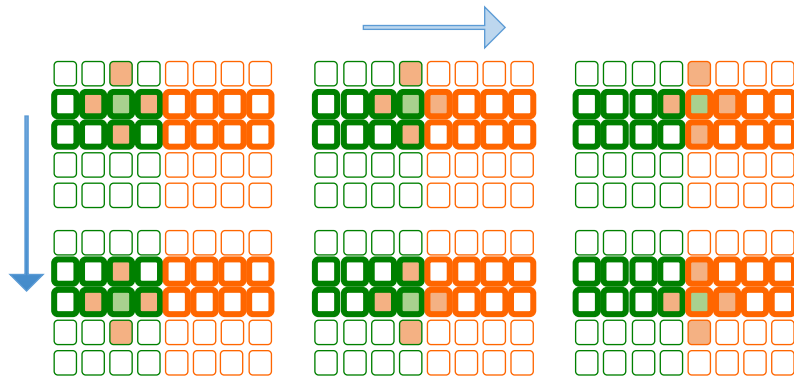
Discussion: Working around the size limitation

Example:

n=500, cache size=300 words

So how do we do this in code?

- What is the width of a strip?
- How many strips?
- How many loops in the code?



```
do j=1, n
  do i=1, n
    y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
  enddo
enddo
```

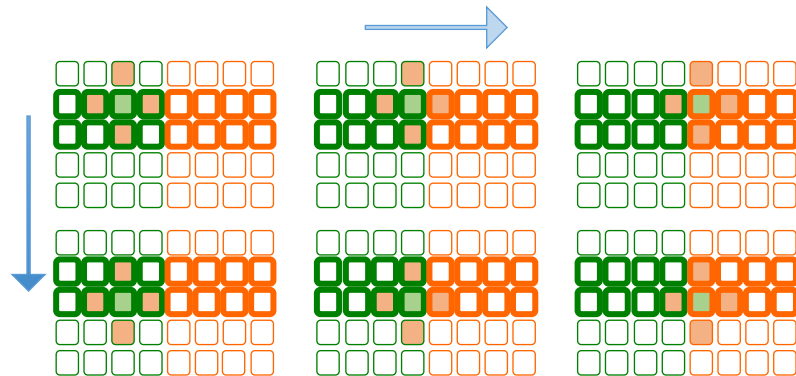

Discussion: Working around the size limitation

Example:

n=500, cache size=300 words

So how do we do this in code?

- What is the width of a strip? 100
- How many strips? 5
- How many loops in the code? 3 (up from 2)



```
n = 500; ns = 100
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
    enddo
  enddo
enddo
```

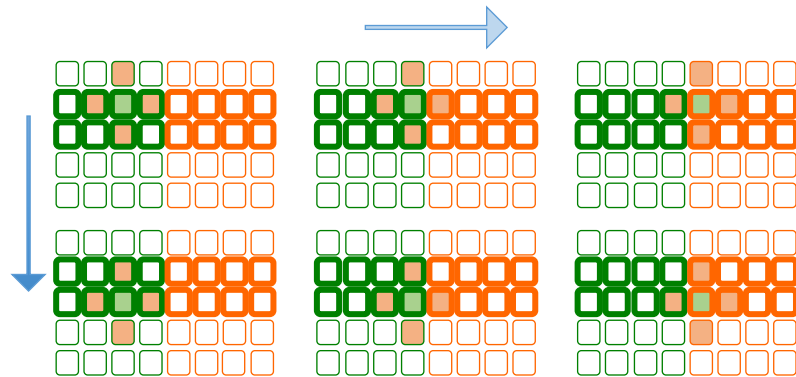
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$n=500$, cache size=300 words

So how do we do this in code?

- What is the width of a strip? 100
- How many strips? 5
- How many loops in the code? 3 (up from 2)



```
n = 500; ns = 100
do iout=1, n/ns
  do j=1, n
    is = (iout-1) * ns + 1      (1, 101, 201, 301, 401)
    ie = iout * ns              (100, 200, 300, 400, 500)
    ie = is + ns - 1            (equivalent formulation)
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
    enddo
  enddo
enddo
```

Discussion: Working around the size limitation

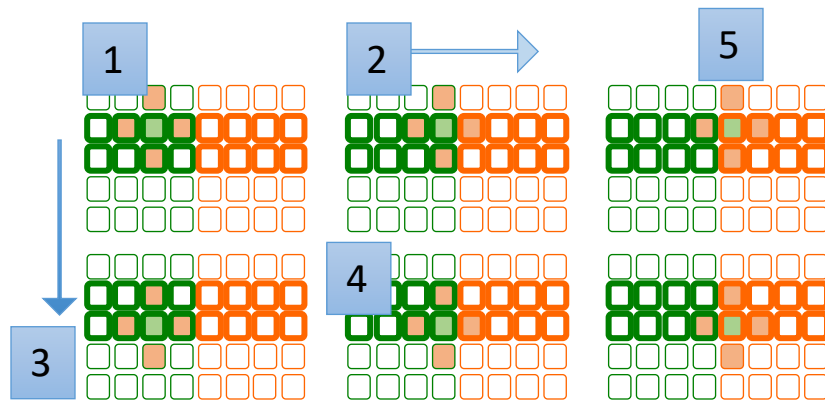
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So how do we do this in code?

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```
n = 500; ns = 100
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 *
    enddo
  enddo
enddo
```



We go left to right fast (**x**-direction)

We go slowly in **y**-direction

Hence left to right is the inner loop. Loop index is '**i**'

The 'fast' loop, i.e. the inner loop 'exceeds' to size of the cache

We split up the inner loop in 2 loops. Indexes '**i**' and '**iout**'

The loop '**j**' that re-uses the data of the inner loop is in the middle

is and **ie** are set so that the pair of loops (**i** and **iout**) covers the whole computational domain, left to right, exactly once

Cache blocking

Re-use data before it is evicted

Breaking a loop into 2 (or more) parts

(There can be cache blocking for multiple loops)

Note:

In our example we have been overly optimistic

Width of the strip stretched to the max

Real application: other data is also stored in cache
(there are also other processes)

Let's fill in the blanks

```
n = 500; ns = 100
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
    enddo
  enddo
enddo
```

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Real application: other data is also stored in cache
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Be aware that for arbitrary pairs (n,ns) the code will be more complicated

Consider:

N=495; ns=100

```
n = 495; ns = 100
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
    enddo
  enddo
enddo
```

Cache blocking

Re-use data before it is evicted

Breaking a loop into 2 (or more) parts

There can be cache blocking for multiple loops

1. Be aware that for arbitrary pairs (n,ns) the code will be more complicated

2. Cache size=300 → ns=100
ns is way(!) too large (by 2×)
Why?

Note:

In our example we have been overly optimistic

Width of the strip stretched to the max

Real application: other data is also stored in cache
(there are also other processes)

In our example, why should the width of the strip (ns) be smaller than 50?

```
n = 500; ns = 100
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
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Cache blocking

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In our example, why should the width of the strip (ns) be smaller than 50?

Usually numerical tests (trials) are used to determine a suitable size for the cache blocking

Tests are repeated, if:

- Architecture changes (different machine)
- Implementation changes (more/less data in loop kernel)

```
n = 500; ns = 100
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
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enddo
```

Cache blocking

Re-use data before it is evicted

Breaking a loop into 2 (or more) parts

There can be cache blocking for multiple loops

2. Cache size=300 → ns=100
ns is way(!) too large (by 2×)
Why?

Everything moving between
memory and CPU is cached:

Not just 'x' but also 'y'

Note:

In our example we have been overly optimistic

Width of the strip stretched to the max

Real application: other data is also stored in cache
(there are also other processes)

In our example, why should the width of the strip (ns) be
smaller than 50?

```
n = 500; ns = 50
do iout=1, ...
  do j=1, n
    is = ...
    ie = ...
    do i=is, ie
      y(i,j) = 0.25 * (x(i-1,j) + x(i+1,j) + x(i,j-1) + x(i,j+1))
    enddo
  enddo
enddo
```


Limitations

Conflicting goals

- Purpose of cache: fast --- low latency/high bandwidth
- Organization of cache: FIFO (First In - First Out) or LRU

Match or no-match?

How do we find a match?

How do we find an element to evict?

4	6	12	11
5	1	14	10
9	8	2	3
7	15	13	16

Problems to tackle

1. Speed
2. FIFO
3. Storage efficiency

For illustration purposes
Cache is drawn as a 2d 'array'
You can imagine that the cache is organized as a 1d array

Basic principle

The cache is small, therefore it can hold data only for a (very) limited time (time in cycles)

How long (# of cycles) and how often data is re-used depends on the code (implementation of the algorithm)

Limitations

Conflicting goals

- Purpose of cache: fast --- low latency/high bandwidth
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Keep in this in mind when thinking about how a cache works:

- The cache stores where the data came from, i.e. the original address
- The cache stores the actual value

These numbers are the addresses, not the actual data
Assume that in this example we encounter the addresses
consecutive and in order.

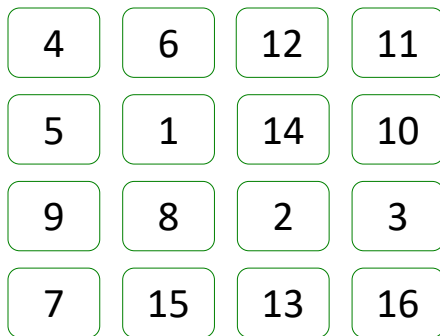
So address '1', and its content, was stored first,
i.e. is the oldest

Address '2', and its content, is the second oldest
Address '16' was stored last

Match or no-match?

How do we find a
match?

How do we find an
element to evict?



4	6	12	11
5	1	14	10
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Problems to tackle

1. Speed
2. FIFO
3. Storage efficiency

For illustration purposes
Cache is drawn as a 2d 'array'
You can imagine that the cache is organized as a (long) 1d array

Example:

Loading element #3: This element is stored in the cache. How do we find element #3

Loading element #17: This is not a match; #17 loaded from memory and will replace oldest element in cache

Limitations: The Cache can be quite large

Conflicting goals

- Purpose of cache: fast --- low latency/high bandwidth
- Organization of cache: FIFO (First In- First Out) or LRU

Note:

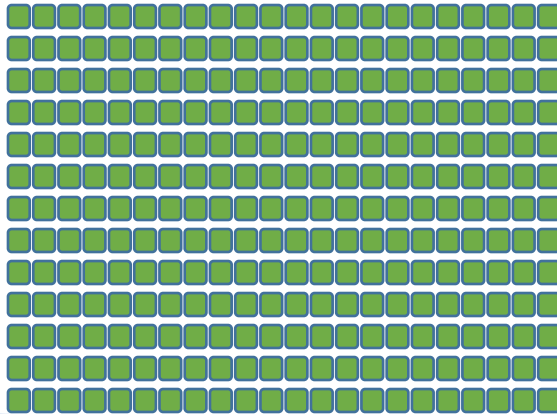
For every cell in the cache the original address must be stored

Address = 1 word

Therefore half the cache stores addresses

Half the cache stores data

... and then some ordering is needed



OK, for a cache holding 16 words we may be able to compare all addresses and also make FIFO work

Cache size may exceed 1Mw

More that a million entries

(1Mw = 4 or 8 Mb)

So how can we devise a fast strategy?

Let's tackle 'fast access' first,
and the add some FIFO
and then storage efficiency

Example: Let's make our cache access fast

Let's make up some address space notation

- Address (main memory) has 6 digits
- Each digit holds a value between 1 and 4
- Example 142314

We encounter addresses in this order

141423

141424

141431

443311

141432

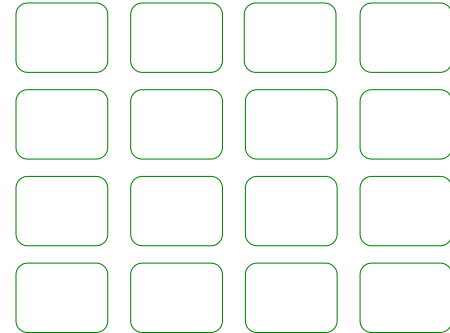
141433

121111

...

How can we **map** our addresses into the cache address space?

Our cache



Example: Let's make our cache fast

Let's make up some address space notation

- Address has 6 digits
- Each digit holds a value between 1 and 4

We encounter addresses in this order

What if I write it like this

1414 23

1414 24

1414 31

4433 11

1414 32

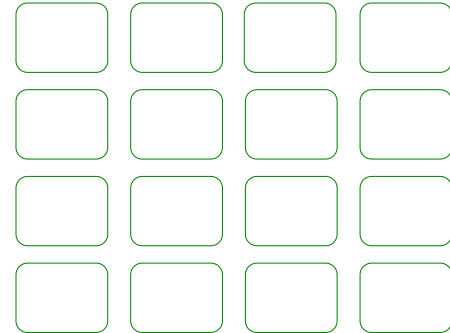
1414 33

1211 11

...

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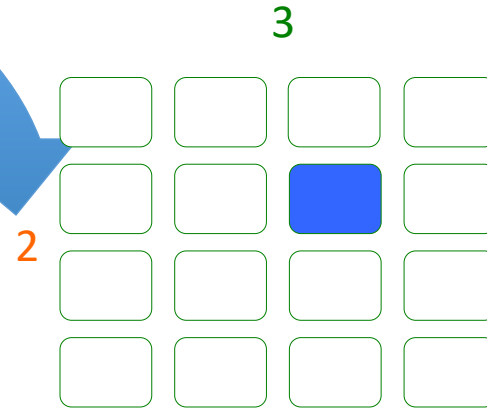
1414 32

1414 33

1211 11

...

How can we **map** our addresses into the cache address space?



Algorithm

CPU reads address

CPU checks if data is stored in cache

(How many storage locations have to be checked?)

1. If yes, read it from there
2. If no, read data from memory and store it also in cache

How does this implementation accelerate data access?

Cache with Direct Mapping

Let's make up some address space notation

- Address has 6 digits
- Each digit holds a value between 1 and 4

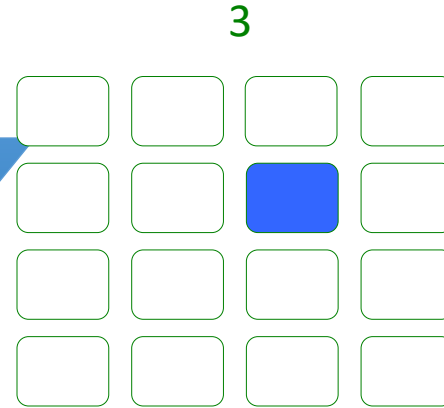
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What if I write it like this

1414 23
1414 24
1414 31
4433 11
1414 32
1414 33
1211 11

...

How can we **map** our addresses into the cache address space?



Direct Mapping (many to one)

Every element in main memory can be stored
In exactly one cache location

Problems

1. No FIFO --- Why?
2. Why do some access patterns render caching ineffective?

Cache with Direct Mapping: Problems

Conflicting goals

- Purpose of cache: fast --- low latency/high bandwidth
- Organization of cache: FIFO (First In- First Out) or LRU

Example: array with 16×16 elements

Assume row major ordering

Loop through the first column

How far are these elements apart in main memory addresses

$a(1,1)$, $a(1,2)$, $a(1,3)$?

or

$a[0,0]$, $a[1,0]$, $a[2,0]$ for column major ordering?

4	6	12	11
5	1	14	10
9	8	2	3
7	15	13	16

Cache with Direct Mapping: Problems

Conflicting goals

- Purpose of cache: fast --- low latency/high bandwidth
- Organization of cache: FIFO (First In- First Out) or LSR

Example: array with 16×16 elements

Assume row major ordering

Loop through the first column

How far are these elements apart in main memory addresses

$a(1,1)$, $a(1,2)$, $a(1,3)$?

Answer: The distance is 16

Example addresses are:

4422 22

4423 22

4424 22

So where are these elements mapped in the cache?

4	6	12	11
5	1	14	10
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Cache with Direct Mapping: Problems

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Example addresses are:

4422 22

4423 22

4424 22

4	6	12	11
5	1	14	10
9	8	2	3
7	15	13	16

So were are these elements mapped in the cache? All to the same element
Therefore our cache has a reduced effective size (In our case just one element)

Cache Associativity

Let's make up some address space notation

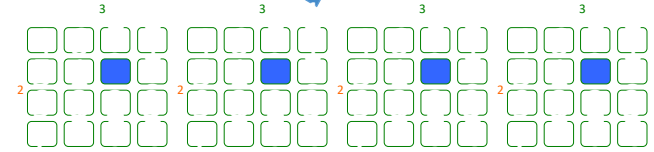
- Address has 6 digits
- Each digit holds a value between 1 and 4

We encounter addresses in this order

What if I store it like this

1414 23
1414 24
1414 31
4433 11
1414 32
1414 33
1211 23
4433 23
...

Example: Cache with 4-way associativity



An element of data may be cached in 1 of 4 locations
FIFO: replace the 'oldest' data element (out of the 4)

Advantages of Caches with Associativity

1. Ineffective mapping alleviated (somewhat)
 2. Compare addresses only for few (4) locations
 3. Eviction policy FIFO or LRU schedule
 4. Keep 'age' for few (4) entries
- (In principle, 'random' eviction could work, too)

Cache: So far

What we have addressed so far

Why caches?

Cache blocking

Address mapping

Associativity

- fully associative, set-associative, direct mapping

Remaining problem

For each 'cell' in the cache we store the

- data (that's what we are interested in)
- where the data came from (i.e. the address in main memory)

50% is useful (to us)

50% is book keeping

We can do better! But how?

Requirements

Know what is stored (full address)

Know how 'old' the data is (within associativity)

Finding data

Compare address with address in cache

Two possibilities

1. Match: load data from cache
2. No match: Load from memory, evict oldest data, store new data in place

Does this help us?

$$a(i) = b(i) + c(i)$$

```
loop with index i  
  a(i) = b(i) + c(i)  
end loop
```

Can data streams help us reducing the overhead
of book keeping?

Improve Cache Efficiency

Let's make up some address space notation

- Address has 6 digits
- Each digit holds a value between 1 and 4

Streams of data: a, b, c

1414 11

1414 12

1414 13

1414 14

3722 31

3722 32

3722 33

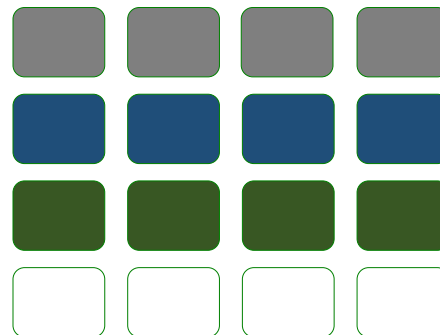
3722 34

2344 21

2344 22

2344 23

2344 24



Consecutive (in memory) elements of a, b, and c are loaded
Elements of a, b, and c are cached in consecutive locations

Improve Cache Efficiency

Let's make up some address space notation

- Address has 6 digits
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1414 11

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3722 32

3722 33

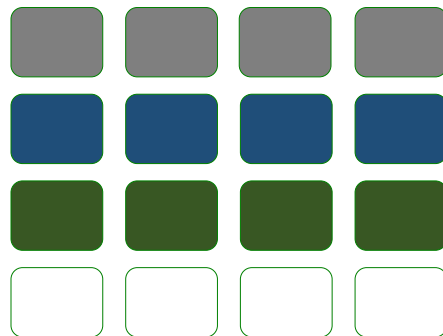
3722 34

2344 21

2344 22

2344 23

2344 24



Consecutive (in memory) elements of a, b, and c are loaded
Elements of a, b, and c are cached in consecutive locations

Let's take advantage and keep only track of consecutive
tuples of 8/16 words (double/single precision), i.e. 512 bits

Cache Lines

Let's make up some address space notation

- Address has 6 digits
- Each digit holds a value between 1 and 4

Streams of data: a, b, c

1414 11

1414 12

1414 13

1414 14

3722 31

3722 32

3722 33

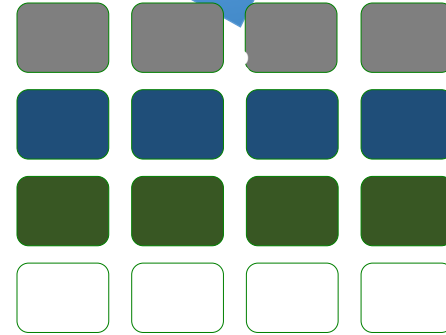
3722 34

2344 21

2344 22

2344 23

2344 24



Complete cache lines are moved between memory, cache, and CPU
1 cache line: 512 bits (x86 architecture), or 8 words (dp), or 16 words (sp)

Book keeping is done per cache line (reduction by 7/8 or 15/16)

Assumption: It is likely that the code uses all elements rather than only 1

$a(i) = b(i) + c(i)$: 3 streams each with consecutive data access

Is this always efficient? What would be a setup (addresses) were this works with limited efficiency?

Cache Lines

Let's make up some address space notation

- Address has 6 digits
- Each digit holds a value between 1 and 4

Streams of data: a, b, c

1414 11

1414 12

1414 13

1414 14

3722 31

3722 32

3722 33

3722 34

2344 21

2344 22

2344 23

2344 24

Complete cache lines are moved between memory, cache, and CPU

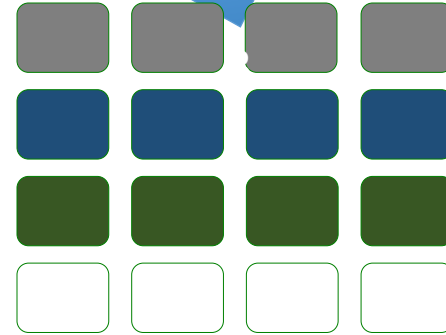
1 cache line: 512 bits, or 8 words (dp), or 16 words (sp)

Book keeping: per cache line (reduction by 7/8 or 15/16)

Assumption: It is likely that the code uses all elements rather than only 1

$a(i) = b(i) + c(i)$: 3 streams each with consecutive data access

Is this always efficient? What would be a setup (addresses) were this works with limited efficiency?



What will happen here?

Loop with index i
 $a(2 \times i) = b(2 \times i) + c(2 \times i)$

Cache Lines

Let's make up some address space notation

- Address has 6 digits
- Each digit holds a value between 1 and 4

Streams of data: a, b, c

1414 11

1414 12

1414 13

1414 14

3722 31

3722 32

3722 33

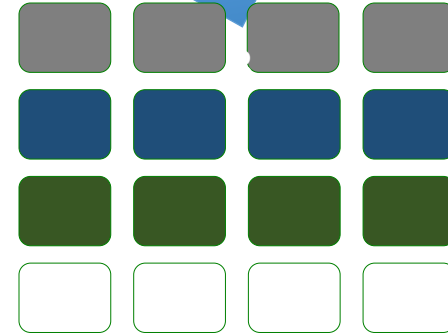
3722 34

2344 21

2344 22

2344 23

2344 24



Complete cache lines are moved between memory, cache, and CPU

1 cache line: 512 bits, or 8 words (dp), or 16 words (sp)

Book keeping: per cache line (reduction by 7/8 or 15/16)

Assumption: It is likely that the code uses all elements rather than only 1

$a(i) = b(i) + c(i)$: 3 streams each with consecutive data access

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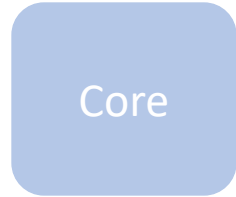
Bandwidth reduced by 2×

But wait ...

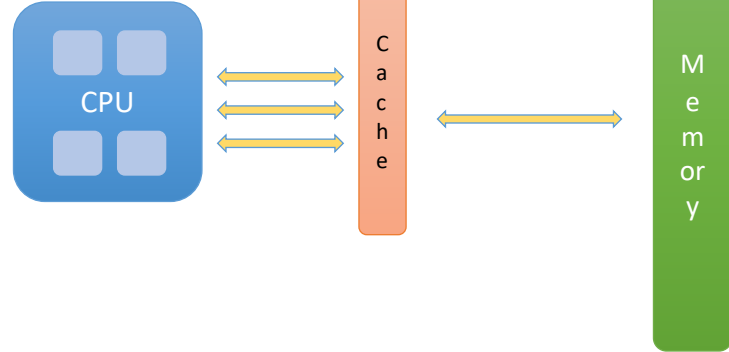
There is more!

about caches

Our Toy Computer with multi-core CPUs



Example with 4 cores



Stampede2

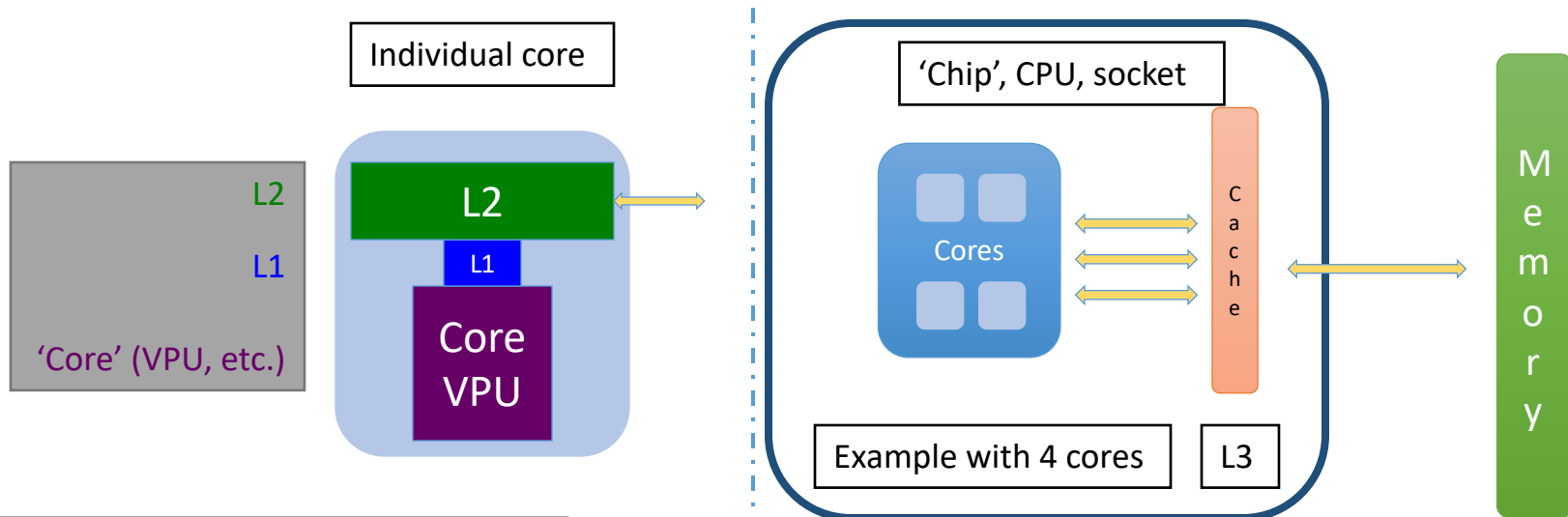
A socket/CPU has 24 cores

The total number of caches is 49

How many caches are there

- Per core?
- Per CPU?

Our Toy Computer with multi-core CPUs



Stampede2

A socket/CPU has 24 cores
The total number of caches per CPU is 49

How many caches are there

- Per core? 2 (L1 and L2)
- Per CPU? 1 (L3)

Feel sorry for the
'bookkeeper' at
least once!

Sizes

L1: 32 KB	very close, very fast
L2: 1MB	close and fast
L3: 33MB	Farther, but still on-chip

Stampede2 nodes have 2 sockets
Total number of caches is 98

More book keeping

Bookkeeping: MOESI Protocol

For now, only consider **reading data**

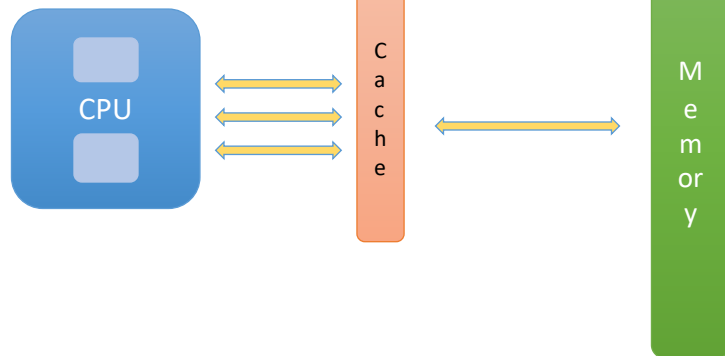
... = $b(i) + \underline{c(i)}$

We start the loop, reading $c(1)$ on core 0

1. Cache line for $c(1:8)$ is in main memory
2. Cache line moves to L3
3. Cache line moves to L2
4. Cache line moves to L1
5. 'somehow' we perform the operation

So where do we read $c(2)$ from?

Example with 2 cores



MOESI Protocol

For now, only consider **reading data**

... = $b(i) + \underline{c(i)}$

We start the loop, reading $c(1)$ on core 0

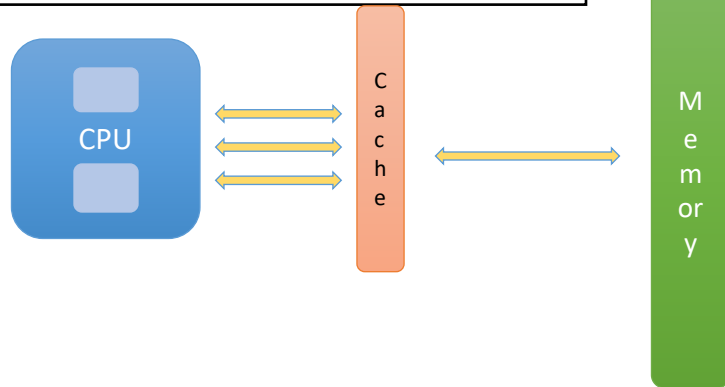
1. Cache line for $c(1:8)$ is in main memory
2. Cache line moves to L3
3. Cache line moves to L2
4. Cache line moves to L1
5. 'somehow' we perform the operation

So where do we read $c(2)$ from?

We continue the loop, reading $c(2)$

1. There are now 4 copies of the cache line
2. We can read the data from any copy, likely reading from L1
3. 'somehow' we perform the operation

Example with 2 cores: core 0 and core 1



MOESI Protocol

For now, only consider **reading data**

... = $b(i) + \underline{c(i)}$

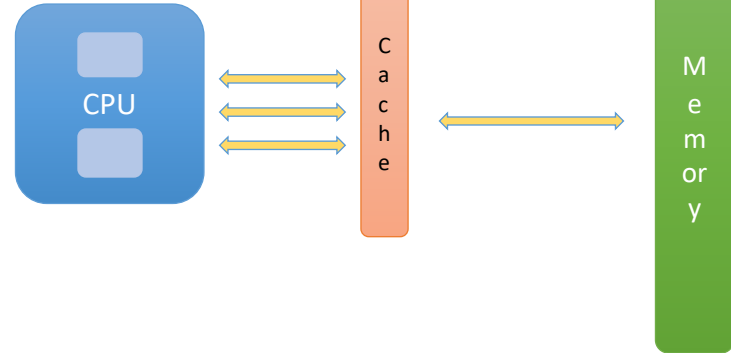
We start the loop, reading $c(1)$ on core 0

1. Cache line for $c(1:8)$ is in main memory
2. Cache line moves to L3
3. Cache line moves to L2
4. Cache line moves to L1
5. 'somehow' we perform the operation

We continue the loop, reading $c(2)$

1. There are now 4 copies of the cache line
2. We can read the data from any copy, likely reading from L1
3. 'somehow' we perform the operation

Example with 2 cores



Process hops to core 1 and

we continue the loop, reading $c(3)$

1. There are now 4 copies of the cache line
2. 2 copies are far away, L1 and L2 of core 0
3. 1 copy is close: L3
4. 1 copy is far away (memory)
5. 'somehow' we perform the operation

We can read from any copy (depending on availability and convenience)

MOESI Protocol

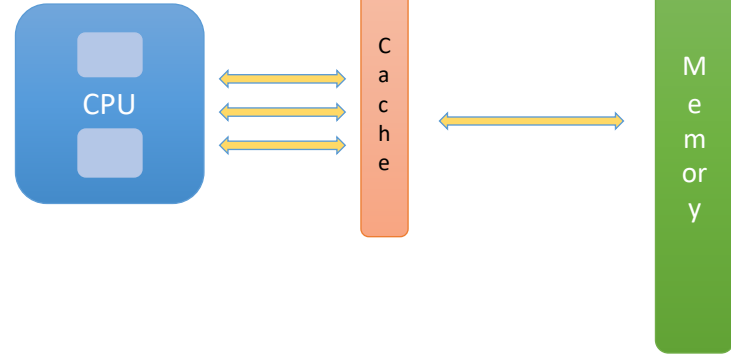
For now, only consider **writing data**

$a(i) = \dots$

We have to bring in cache line first (more later)

1. Cache line for $a(1:8)$ is in main memory
2. Cache line moves to L3
3. Cache line moves to L2
4. Cache line moves to L1
5. 'somehow' we perform the operation
6. $a(1)$ is modified
7. Modified cache line moves back to L1

Example with 2 cores



Process hops to core 1 and we continue the loop, modifying $a(2)$

1. Again there are now 4 copies of the cache line
2. Which one do we use?

MOESI Protocol

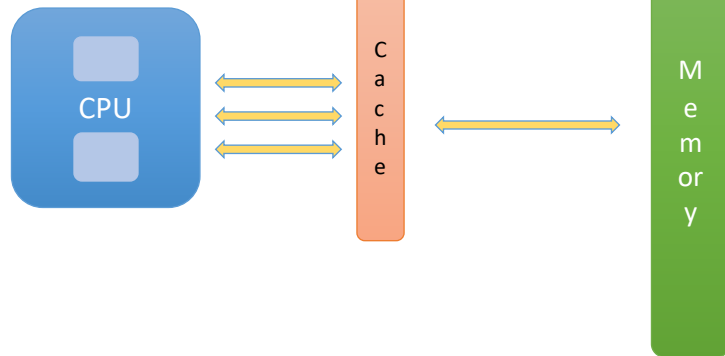
For now, only consider **writing data**

a(i) = ...

We have to bring in cache line first (more later)

1. Cache line for a(1:8) is in main memory
2. Cache line moves to L3
3. Cache line moves to L2
4. Cache line moves to L1
5. 'somehow' we perform the operation
6. a(1) is modified
7. Cache line moves back to L1

Example with 2 cores



Process hops to core 1 and we continue the loop, modifying a(2)

1. Again there are now 4 copies of the cache line
2. Which one do we use?
3. 3 of the 4 copies are invalid
4. Only the copy in L1 of core 0 is 'good to go'

MO(E)SI Protocol

A cache line can be in one of these states

- Modified (M): Only one cache has a valid copy (which has been modified). All other copies are invalid
- Owned (O): Multiple caches hold a copy, which may or may not be valid. Only one cache 'owns' the cache line
- Exclusive (E): Only one cache holds an exclusive copy
- Shared (S): Multiple caches hold a copy of the cache line
- Invalid (I): A copy of the cache line that is invalid

Writing

Before a process can modify data, it has to own the cache line. Then the modification renders all other copies invalid

Reading

To read from a cache line, the status of the cache line has to be 'shared', or 'owned', or 'modified', but not 'invalid'!

Complexity: very large

49 caches per socket (per CPU)

2 sockets: lot's of traffic between sockets (cache snooping)

Cache coherency

MOESI protocol ensures cache coherency

Programmer not responsible for managing cache lines

Cornerstone of **any** shared-memory platform

Backbone of any thread-based parallel computing

Performance/programming implications from MO(E)SI

Parallel computing is not part of this class (see PCSE in the Spring)

Nevertheless there is one implication that I'd like to discuss.

Imagine your code executes on 2 cores

- Two 'thingies' are executing. These 'thingies' are called threads (reference to OpenMP)
- A loop is split in two halves. Each thread is executing $\frac{1}{2}$ of the loop → 2x speed-up (theoretically)

Which solution will work better? (having cache-coherency in mind)

Scenario 1: Loop split into 2

Thread 0

```
do i=1, n/2
  a(i) = b(i) + c(i)
enddo
```

Thread 1

```
do i=n/2+1, n
  a(i) = b(i) + c(i)
enddo
```

Scenario 2: Loops for odd and even elements

Thread 0 (odd)

```
do i=1, n, 2
  a(i) = b(i) + c(i)
enddo
```

Thread 1 (even)

```
do i=2, n, 2
  a(i) = b(i) + c(i)
enddo
```

General syntax: Do <start>, <end>, <increment> (default increment is +1)

Odd elements: do i=1, n, 2 (1, 3, 5, 7, ...)

Even elements: do i=2, n, 2 (2, 4, 6, 8, ...)