CS3101b – Theory of High-performance Computing

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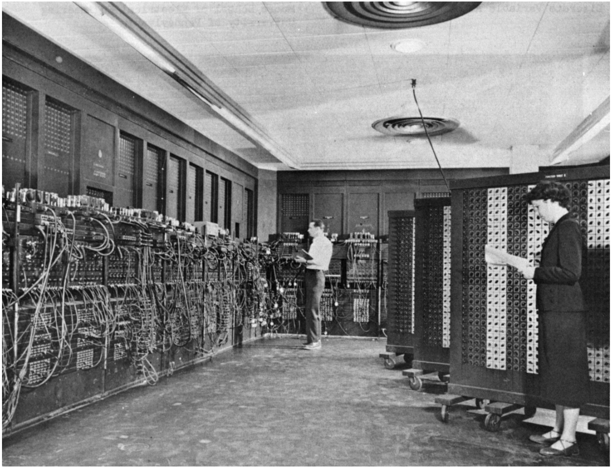
CS3101

Plan

1. Hardware Acceleration Technologies
2. Distributed computing with `Julia`
3. Optimizing Code for Data Locality: A Case Study
4. Multicore Programming with `CilkPlus`
5. CS3101 Course Outline

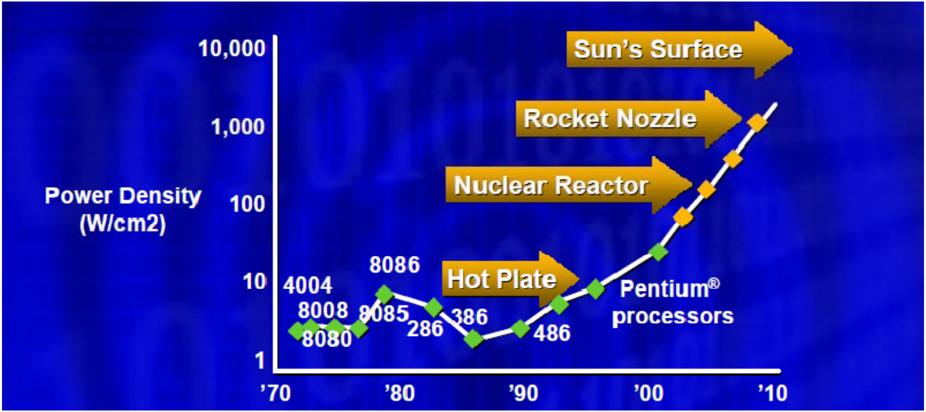
Plan



Electronic Numerical Integrator And Computer (ENIAC). The first general-purpose, electronic computer. It was a Turing-complete, digital computer capable of being reprogrammed and was running at 5,000 cycles per second for operations on the 10-digit numbers.

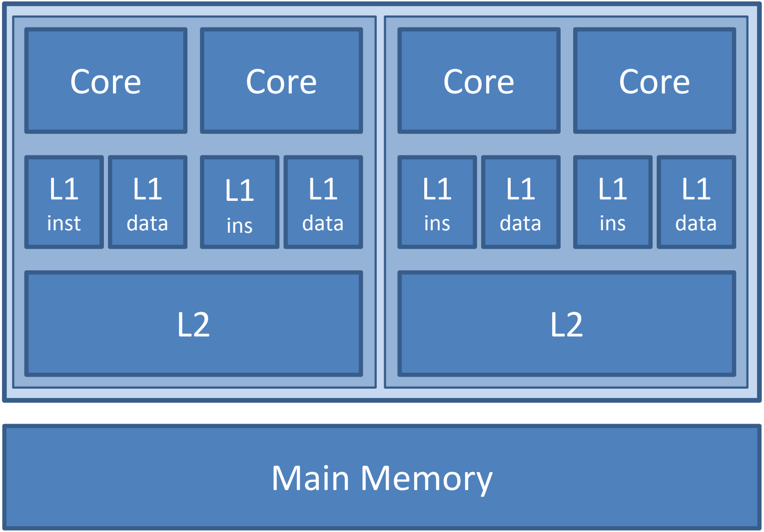
The IBM Personal Computer, commonly known as the IBM PC (Introduced on August 12, 1981).

The Pentium Family.



Power Density (W/cm2)
10,000
1,000
100
10
1
'70
'80
'90
'00
'10
Sun's Surface
Rocket Nozzle
Nuclear Reactor
Hot Plate
4004
8008
8080
8085
8086
286
386
486
Pentium® processors


INTEL Ⓜ © '05 Q6600
INTEL® CORE™2 QUAD
SLACR MALAY
2.40GHZ/8M/1066/05A
L738B526


Core
Core
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L1
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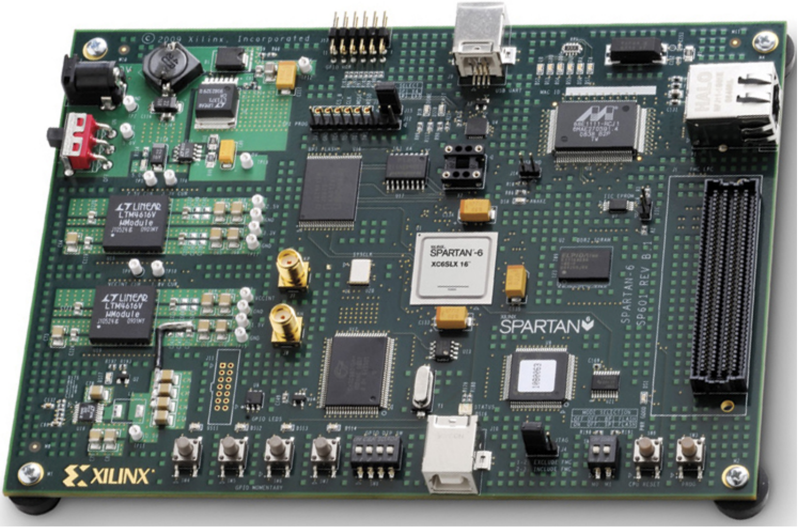
L2
Main Memory


94V-0
MADE IN CHINA
NVIDIA
RoHS
COMPLIANT


SPARTAN-6
XC6SLX 16
SPARTAN
XILINX
LINEAR
LTM4616V
SP601 REV B.1
SPARTAN-6

Capacity
Access Time
Cost

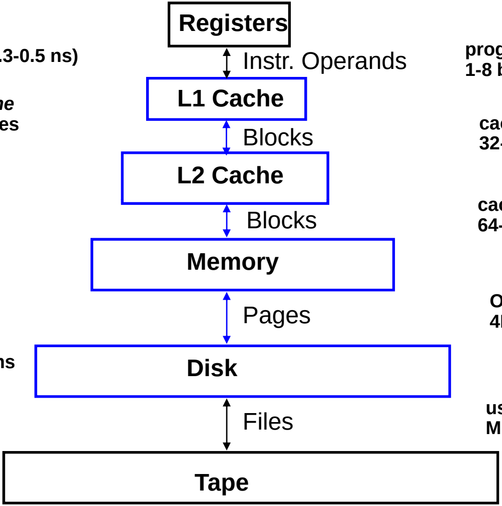
CPU Registers
100s Bytes
300 – 500 ps (0.3-0.5 ns)

L1 and L2 Cache
10s-100s K Bytes
~1 ns - ~10 ns
$1000s/ GByte

Main Memory
G Bytes
80ns- 200ns
~ $100/ GByte

Disk
10s T Bytes, 10 ms
(10,000,000 ns)
~ $1 / GByte

Tape
infinite
sec-min
~$1 / GByte



Staging
Xfer Unit

prog./compiler
1-8 bytes

cache cntl
32-64 bytes

cache cntl
64-128 bytes

OS
4K-8K bytes

user/operator
Mbytes

Upper Level

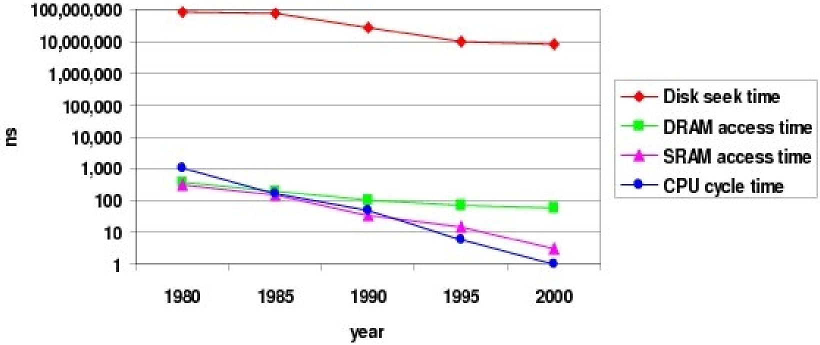
faster

Larger

Lower Level

The CPU-Memory Gap

The increasing gap between DRAM, disk, and CPU speeds.



Once uopn a time, every thing was slow in a computer . . .

Plan

Tasks (aka Coroutines)

Tasks

- Tasks are a control flow feature that allows computations to be suspended and resumed in a flexible manner
- This feature is sometimes called by other names, such as symmetric coroutines, lightweight threads, cooperative multitasking, or one-shot continuations.
- When a piece of computing work (in practice, executing a particular function) is designated as a Task, it becomes possible to interrupt it by switching to another Task.
- The original Task can later be resumed, at which point it will pick up right where it left off

Producer-consumer scheme example

```
function producer()
  produce("start")
  for n=1:2
    produce(2n)
  end
  produce("stop")
end
```

To consume values, first the producer is wrapped in a Task, then consume is called repeatedly on that object:

```
ulia> p = Task(producer)
Task

julia> consume(p)
"start"

julia> consume(p)
2

julia> consume(p)
4

julia> consume(p)
"stop"
```

Julia's message passing principle

Julia's message passing

- Julia provides a multiprocessing environment based on message passing to allow programs to run on multiple processors in shared or distributed memory.
- Julias implementation of message passing is one-sided:
    - the programmer needs to explicitly manage only one processor in a two-processor operation
    - these operations typically do not look like message send and message receive but rather resemble higher-level operations like calls to user functions.

Remote references and remote calls: example

```
moreno@gorgosaurus:~$ julia -p 4

julia> r = remotecall(2, rand, 2, 2)
RemoteRef(2,1,6)

julia> fetch(r)
2x2 Array{Float64,2}:
 0.675311  0.735236
 0.682474  0.569424

julia> s = @spawnat 2 1+fetch(r)
RemoteRef(2,1,8)

julia> fetch(s)
2x2 Array{Float64,2}:
 1.67531  1.73524
 1.68247  1.56942
```

Commnets on the example

- Starting with `julia -p n` provides n processors on the local machine.
- The first argument to `remote_call` is the index of the processor that will do the work.
- The first line we asked processor 2 to construct a 2-by-2 random matrix, and in the third line we asked it to add 1 to it.
- The `@spawnat` macro evaluates the expression in the second argument on the processor specified by the first argument.

Distributed arrays and parallel reduction (1/4)

```
[moreno@compute-0-3 ~]$ julia -p 5
               _
   _       _ _(_)_     |  A fresh approach to technical computing
  (_)     | (_) (_)    |  Documentation: http://docs.julialang.org
   _ _   _| |_  __ _   |  Type "help()" to list help topics
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 0.2.0-prerelease+3622
 _/ |\__'_|_|_|\__'_|  |  Commit c9bb96c 2013-09-04 15:34:41 UTC
|__/                   |  x86_64-redhat-linux

julia> da = @parallel [2i for i = 1:10]
10-element DArray{Int64,1,Array{Int64,1}}:
  2
  4
  6
  8
 10
 12
 14
 16
 18
 20
```

Distributed arrays and parallel reduction (2/4)

```
julia> procs(da)
4-element Array{Int64,1}:
 2
 3
 4
 5

julia> da.chunks
4-element Array{RemoteRef,1}:
 RemoteRef(2,1,1)
 RemoteRef(3,1,2)
 RemoteRef(4,1,3)
 RemoteRef(5,1,4)

julia>

julia> da.indexes
4-element Array{(Range1{Int64},),1}:
 (1:3,)
 (4:5,)
 (6:8,)
 (9:10,)

julia> da[3]
6

julia> da[3:5]
3-element SubArray{Int64,1,DArray{Int64,1,Array{Int64,1}},(Range1{Int64},)}:
  6
  8
 10
```

Distributed arrays and parallel reduction (3/4)

```
julia> fetch(@spawnat 2 da[3])
6

julia>

julia> { (@spawnat p sum(localpart(da))) for p=procs(da) }
4-element Array{Any,1}:
 RemoteRef(2,1,71)
 RemoteRef(3,1,72)
 RemoteRef(4,1,73)
 RemoteRef(5,1,74)

julia>

julia> map(fetch, { (@spawnat p sum(localpart(da))) for p=procs(da) })
4-element Array{Any,1}:
 12
 18
 42
 38

julia>

julia> sum(da)
110
```

Distributed arrays and parallel reduction (4/4)

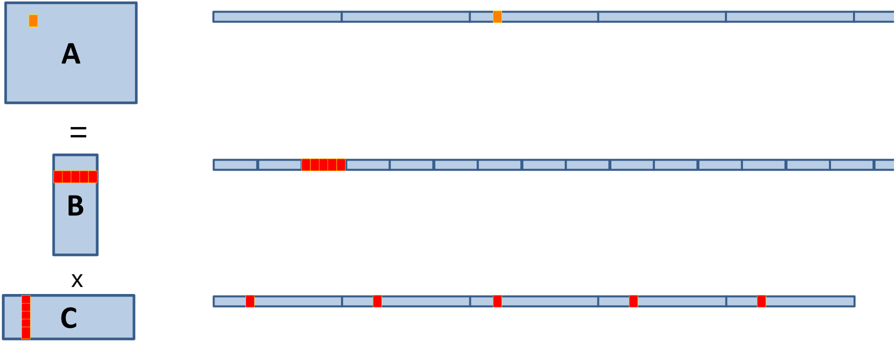
```
julia> reduce(+, map(fetch,
                 { (@spawnat p sum(localpart(da))) for p=procs(da) }))
110

julia>

julia> preduce(f,d) = reduce(f,
                             map(fetch,
                               { (@spawnat p f(localpart(d))) for p=procs(d) }))
# methods for generic function preduce
preduce(f,d) at none:1

julia> function Base.minimum(x::Int64, y::Int64)
       min(x,y)
       end
minimum (generic function with 10 methods)

julia> preduce(minimum, da)
2
```

Plan

A typical matrix multiplication C code

```
#define IND(A, x, y, d) A[(x)*(d)+(y)]
uint64_t testMM(const int x, const int y, const int z)
{
  double *A;  *B; *C;
        long started, ended;
        float timeTaken;
        int i, j, k;
        srand(getSeed());
        A = (double *)malloc(sizeof(double)*x*y);
        B = (double *)malloc(sizeof(double)*x*z);
        C = (double *)malloc(sizeof(double)*y*z);
        for (i = 0; i < x*z; i++) B[i] = (double) rand() ;
        for (i = 0; i < y*z; i++) C[i] = (double) rand() ;
        for (i = 0; i < x*y; i++) A[i] = 0 ;
        started = example_get_time();
        for (i = 0; i < x; i++)
          for (j = 0; j < y; j++)
             for (k = 0; k < z; k++)
                    //  A[i][j] += B[i][k] + C[k][j];
                    IND(A,i,j,y) += IND(B,i,k,z) * IND(C,k,j,y);
        ended = example_get_time();
        timeTaken = (ended - started)/1.f;
  return timeTaken;
}
```

Issues with matrix representation

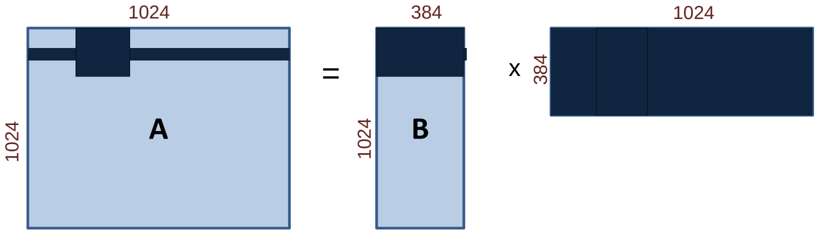


- Contiguous accesses are better:
  - Data fetch as cache line (Core 2 Duo 64 byte per cache line)
  - With contiguous data, a single cache fetch supports 8 reads of doubles.
  - Transposing the matrix `C` should reduce L1 cache misses!

Transposing for optimizing spatial locality

```
float testMM(const int x, const int y, const int z)
{
  double *A; double *B; double *C; double *Cx;
        long started, ended; float timeTaken; int i, j, k;
        A = (double *)malloc(sizeof(double)*x*y);
        B = (double *)malloc(sizeof(double)*x*z);
        C = (double *)malloc(sizeof(double)*y*z);
        Cx = (double *)malloc(sizeof(double)*y*z);
        srand(getSeed());
        for (i = 0; i < x*z; i++) B[i] = (double) rand() ;
        for (i = 0; i < y*z; i++) C[i] = (double) rand() ;
        for (i = 0; i < x*y; i++) A[i] = 0 ;
        started = example_get_time();
        for(j =0; j < y; j++)
          for(k=0; k < z; k++)
            IND(Cx,j,k,z) = IND(C,k,j,y);
        for (i = 0; i < x; i++)
          for (j = 0; j < y; j++)
             for (k = 0; k < z; k++)
               IND(A, i, j, y) += IND(B, i, k, z)*IND(Cx, j, k, z);
        ended = example_get_time();
        timeTaken = (ended - started)/1.f;
  return timeTaken;
}
```

Issues with data reuse



- Naive calculation of a row of `A`, so computing 1024 coefficients: 1024 accesses in `A`, 384 in `B` and $1024 \times 384 = 393,216$ in `C`. Total $= 394,524$.
- Computing a 32×32-block of `A`, so computing again 1024 coefficients: 1024 accesses in `A`, 384×32 in `B` and 32×384 in `C`. Total $= 25,600$.
- The iteration space is traversed so as to reduce memory accesses.

Blocking for optimizing temporal locality

```
float testMM(const int x, const int y, const int z)
{
        double *A; double *B; double *C;
        long started, ended; float timeTaken; int i, j, k, i0, j0, k0;
        A = (double *)malloc(sizeof(double)*x*y);
        B = (double *)malloc(sizeof(double)*x*z);
        C = (double *)malloc(sizeof(double)*y*z);
        srand(getSeed());
        for (i = 0; i < x*z; i++) B[i] = (double) rand() ;
        for (i = 0; i < y*z; i++) C[i] = (double) rand() ;
        for (i = 0; i < x*y; i++) A[i] = 0 ;
        started = example_get_time();
        for (i = 0; i < x; i += BLOCK_X)
          for (j = 0; j < y; j += BLOCK_Y)
            for (k = 0; k < z; k += BLOCK_Z)
              for (i0 = i; i0 < min(i + BLOCK_X, x); i0++)
                for (j0 = j; j0 < min(j + BLOCK_Y, y); j0++)
                   for (k0 = k; k0 < min(k + BLOCK_Z, z); k0++)
                       IND(A,i0,j0,y) += IND(B,i0,k0,z) * IND(C,k0,j0,y);
         ended = example_get_time();
         timeTaken = (ended - started)/1.f;
   return timeTaken;
}
```

Transposing and blocking for optimizing data locality

```
float testMM(const int x, const int y, const int z)
{
        double *A; double *B; double *C, double *Cx;
        long started, ended; float timeTaken; int i, j, k, i0, j0, k0;
        A = (double *)malloc(sizeof(double)*x*y);
        B = (double *)malloc(sizeof(double)*x*z);
        C = (double *)malloc(sizeof(double)*y*z);
        srand(getSeed());
        for (i = 0; i < x*z; i++) B[i] = (double) rand() ;
        for (i = 0; i < y*z; i++) C[i] = (double) rand() ;
        for (i = 0; i < x*y; i++) A[i] = 0 ;
        started = example_get_time();
        for(j =0; j < y; j++)
          for(k=0; k < z; k++)
            IND(Cx,j,k,z) = IND(C,k,j,y);
        for (i = 0; i < x; i += BLOCK_X)
          for (j = 0; j < y; j += BLOCK_Y)
            for (k = 0; k < z; k += BLOCK_Z)
              for (i0 = i; i0 < min(i + BLOCK_X, x); i0++)
                for (j0 = j; j0 < min(j + BLOCK_Y, y); j0++)
                   for (k0 = k; k0 < min(k + BLOCK_Z, z); k0++)
                       IND(A,i0,j0,y) += IND(B,i0,k0,z) * IND(Cx,j0,k0,z);
        ended = example_get_time();
        timeTaken = (ended - started)/1.f;
```

Experimental results

Computing the product of two $n \times n$ matrices on my laptop (Quad-core Intel i7-3630QM CPU @ 2.40GHz L2 cache 6144 KB, 8 GBytes of RAM)

n	naive	transposed	8×8-tiled	t. & t.
1024	7854	1086	1105	999
2048	8335	8646	10166	7990
4096	747100	69149	100538	69745
8192	6914349	546585	823525	562433

Timings are in milliseconds.

The cache-oblivious multiplication (more on this later) and the titled multiplication have simiilar performance.

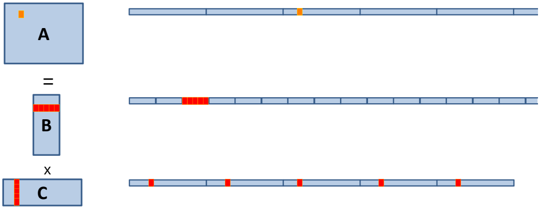
Other performance counters

Hardware count events

- CPI Clock cycles Per Instruction: the number of clock cycles that happen when an instruction is being executed. With pipelining we can improve the CPI by exploiting instruction level parallelism
- L1 and L2 Cache Miss Rate.
- Instructions Retired: In the event of a misprediction, instructions that were scheduled to execute along the mispredicted path must be canceled.

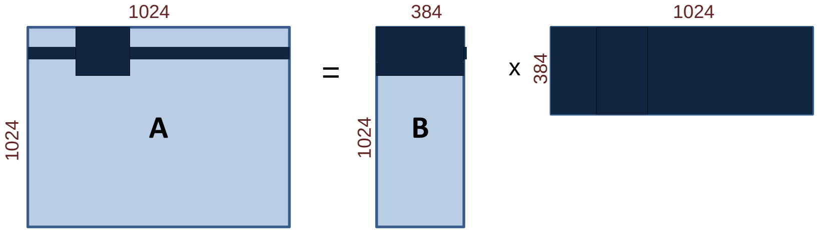
	CPI		L1 Miss Rate		L2 Miss Rate	Percent SSE Instructions	Instructions Retired	
In C	4.78		0.24		0.02	43%	13,137,280,000	
		5x		2x				1x
Transposed	1.13		0.15		0.02	50%	13,001,486,336	
		3x		8x				0.8x
Tiled	0.49		0.02		0	39%	18,044,811,264	

Analyzing cache misses in the naive and transposed multiplication



- Let A, B and C have format (m, n), (m, p) and (p, n) respectively.
- A is scanned once, so mn/L cache misses if L is the number of coefficients per cache line.
- B is scanned n times, so mnp/L cache misses if the cache cannot hold a row.
- C is accessed "nearly randomly" (for m large enough) leading to mnp cache misses.
- Since $2m\,n\,p$ arithmetic operations are performed, this means roughly **one cache miss per flop!**
- If C is transposed, then the ratio improves to 1 for L.

Analyzing cache misses in the tiled multiplication



- Let A, B and C have format (m, n), (m, p) and (p, n) respectively.
- Assume all tiles are square of order b and three fit in cache.
- If C is transposed, then loading three blocks in cache cost $3b^2/L$.
- This process happens n^3/b^3 times, leading to $3n^3/(bL)$ cache misses.
- Three blocks fit in cache for $3b^2 < Z$, if Z is the cache size.
- So $O(n^3/(\sqrt{Z}L))$ cache misses, if b is well chosen, which is optimal.

Plan

Cilk and CilkPlus

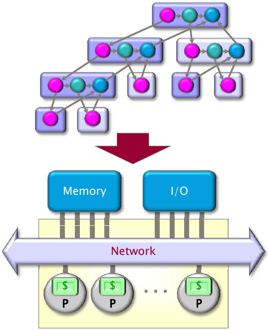
- Cilk has been developed since 1994 at the MIT Laboratory for Computer Science by Prof. Charles E. Leiserson and his group, in particular by Matteo Frigo.
- Cilk has been integrated into Intel C compiler under the name CilkPlus, see http://www.cilk.com/
- CilkPlus (resp. Cilk) is a small set of linguistic extensions to C++ (resp. C) supporting fork-join parallelism
- Both Cilk and CilkPlus feature a provably efficient work-stealing scheduler.
- CilkPlus provides a hyperobject library for parallelizing code with global variables and performing reduction for data aggregation.
- CilkPlus includes the Cilkscreen race detector and the Cilkview performance analyzer.

Nested Parallelism in CilkPlus

```
int fib(int n)
{
   if (n < 2) return n;
   int x, y;
   x = cilk_spawn fib(n-1);
   y = fib(n-2);
   cilk_sync;
   return x+y;
}
```

- The named child function `cilk_spawn fib(n-1)` may execute in parallel with its parent
- CilkPlus keywords `cilk_spawn` and `cilk_sync` grant permissions for parallel execution. They do not command parallel execution.

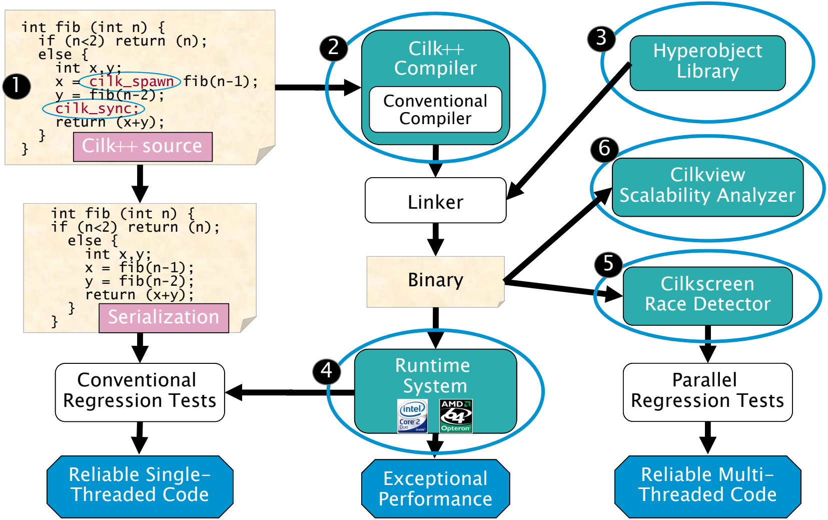
Scheduling



A **scheduler**'s job is to map a computation to particular processors. Such a mapping is called a **schedule**.

- If decisions are made at runtime, the scheduler is *online*, otherwise, it is *offline*
- `Cilk++`'s scheduler maps strands onto processors dynamically at runtime.

The CilkPlus Platform



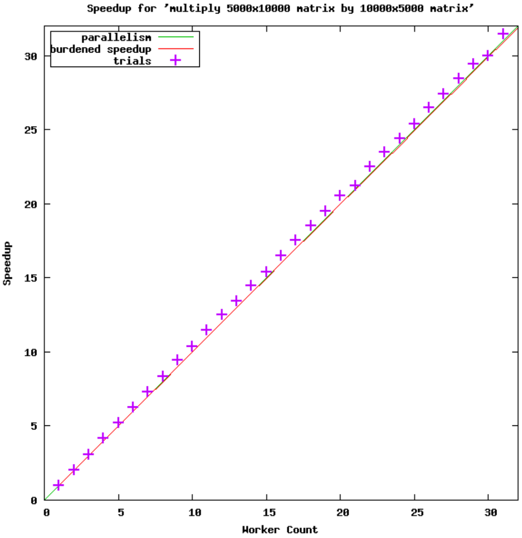
Benchmarks for the parallel version of the divide-n-conquer mm

Multiplying a 4000x8000 matrix by a 8000x4000 matrix

- on 32 cores = 8 sockets x 4 cores (Quad Core AMD Opteron 8354) per socket.
- The 32 cores share a L3 32-way set-associative cache of 2 Mbytes.

#core	Elision (s)	Parallel (s)	speedup
8	420.906	51.365	8.19
16	432.419	25.845	16.73
24	413.681	17.361	23.83
32	389.300	13.051	29.83

Benchmarks using Cilkview



Plan

Course Topics

Week 1: Course presentation and orientation

Week 2-3: Distributed and parallel computing with the Julia interactive system

Week 4-5: Multicore architectures and the fork-join multithreaded parallelism

Week 6: Analyzing the cache complexity of algorithms

Weeks 7-8: Cache memories and their impact on the performance of computer programs

Week 9-10: Fundamental models of concurrent computations (PRAM and its variants)

Week 11: Highly data parallel architecture models (pipeline, stream, vector, etc.)

Weeks 12: Many-core processors (GPGPUs) with an overview of many-core programming

About this course

- Prerequisites: Computer Science 2101A/B or 2211A/B.
- Objectives: introducing students to the necessary theoretical background (architectures, models of computations, algorithms) in order to understand and practice high-performance computing.
- This course can be seen as extension of other CS courses such as 3331A - Foundations of Computer Science I 3305B - Operating Systems 3340B - Analysis of Algorithms I 3350B - Computer Architecture, providing the parallel dimension of Today's Computer Science.
- In the future, it should become a preliminary requirement to 4402B - Distributed and Parallel Systems.
- We will cover a large variety of materials and we will have tutorial every week.

High-performance computing and symbolic computation

Basic Polynomial Algebra Subprograms

www.bpaslib.org

www.metafork.org

www.cumodp.org

www.regularchains.org

Acknowledgments and references

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- Charles E. Leiserson (MIT), Matteo Frigo (Axis Semiconductor) Saman P. Amarasinghe (MIT) and Cyril Zeller (NVIDIA) for sharing with me the sources of their course notes and other documents.
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References.

- *The Implementation of the Cilk-5 Multithreaded Language* by Matteo Frigo Charles E. Leiserson Keith H. Randall.
- *Cache-Oblivious Algorithms* by Matteo Frigo, Charles E. Leiserson, Harald Prokop and Sridhar Ramachandran.
- *The Cache Complexity of Multithreaded Cache Oblivious Algorithms* by Matteo Frigo and Volker Strumpen.
- *How To Write Fast Numerical Code: A Small Introduction* by Srinivas Chellappa, Franz Franchetti, and Markus Pueschel.
- *Models of Computation: Exploring the Power of Computing* by John E. Savage.
- `http://developer.nvidia.com/category/zone/cuda-zone`
- `http://www.csd.uwo.ca/~moreno/HPC-Resources.html`