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- architectures
- real machines
- computing concepts
- parallel programming

architectures

- real machines
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- parallel programming



serial machine





obtained from compilers or interpreters of higher-level languages

serial machine





<u>CPU:</u>

- very primitive commands, obtained from compilers or interpreters of higher-level languages
- cycle chain:
 - **fetch** get instruction and/or data from memory
 - decode store instruction and/or data in register
 - execute perform instruction

serial machine





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arithmetical/logical instructions: +, -, *, /, bitshift, if

serial machine





<u>CPU:</u>

- very primitive commands, obtained from compilers or interpreters of higher-level languages
- cycle chain:
 - **fetch** get instruction and/or data from memory
 - decode store instruction and/or data in register
 - **execute** perform instruction
- some CPU allow multi-threading,
 i.e. already fetch next instruction while still executing



serial machine



speed-ups:

improve your algorithm to require less instructions

example:

a factor like "3/(8piG)" inside a for-loop should be avoided; define FAC=3/(8piG) outside the loop and use FAC inside the loop instead...

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example: avoid at all costs pow(), log(), etc., e.g. pow(x, 2) should be replaced with x*x

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speed-ups:

buy a machine with higher clock-frequency

serial machine



speed-ups: improve your algorithm!

serial machine



speed-ups:

...or wait for technology to advance ;-)

serial machine



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten New plot and data collected for 2010-2015 by K. Rupp

serial machine



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- storage in binary system:
 - I bit = 0 or I
 - 8 bits = 1 byte
 - 4 bytes = 1 float (=32 bits, standard for 32-bit architectures)
 - 8 bytes = 1 double (=64 bits, standard for 64-bit architectures)





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serial machine





RAM:

- Random Access Memory, i.e. read and write
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serial machine





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- Iatency = time for memory access (bus width also relevant)
- speed-ups:
 - multi-threading CPU's
 - larger bus width:
 - '80s 8-bit wide
 '90s 16-bit wide
 '00s 32-bit wide
 (internal 'highway' for data transfer)
 - today 64-bit wide

ARCHITECTURES

Computer Architectures

serial machine





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serial machine





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serial machine





Cache:

- Random Access Memory, i.e. read and write
- built into motherboard next to CPU
- when 'fetch a[i]' also 'fetch a[i+1]' into Cache (in fact, full lines or pages are "cached")
- nowadays multiple Cache levels
- bad programming will lead to "Cache misses":



Cache hit rate

Cache access time RA

RAM access time

serial machine





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Cache hit rate

Cache access time RAM access time

example:

 $t_{Cache} = 10ns, \quad t_{RAM} = 100ns$ $t_{Cache} = 10ns, \quad t_{RAM} = 100ns$

• $t = f \times t_{Cache} + (1 - f) \times t_{RAM}$

serial machine





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Cache hit rateCache access timeexample: $f = 0.1, t_{Cache} = 10ns, t_{RAM} = 100ns$ $f = 0.9, t_{Cache} = 10ns, t_{RAM} = 100ns$

serial machine





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Cache hit rateCache access timeRAM access timeexample: $f = 0.1, t_{Cache} = 10ns, t_{RAM} = 100ns \Rightarrow 91ns$ $f = 0.9, t_{Cache} = 10ns, t_{RAM} = 100ns \Rightarrow 19ns$

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serial machine





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• $t = f \times t_{Cache} + (1 - f) \times t_{RAM}$

Cache hit rate Cache access time

s time RAM access time

example:

 $f = 0.1, \quad t_{Cache} = 10ns, \quad t_{RAM} = 100ns \implies 91ns$ $f = 0.9, \quad t_{Cache} = 10ns, \quad t_{RAM} = 100ns \implies 19ns$ factor of 4.5!

serial machine





Cache:

- Random Access Memory, i.e. read and write
- built into motherboard next to CPU
- when 'fetch a[i]' also 'fetch a[i+1]' into Cache (in fact, full lines or pages are "cached")
- nowadays multiple Cache levels
- bad programming will lead to "Cache misses":



design your code in order to access contiguous memory blocks!



- Cache hits and misses:
 - 2D array in C: density[2][3]



- Cache hits and misses:
 - 2D array in C: density[2][3]
 - memory alignment:





- Cache hits and misses:
 - 2D array in C: density[2][3]



serial machine



Cache hits and misses:

for(i=0; i<3; i++)
 for(j=0; j<2; j++)
 whatever(density[j][i]);</pre>

2D array in C: density[2][3]
memory alignment: density[0][2] ... density[1][0] ...

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Cache hits and misses:

for(j=0; j<2; j++)
for(i=0; i<3; i++)
whatever(density[j][i]);</pre>





serial machine





CPU clock frequency vs. bus frequency:

- CPU frequency determines execution speed of commands
- bus frequency determines how quickly to get new commands/data
serial machine





CPU clock frequency vs. bus frequency:

- CPU frequency determines execution speed of commands
- bus frequency determines how quickly to get new commands/data
 - => bus frequency (and width) is more relevant for actual speed!

serial machine





serial machine



possible speed-ups by the programmer:

- improve your algorithm to require less instructions, e.g. f=4*PI/Grav
- improve your algorithm to use more adequate instructions, e.g. x^*x instead of pow(x,2)
- proper usage of cache, e.g. check memory alignment

serial machine



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serial machine









- shared memory architecture
 - easy to adapt existing serial code
 - limited by RAM to be placed into a single machine



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- shared memory architecture
 - easy to adapt existing serial code
 - limited by RAM to be placed into a single machine
- OpenMP www.openmp.org
 - most commonly used standard to parallelize code on shared memory architectures
 - primarily distribute for-loop components onto different CPU's
 - natively by supported by gcc since v4.2



- shared memory architecture
 - easy to adapt existing serial code
 - limited by RAM to be placed into a single machine
- OpenMP www.openmp.org
 - most commonly used standard to pe
 - you(!) have to add extra commands to the code ctures ted by gcc since v4.2







- distributed memory architecture:
 - existing code difficult to adapt
 - easy to built (cluster of PC's)
 - speed-up limited by inter-computer communication







- distributed memory architecture:
 - existing code difficult to adapt
 - easy to built (cluster of PC's)
 - speed-up limited by inter-computer communication $\overset{\downarrow \downarrow}{\overset{\downarrow}}$
- MPI Message Passing Interface
 - "standard" library for work dispersal on distributed memory architectures
 - e.g., www.open-mpi.org







architectures

real machines

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parallel machine in reality = multi-level hybrid machines

IBM Blue Gene/L

(131072 CPU's in total!)



REAL MACHINES

Computer Architectures

parallel machine in reality = multi-level hybrid machines



www.top500.org



www.top500.org

#136 in 06/2011

Name:MageritVendor:IBM#CPU's:3920performance:I00 Tflops/sec

<u>#170 in 06/2011</u>

Name:MareNostrumVendor:IBM#CPU's:10240performance:60 Tflops/sec

www.top500.org

<u>#136 in 06/2011</u>

<u>#170 in 06/2011</u>

Name:	Magerit	Name:	MareNostrum	
Vendor:	IBM	Vendor:	IBM	
#CPU's:	3920	#CPU's:	10240	17
performance:	100 Tflops/sec	performance:	60 Tflops/sec	J•

www.top500.org

#136 in 06/2011

Name:MageritVendor:IBM#CPU's:3920performance:I00 Tflops/sec

interconnect: Infiniband, up to 1500 Gbits/sec

<u>#170 in 06/2011</u>

Name:MareNostrumVendor:IBM#CPU's:10240performance:60 Tflops/sec

interconnect: Myrinet, ca. 2Gbit/sec

architectures

real machines

computing concepts

parallel programming

GRID computing / Cloud computing?

• GRID computing:

• distributed computing where resources are linked together to solve a single problem



- GRID computing:
 - distributed computing where resources are linked together to solve a single problem
- Cloud computing:
 - use remote resources for your (personal) needs (music storage, email correspondence, ...)





- GRID computing: ⇒ actually running simulations
 - distributed computing where resources are linked together to solve a single problem
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first GRID computing?

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GRID computing: A actually running simulations

• distributed computing where resources are linked together to solve a single problem



- GRID computing: ⇒ actually running simulations
 - distributed computing where resources are linked together to solve a single problem
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there actually exists a GRID network with 21×10^6 Pflops* !!!!!!

- GRID computing: ⇒ actually running simulations
 - distributed computing where resources are linked together to solve a single problem
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there actually exists a GRID network with 21×10^6 Pflops:

Bitcoin Network

- GRID computing: ⇒ actually running simulations
 - distributed computing where resources are linked together to solve a single problem
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• how to program such machines?
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your algorithm must be parallel,

then it's only a matter of using parallel libraries to distribute the work...

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your algorithm must be parallel,

then it's only a matter of using parallel libraries to distribute the **work**...

data parallelisation:

all CPUs execute the same code, but have different parts of the data

task parallelisation

all CPUs have the same data, but execute different calculations

how to program such machines?

your algorithm must be parallel,

then it's only a matter of using parallel libraries to distribute the **work**...

data parallelisation:

all CPUs execute the same code, but have different parts of the data

• how to program such machines?



• how to program such machines?



how to program such machines?

serial algorithm

```
a[0] = STARTVALUE;
for(i=1; i<N; i++) {
    a[i] = function(a[i-1]);
}
```



}

how to program such machines?

serial algorithm

```
a[0] = STARTVALUE;
for(i=1; i<N; i++) {
    a[i] = function(a[i-1]);
```

⇒ not parallelizable as a[i] depends on all previous a[]'s!



}

serial algorithm

```
a[0] = STARTVALUE;
```

```
for(i=1; i<N; i++) {</pre>
```

```
a[i] = function(a[i-1]);
```

⇒ not parallelizable as a[i] depends on all previous a[]'s!

general remark: recursion is elegant yet not parallelizable...





how to program such machines?

serial algorithm

```
parallel algorithm
```

```
a[0] = STARTVALUE;
```

```
for(i=1; i<N; i++) {</pre>
```

```
a[i] = function(a[i-1]);
```

}



how to program such machines?

serial algorithm

```
parallel algorithm
```

a[0] = STARTVALUE;

```
for(i=1; i<N; i++) {</pre>
```

```
a[i] = function(a[i-1]);
```

}



each CPU runs the same code, but on a different part of the problem...

}

how to program such machines?

serial algorithm

```
a[0] = STARTVALUE;
```

```
for(i=1; i<N; i++) {</pre>
```

```
a[i] = function(a[i-1]);
```

```
example:
shared memory architecture
```

CPU #I CPU #2 CPU #3 a[0] a[1] a[2] a[3] a[4] a[5] a[6] a[7] ID array

parallel algorithm

(i.e. all CPU's can access the same memory)

}

how to program such machines?

serial algorithm

```
a[0] = STARTVALUE;
for(i=1; i<N; i++) {
    a[i] = function(a[i-1]);
```

```
PARALLEL PROGRAMMING
```

ID array

parallel algorithm

```
a[0] = STARTVALUE;
for(i=1; i<N; i++) {
    b = a[0];
    for(j=0; j<i; j++) {
        b = function(b);
     }
     a[i] = b;
}
```



how to program such machines?

serial algorithm

```
parallel algorithm
```



the i-loop can now be parallelized as all a[i] are calculated independently



a[0] = STARTVALUE;

for(i=1; i<N; i++) {</pre>

Computer Architectures

}

how to program such machines?

serial algorithm

a[i] = function(a[i-1]);



parallel algorithm

```
for(i=1; i<N; i++) {
    b = a[0];
    for(j=0; j<i; j++) {
        b = function(b);
     }
     a[i] = b;
}</pre>
```

we eliminated the recursion/dependence by expanding it explicitly. (by introducing yet another recursion, but c'est la vie...)

how to program such machines?

serial algorithm

<u>parallel algorithm</u>



how to program such machines?

serial algorithm





each CPU gets its own private copy of these variables



how to program such machines?

serial algorithm

parallel algorithm





how to program such machines?

serial algorithm





ID array

parallel algorithm

how to program such machines?

serial algorithm

parallel algorithm



• how to program such machines?





how to program such machines?













```
double calc_b(int i, double sv)
{
    double b;
    int j;
    b = sv;
    for(j=0; j<i; j++) {
        b = function(b);
    }
    return(b);
}</pre>
```













• how to program such machines (OpenMP standard):

#pragma omp parallel for private() shared()

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#pragma omp parallel for private() shared() start parallel environment

(can be started everywhere in code...)

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parallel environment only for next for-loop

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parallel environment only for next for-loop each thread stores its own local copy of these variables

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variables accessible by each thread

• how to program such machines (OpenMP standard):



parallel environment only for next for-loop each thread stores its own local copy of these variables

variables accessible by each thread

<u>Note:</u>

- if you only read the value of a variable, it can be 'shared'
- if you write into a variable, think carefully about its status!

• how to program such machines (OpenMP standard):



```
a[i] = b;
```

• if you **write** into a variable, think carefully about its status

a[i] = b;

• how to program such machines (OpenMP standard):



• if you write into a variable, think carefully about its status

• how to program such machines (OpenMP standard):



• how to program such machines (OpenMP standard):

```
a[0] = STARTVALUE;
#pragma omp parallel for private(i,j,b) shared(a,N)
for(i=1; i<N; i++) {
    b = a[0];
    for(j=0; j<i; j++) {
        b = function(b);
      }
    a[i] = b;
}</pre>
```

• how to program such machines (OpenMP standard):

```
a[0] = STARTVALUE;
```

a[i] = b;

}

```
#pragma omp parallel for private(i,j,b) shared(a,N)
for(i=1; i<N; i++) {</pre>
```

put this into a function!

```
b = a[0];
for(j=0; j<i; j++) {
    b = function(b);
}
```
• how to program such machines (OpenMP standard):

```
a[0] = STARTVALUE;
```

```
#pragma omp parallel for private(i,j,b) shared(a,N)
for(i=1; i<N; i++) {</pre>
```

	<pre>b = a[0]; for(j=0; j<i; j++)="" {<br="">b = function(b);</i;></pre>	put this into a function:	<pre>double calc_b(int i, double sv) {</pre>
	}		double b;
	a[i] = b;		int j;
}			b = sv;
			<pre>for(j=0; j<i; b="function(b);" j++)="" pre="" {="" }<=""></i;></pre>
			}

```
return(b);
```

}

```
a[0] = STARTVALUE;
#pragma omp parallel for private(i,j,b) shared(a,N)
for(i=1; i<N; i++) {</pre>
                                                     double calc b(int i, double sv)
                                                     {
                                                        double b;
                                                        int j;
   a[i] = calc_b(i, a[0]);
}
                                                        b = sv;
                                                        for(j=0; j<i; j++) {</pre>
                                                           b = function(b);
                                                        }
                                                        return(b);
                                                     }
```

```
a[0] = STARTVALUE;
#pragma omp parallel for private(i, shared(a,N)
for(i=1; i<N; i++) {</pre>
                                                    double calc b(int i, double sv)
                                                    {
                                                       double b;
                                                       int j;
   a[i] = calc_b(i, a[0]);
}
                                                       b = sv;
                                                       for(j=0; j<i; j++) {</pre>
                                                           b = function(b);
                                                        }
                                                       return(b);
                                                    }
```

```
a[0] = STARTVALUE;
#pragma omp parallel for private(i) shared(a,N)
for(i=1; i<N; i++) {</pre>
   a[i] = calc b(i, a[0]);
}
                                                     double calc b(int i, double sv)
                                                     {
                                                        double b;
                                                        int j;
                                                        b = sv;
                                                        for(j=0; j<i; j++) {</pre>
                                                            b = function(b);
                                                        }
                                                        return(b);
                                                     }
```

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a[0] = STARTVALUE;
#pragma omp parallel for private(i) shared(a,N)
for(i=1; i<N; i++) {</pre>
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}
                                                      double calc b(int i, double sv)
                                                      {
                                                         double b;
                                                         int j;
                                                         b = sv;
                                                         #pragma omp parallel for...
                                                         for(j=0; j<i; j++) {</pre>
                                                             b = function(b);
                                                         }
                                                         return(b);
                                                      }
```

• how to program such machines (OpenMP standard):

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a[0] = STARTVALUE;
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```

2 reasons for not parallelizing this for-loop...

```
double calc_b(int i, double sv)
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    <u>"pragma omp parallel for...
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        b = function(b);
    }
    return(b);
}</pre></u>
```

```
a[0] = STARTVALUE;
#pragma omp parallel for private(i) shared(a,N)
for(i=1; i<N; i++) {
    a[i] = calc_b(i, a[0]);
}
dc
{
    2 reasons for not parallelizing this for-loop:
        it is a recursion
        we already parallelized outside of calc_b()
    ?:
</pre>
```

```
double calc_b(int i, double sv)
{
    double b;
    int j;
    b = sv;
    <u>"#pragma omp parallel for..."
    for(j=0; j<i; j++) {
        b = function(b);
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    return(b);
}</pre></u>
```

• how to program such machines (OpenMP standard):

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a[0] = STARTVALUE;
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}</pre>
```

general advise:

- make your code modular, i.e. use functions
- modular code is easier to parallelize

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double calc_b(int i, double sv)
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    int j;
    b = sv;
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        b = function(b);
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    return(b);
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• how to program such machines?



but how to divide the domain?

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but how to divide the domain: distribute the **work** evenly!

• how to program such machines?



but how to divide the domain: distribute the **work** evenly!

```
b = a[0];
for(j=0; j<i; j++) {
    b = function(b);
}
=> CPU's dealing with higher i 's have more work to do!
```

• how to program such machines?

OpenMP work distribution:

```
schedule(dynamic): loop index = 0-Nthreads-I \checkmark Nthreads \checkmark Nthreads+I \checkmark etc.
```

schedule (static): evenly divide loop index amongst Nthreads

<u>usage:</u>

#pragma omp parallel for private(...) shared(...) schedule(...)

```
b = a[0];
for(j=0; j<i; j++) {
    b = function(b);
} => CPU's dealing with higher i 's have more work to do!
```

```
ID array
```









• how to program such machines?

*this is not to be confused with domain discretisation!

• how to program such machines?



how to check the speed-up of your program?

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strong scaling

weak scaling

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you keep the problem size fixed, but increase the number of CPU's you keep the number of CPU's fixed, but increase the problem size

• how to check the speed-up of your program?

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weak scaling

you keep the problem size fixed, but increase the number of CPU's

you aim at running a given problem as fast as possible... you keep the number of CPU's fixed, but increase the problem size

you aim at running the largest possible problem in a given amount of time...

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strong scaling

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you aim at running a given problem as fast as possible...

weak scaling

you keep the number of CPU's fixed, but increase the problem size

you aim at running the largest possible problem in a given amount of time...

actually more important nowadays

how to actually write a program?

Computer Architectures

- how to actually write a program?
 - define the problem
 - decide on organisation
 - o choose essential elements (variables, structures, etc.)
 - \circ shape relevant tasks
 - o design your algorithm to be parallelizable
 - $\,\circ\,$ draw a flowchart
 - code in your preferred language
 - test code using simple/known test cases

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try to break problem down into pieces/modules that can be coded separately from each other...

shaping relevant tasks?

Computer Architectures

shaping relevant tasks – data

Computer Architectures

shaping relevant tasks – data

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shaping relevant tasks – data





Computer Architectures

shaping relevant tasks – data





Computer Architectures

shaping relevant tasks – data







modular and hence more flexible!

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each CPU runs the same code, but on a different part of the problem...
CPU#I

CPU#2

Computer Architectures



Calculation(Data2)

design your algorithm to be parallelizable!





- some coding recommendations:
 - make proper use of the Cache (see above)
 - $\ensuremath{\circ}$ avoid complicated indices
 - \circ know how arrays are aligned in memory
 - avoid conditions, I/O, and (sub-)routine calls inside loops
 - avoid unnecessary operations inside loops in general
 - use multiplications rather than divisions or powers
 - keep it simple!



let's put our knowledge into action:

write a code that calculates

$$\pi \approx \sqrt{12} \sum_{k=0}^{\infty} \left(-\frac{1}{3}\right)^k \frac{1}{2k+1}$$

k=0,1,2,3,4
pi += pow(-1.0/3.0, (double)k) / (2.*(double)k+1.);

k=5,6,7,8,9
pi += pow(-1.0/3.0, (double)k) / (2.*(double)k+1.);

k=10,11,12,13
pi += pow(-1.0/3.0, (double)k) / (2.*(double)k+1.);