Setting up the computing environment

- I will be demonstrating on MAC.
- Linux environment is very similar to MAC and should be easy to follow
- Windows might be hardest to set up

In the past we provided virtual machine, *light linux ubuntu*, with all software installed. Such virtual machine can be run on any operating system. If there is sufficient interest for a virtual machine, we will create it. Native installation is more efficient, and probably a good idea to try it out.

Essential Software:

- `Python`, and its packages : `numpy, scipy, matplotlib & jupyter` notebooks (easy installation with Anaconda www.anaconda.com)
- `C++` compiler, such as `gcc`, but other `C++` compilers should be fine too.
- Text editor for coding (anaconda includes `Spyder`, which I am learning, `Emacs, Aquamacs,` or similar)
- `make` to execute makefiles

Recommended Software:

- `Fortran` compiler, such as `gfortran`, or intel fortran (it is getting harder to install nowadays).
- `blas&lapack` libraries. They come preinstalled in most computers or one needs to install vendors libraries (intel mkl for linux). On mac it is contained in Xcode
- `openMP` enabled C++ compiler (native gcc rather than apple clang, which is invoked by `gcc,g++`)
  (It is possible to turn native clang to support openMP, but it is hard. See: *OpenMP on macOS with Xcode tools* https://mac.r-project.org/openmp/)
- `gnuplot` for fast plotting.

Installation on MAC:

- Install `Xcode` package from App Store (E*ssential*)

- We will need specific part of `Xcode` namely "`Command Line Tools`", which might be already installed in your distribution. To check if they are, type:

```
xcode-select --print-path
```

If you do not find them, install by

```
xcode-select --install
```

`Xcode` contains C/C++ compiler (gcc/g++). It is just a link to apples native Clang.
`Xcode` also contains many libraries. For example, it should include `BLAS` and `LAPACK` libraries. To use these libraries, we will use a linker option: `-framework Accelerate`.
For more information see (https://developer.apple.com/accelerate/)
`Xcode` also includes `make`.

Installation on MAC:

Multicore openMP *execution:*

However, Xcode does not come anymore with gnu compilers (such as gnu-c==gcc and gnu-c++==g++). Instead gcc and g++ point to apple's own Clang compiler. Unfortunately Clang does not support openMP (multicore) instructions. Moreover, Clang does not include fortran compiler, such as gnu compiler (gfortran). (see https://mac.r-project.org/openmp/)

Recommended:

To install openMP, fortran & gnuplot we will use homebrew.

The long instructions of how to install the homebrew are available at http://brew.sh

In summary, you need to paste the following into the terminal prompt:

```
/bin/bash -c "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/HEAD/install.sh)"
```

and follow the instructions.

After installing homebrew, you can check for any issues with the install by typing

```
brew doctor
```

Installation on MAC:

On some OSX versions you may run into file permission issues with OSX's SIP process. If you see permission issues that does not allow you to install homebrew, you might need to change ownership on the homebrew directory by typing:

```
sudo chown -R $(whoami):admin /usr/local
```

Recommended:

Now that homebrew is installed, we can install gcc and gfrortran

First check that gcc package exists, you can type in the Terminal prompt

```
brew search gcc
```

To actually install gcc and gfortran, please type:

```
brew install gcc
```

If you arelady installed gcc before, but is not up-to-date, you can type:

```
brew reinstall gcc
```

Warning: the installation of gcc will take a lot of time.

Check installation after complete:

```
gcc-12 --version
gfortran --version
```

Installation on MAC:

Recommended:

Installing gnuplot using homebrew:

```
brew install gnuplot
```

If you get annoying warning "*Populating font family aliases took 96 ms*", you can add to ~/.gnuplot the following line:

```
set term qt font "Helvetica Neue"
```

Installing gsl (gnu scientific library, which contains many numerics algorithms & random number generators) using homebrew:

```
brew install gsl
```

Installation for any platform:

Essential:

Finally, we will install Python with its packages. Some basic version should already be installed by Xcode package. Xcode comes with a stripped-down version of Python, however, this native version of python usually does not contain scipy&jupyter support. To check the current python installation, you can type

```
python
import scipy
scipy.test()
```

If it survives a minute or or more, the installation is OK. If not, follow the instructions below.

As of this writing, the Anaconda distribution is most user friendly and easy to install, available for **all operating systems**:

https://www.anaconda.com "Download", "Graphical installer"

Once installed, open: 

It already includes all packages we need: scipy, numpy, matplotlib, ipython,jupyter

Installation for MAC:

Recommended:

Installing pybin11 in anaconda:

```
conda install -c conda-forge pybind11
```

Alternatively, one can use graphical interface and navigate to “Environments/Search Packages” type pybind11

This is one of the easier methods to speed-up python codes through C++

More information : https://pybind11.readthedocs.io/en/latest/index.html

Installing numba in anaconda:

Usually it is already installed. Check:

```
conda list|grep numba
```

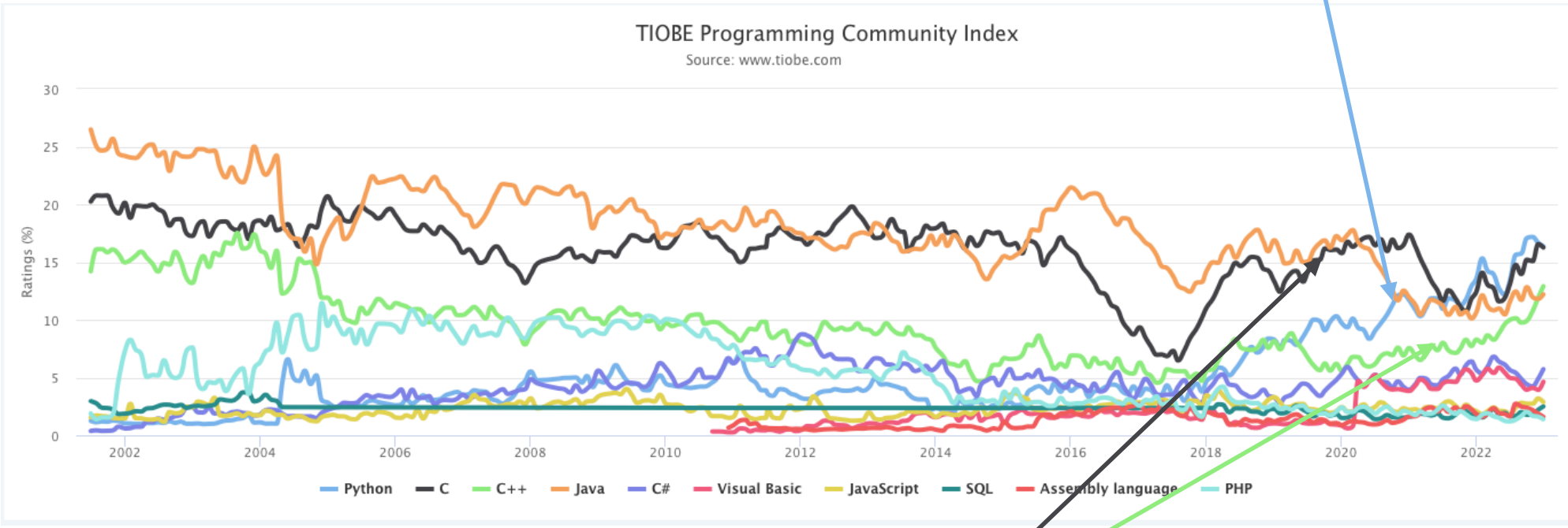
In nothing is listed, type:

```
conda install numba
```

Testing of our installation with a concrete example

Which language is most popular?

https://www.tiobe.com/tiobe-index/



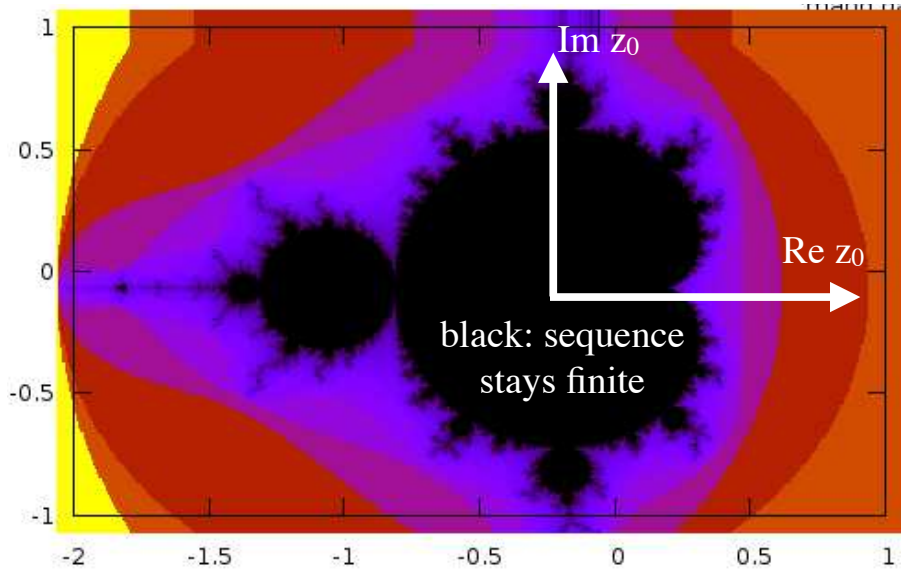
Python is climbing up fast

C/C++ are basis of operating systems and standard for back-end

C++ modernized a lot recently and has overtaken java for the first time (Hall of Fame 2022).

Comparison of languages by generating Mandelbrot set:

Wikipedia: The Mandelbrot set M is defined by a family of complex quadratic polynomials $f(z) = z^2 + z_0$ where z_0 is a complex parameter. For each z_0, one considers the behavior of the sequence $(0, f(0), f(f(0)), f(f(f(0))), \cdots)$ obtained by iterating $f(z)$ starting at $z = 0$, which either escapes to infinity or stays within a disk of some finite radius. The Mandelbrot set is defined as the set of all points z_0 such that the above sequence does not escape to infinity.



Implementation in Fortran (mandf.f90)

```
INTEGER Function Mandelb(z0, max_steps)
  IMPLICIT NONE ! Every variable needs to be declared. It is very prudent to use that.
  COMPLEX*16, intent(in) :: z0
  INTEGER, intent(in)    :: max_steps
  ! locals
  COMPLEX*16 :: z
  INTEGER    :: i
  z=0.
  do i=1,max_steps
     if (abs(z)>2.) then
        Mandelb = i-1
        return
     end if
     z = z*z + z0
  end do
  Mandelb = max_steps
  return
END Function Mandelb
```

Main function which defines how many steps are needed before the value $f(f(\ldots f(z_0)))$ explodes.

This is how we use the above function in the main part of the program.

Note !$OMP directives for multicore execution.

We print 2D array to the standard output, which contains 1/#steps needed before value explodes.

```
program mand
  use omp_lib
  IMPLICIT NONE
  ! external function
  INTEGER :: Mandelb ! Need to declare the external function
  ! locals
  INTEGER :: i, j
  REAL*8  :: x, y
  COMPLEX*16  :: z0
  INTEGER, parameter :: Nx = 1000
  INTEGER, parameter :: Ny = 1000
  INTEGER, parameter :: max_steps = 1000
  REAL*8  :: ext(4) = (/-2., 1., -1., 1./) ! The limits of plotting
  REAL*8  :: mande(Nx,Ny)
  REAL    :: start, finish, startw, finishw

  call cpu_time(start)
  startw  = OMP_get_wtime()

  !$OMP PARALLEL DO  PRIVATE(j,x,y,z0)
  do i=1,Nx
     do j=1,Ny
        x = ext(1) + (ext(2)-ext(1))*(i-1.)/(Nx-1.)
        y = ext(3) + (ext(4)-ext(3))*(j-1.)/(Ny-1.)
        z0 = dcmplx(x,y)
        mande(i,j) = Mandelb(z0, max_steps)
     enddo
  enddo
  !$OMP END PARALLEL DO

  finishw = OMP_get_wtime()
  call cpu_time(finish)
  WRITE(0, '("clock time : ",f6.3,"s  wall time=",f6.3,"s")') finish-start, finishw-startw

  do i=1,Nx
     do j=1,Ny
        x = ext(1) + (ext(2)-ext(1))*(i-1.)/(Nx-1.)
        y = ext(3) + (ext(4)-ext(3))*(j-1.)/(Ny-1.)
        print *, x, y, 1./mande(i,j)
     enddo
  enddo
end program mand
```

Testing example

```
gfortran -O3 -fopenmp -o mandf mandf.f90
```

Execute and check the time:

```
./mandf > mand.dat
clock time : 1.30075s with wall time=0.218432s
```

Finally plot:

```
gnuplot gnu.sh
```

The codes produce three column output x, y, color and need a plotting program to display results. In `gnuplot` the following command plots the output:

```
set view map
splot 'mand.dat' with p ps 3 pt 5 palette
```

or call the script by

```
gnuplot gnu.sh
```

Why do we still bother with Fortran?

↑ A lot of scientific code written in fortran → we need to use it and be able to occasionally adapt it.

↑ It is very easily integrated with `Python/numpy` through `f2py/f2py3`, hence useful in combination with Python.

↓ For todays standards, it is obsolete, i.e, developed by IBM in the 1950s (John W. Backus 1953).

↓ Many releases (Fortran, Fortran II, Fortran III, Fortran 66, Fortran 77, Fortran 90, Fortran 95, Fortran 2003, Fortran 2008).

↓ The language keeps changing substantially, but maintains backward compatibility, with several implementations, but no standard compiler: Intel fortran, gnu, PGI fortran,...

Implementation in C++ (mandc.cc)

Bunch of includes from header files, which contain function/class definitions

need to state that complex and basic printing is in std namespace

`for` loop is almost the same as `do` loop in fortran, except that in C/C++ we always start at 0 rather than 1. This is because of array index starts with a(0) and not a(1) as in fortran.

```
#include <iostream>
#include <complex>
#include <ctime>
#include <vector>
#include <omp.h>
using namespace std;

int Mandelb(const complex<double>& z0, int max_steps)
{
  complex<double> z=0;
  for (int i=0; i<max_steps; i++){
    if (abs(z)>2.) return i;
    z = z*z + z0;
  }
  return max_steps;
}
```

continuation C++:

This is how we use the above function in the main part of the program.

We use native vector<int> data, which is 1D array. C++ still does not have native 2D arrays! Blitz++ or puma can be used, but is not included in standard C++.

Note #pragma omp directives for multicore execution.

We print 1D/2D array to the standard output, which contains 1/#steps needed before value explodes.

```
int main()
{
  const int Nx = 1000;
  const int Ny = 1000;
  int max_steps = 1000;
  double ext[]={-2,1,-1,1};

  vector<int> mand(Nx*Ny);
  clock_t startTimec = clock();
  double start = omp_get_wtime();

  #pragma omp parallel for
  for (int i=0; i<Nx; i++){
    for (int j=0; j<Ny; j++){
      double x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.);
      double y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.);
      mand[i*Ny+j] = Mandelb(complex<double>(x,y), max_steps);
    }
  }

  clock_t endTimec = clock();
  double diffc = double(endTimec-startTimec)/CLOCKS_PER_SEC;
  double diff = omp_get_wtime()-start;

  clog<<"clock time : "<<diffc<<"s"<<" with wall time="<<diff<<"s "<<endl;

  for (int i=0; i<Nx; i++){
    for (int j=0; j<Ny; j++){
      double x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.);
      double y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.);
      cout<<x<<" "<<y<<" "<< 1./mand[i*Ny+j] << endl;
    }
  }
}
```

Testing example

Compile:

```
g++-12 -fopenmp -O3 -o mandc mandc.cc
```

Execute and check the time:

```
mandf > mand.dat
clock time : 1.30075s with wall time=0.218432s

time mandc > mand.dat
clock time :  1.256s  wall time= 0.219s
```

Finally plot:

```
gnuplot gnu.sh
```

- C++ and fortran timings very similar

Alternative compilation with makefile

Both C++ and fortran code can be simultaneously compiled with a help of makefile (compilation allows optimization):

my C++ executable is g++-10

my fortran compiler

all instructions that need to be processed

both instructions defined above but specified here

useful to know how to clean compilation

```
CC = g++-12
F90 = gfortran

all : mandc mandf

mandc : mandc.cc
  $(CC) -O3 -fopenmp -o mandc mandc.cc

mandf : mandf.f90
  $(F90) -O3 -fopenmp -o mandf mandf.f90


clean :
  rm mandc mandf
```

Implementation in Perl (mandp.pl)

Perl code does not need to be compiled. It is interpreter.
The call to subroutine is skipped due to optimization.
The execution very very slow.

```
#!/usr/bin/perl
use Math::Complex;

$Nx=100;
$Ny=100;
$max_steps=50;

for ($i=0; $i<$Nx; $i++){
    for ($j=0; $j<$Ny; $j++){
  $x = -2. + 3.*$i/($Nx-1.);
  $y = -1. + 2.*$j/($Ny-1.);
  $z0 = $x + $y*i;
  $z=0;
  for ($itr=0; $itr<$max_steps; $itr++){
      if (abs($z)>2.){last;}
      $z = $z*$z + $z0;
  }
  print "$x  $y  $itr \n";
    }
}
```

Implementation in Python (manp.py)

Python is interpreter as well.

```
from scipy import *
from pylab import *
import time

def Mand(z0, max_steps):
    z = 0j
    for itr in range(max_steps):
        if abs(z)>2.:
            return itr
        z = z*z + z0
    return max_steps

if __name__ == '__main__':

    Nx = 1000
    Ny = 1000
    max_steps = 1000 #50

    ext = [-2,1,-1,1]
    t0 = time.time()

    data = zeros( (Nx,Ny) )

    for i in range(Nx):
        for j in range(Ny):
            x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.)
            y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.)
            data[i,j] = Mand(x + y*1j, max_steps)
print ('clock time: '+str( time.time()-t0) )
imshow(transpose(1./data), extent=ext)
show()
```

2D array initialized

2D array filled

No openMP hence clock and wall time equal

Here we are plotting directly

Testing examples

Execute and check the time:

```
./mandf > mand.dat
clock time : 1.30075s with wall time=0.218432s

./mandc > mand.dat
clock time :  1.256s  wall time= 0.219s

perl mandp.pl > mand.dat
clock time : 5361.4s

python manp.py
clock time : 24.6s
```

- Both interpreters are substantially slower than compilers.
- Python is substantially faster than perl.
- C++ and fortran timings very similar, and much faster than interpreters.

Homework:

Set up your environment: C++, Python, fortran, BLAS&LAPACK (or "`Command Line Tools`" on mac).

- If you are familiar with coding, write your own mandelbrot version of the code.
  If not, download Mandelbrot code written in fortran, C++, perl and python. Execute them and check that they work properly.
- Test your `gnuplot` by plotting mandelbrot set from generated file `mand.dat`.

Improving Python

Python can be speed up. Here are the main strategies:

1) Find numpy/scipy routines which can replace slow python code and for loops
2) Try using `numba` : https://numba.pydata.org
    1) helps when there are slow for loops
    2) many repeated operations in an area
    3) one needs to experiment with `numba`/Python code (sometimes slower Python leads to faster numba)
3) Recode the slow loop in fortran, and use `f2py`
4) Recode the slow part in C++, and use `pybind11`
5) [In Python2 there was `weave` "small inline C++ code"]

For mandelbrot we do not have scipy/numpy routine.
We will first try `numba` : https://numba.pydata.org

Improving Python: Numba

https://numba.pydata.org

Just need to add two lines: import + single line before function

```
from numba import jit

@jit(nopython=True)
```

Limitations of Numba

- Numba only accelerates code that uses scalars or (N-dimensional) arrays. You can't use built-in types like `list` or `dict` or your own custom classes.
- You can't allocate new arrays in accelerated code.
- You can't use recursion.

Most of those limitations are removed if using Cython.

Numba has been getting a lot better, even just over the past few months (e.g., they recently added support for generating random numbers).

But first we will rewrite Python code into a single function with two loops, which will make Numba faster and can also be used with C++/fortran to substantially speed up the code.

Improving Python

We now have three nested for loops
All three can be optimized with any of available tools

The code appears slower now (90s versus 25s).
This might vary between different computers.

```
from scipy import *
from numpy import *
from pylab import *
import time

def MandPyth(ext, max_steps, Nx, Ny):
    data = ones( (Nx,Ny) )*max_steps
    for i in range(Nx):
        for j in range(Ny):
            x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.)
            y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.)
            z0 = x+y*1j
            z = 0j
            for itr in range(max_steps):
                if abs(z)>2.:
                    data[j,i]=itr
                    break
                z = z*z + z0
    return data
if __name__ == '__main__':
    Nx = 1000
    Ny = 1000
    max_steps = 1000 # 50

    ext = [-2,1,-1,1]

    t0 = time.time()
    data = MandPyth(array(ext), max_steps, Nx, Ny)
    t1 = time.time()
    print('Python: ', t1-t0)
    imshow(1./data, extent=ext)
    show()
```

Improving Python: Numba

The two lines added here

```
from scipy import *
from numpy import *
from pylab import *
import time
from numba import jit  # This is the new line with numba

@jit(nopython=True)    # This is the second new line with numba
def MandNumba(ext, max_steps, Nx, Ny):
    data = ones( (Nx,Ny) )*max_steps
    for i in range(Nx):
        for j in range(Ny):
            x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.)
            y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.)
            z0 = x+y*1j
            z = 0j
            for itr in range(max_steps):
                if abs(z)>2.:
                    data[j,i]=itr
                    break
                z = z*z + z0
    return data
if __name__ == '__main__':
    Nx = 1000
    Ny = 1000
    max_steps = 1000 # 50

    ext = [-2,1,-1,1]

    t0 = time.time()
    data = MandNumba(array(ext), max_steps, Nx, Ny)
    t1 = time.time()
    print('Python: ', t1-t0)
    imshow(1./data, extent=ext)
    show()
```

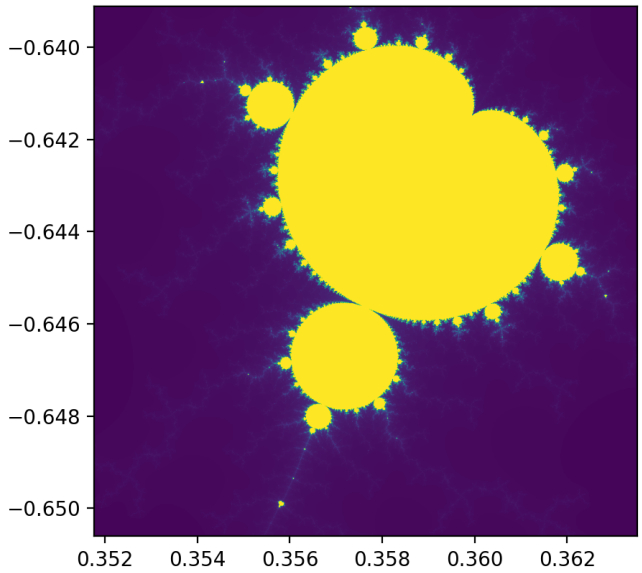
Speed goes from 90s to 1.5s, i.e., 60-times.
Also, compared to previous code (25s) 16-times.

Impressive performance for the effort
(but it does not not always perform so great)

Dynamic update of selected region: self-similarity

We want to create a figure, which can be dynamically zoomed-in and enlarged, to follow self-similarity of fractal plot.

Example:



Dynamic update of selected region: self-similarity

We want to create a figure, which can be dynamically zoomed-in and enlarged, to follow self-similarity of fractal plot.

We will connect a function `ax_update(ax)` with the event of changing xlim or ylim using `callbacks.connect` function, which is defined for axis class in matplotlib library.

Below are the lines we will add/change in the existing Python/Numba implementation:

```
……
def ax_update(ax):  # actual plotting routine
    ax.set_autoscale_on(False) # Otherwise, infinite loop

if __name__ == '__main__':
    ……
    #imshow(1./data, extent=ext)
    fig,ax=subplots(1,1)
    ax.imshow(data, extent=ext,aspect='equal',origin='lower')

    ax.callbacks.connect('xlim_changed', ax_update)
    ax.callbacks.connect('ylim_changed', ax_update)
    show()
```

Current code does not work yet, because we did not replot the fractal once the function `ax_update` is called.
Now we need to find the size of the region we zoom-in, and replot the fractal for the new region.

Dynamic update of selected region: self-similarity

dimensions of the window

creating our new limits

actual recalculation of fractal

set the data to the right place

connecting the mouse event with the above function

```
.....
def ax_update(ax):  # actual plotting routine
    ax.set_autoscale_on(False) # Otherwise, infinite loop
    # Get the range for the new area
    xstart, ystart, xdelta, ydelta = ax.viewLim.bounds
    xend = xstart + xdelta
    yend = ystart + ydelta
    ext=array([xstart,xend,ystart,yend])
    data = MandNumba(ext, max_steps, Nx, Ny) # actually producing new fractal

    # Update the image object with our new data and extent
    im = ax.images[-1]  # take the latest object
    im.set_data(data)   # update it with new data
    im.set_extent(ext)           # change the extent
    ax.figure.canvas.draw_idle() # finally redraw

if __name__ == '__main__':
    .........
    #imshow(1./data, extent=ext)
    fig,ax=subplots(1,1)
    ax.imshow(data, extent=ext,aspect='equal',origin='lower')

    ax.callbacks.connect('xlim_changed', ax_update)
    ax.callbacks.connect('ylim_changed', ax_update)
    show()
```

Homework:

Implement the dynamic version of the mandelbrot cell

Improving Python

The idea: Write most of the code in Python. Allocate all arrays in Python, to avoid annoying bookeeping of allocation/deallocation of memory. Speed-up the innermost loop by fortran/C++.

Python is used as ”glue” for C++ and fotran code. Can combined modules obtained by either of the two or other tools.

Several available tools:

- `f2py` for fortran
- `pybind11` :https://github.com/pybind/pybind11 very powerful for C++ to Python-library conversion. Needs newer C++-11 compiler. It requires only a few header files, and no libraires or compilation. Efficient, and not too hard to use.
- `weave` : was removed in Python3. It used to be part of scipy, later removed from scipy, but included in stand alone Python packages. In python3 abandoned. Very simple to use and very efficient results. But code is a string, which is very clumsy for writting more than 10 lines of code.
- `Swig` : very general. It can glue almost everything with everything. It is demanding to master.
- `PyCXX` : smaller, intented only for C/C++ < – > Python conversion. Looks quite simple, but very limited numpy support.
- `Cython` : http://cython.org/ (very popular with similar performance as numba, but much easier to port. However, a bit harder to use —almost like a new compiler for python). We do not write real C++ code, but code similar to C++, which is being compiled.

Improving Python with fortran (f2py)

Normal fortran subroutine, which can be called by fortran main code.

We can add some comments that make nicer python modules
!f2py optional
!f2py intent(hide)

!$OMP directive allows openMP parallelization

```
!-----------------------------------------------------
! Produces Mandelbrot plot in the range [-ext[0]:ext[1]]x[ext[2]:ext[3]]
! It uses formula z = z*z + z0 iteratively until
! asb(z) gets bigger than 2
! (deciding that z0 is not in mandelbrot)
! The value returned is 1/(#-iterations to escape)
!-----------------------------------------------------
SUBROUTINE Mandelb(data, ext, Nx, Ny, max_steps)
  IMPLICIT NONE ! Don't use any implicit names of variables!
  ! Function arguments
  REAL*8, intent(out) :: data(Nx,Ny)
  REAL*8, intent(in)  :: ext(4)              ! [xa,xb,ya,yb]
  INTEGER, intent(in) :: max_steps
  INTEGER, intent(in) :: Nx, Ny
  !f2py integer optional, intent(in)          :: max_steps=1000
  !  !f2py integer intent(hide), depend(data) :: Nx=shape(data,0)  ! it will be hidden automaticall
  !  !f2py integer intent(hide), depend(data) :: Ny=shape(data,1)  ! it will be hidden automaticall
  ! Local variables
  INTEGER    :: i, j, itt
  COMPLEX*16 :: z0, z
  REAL*8     :: x, y
  data(:,:) = max_steps
  !$OMP PARALLEL DO  PRIVATE(j,x,y,z0,z,itt)
  DO i=1,Nx
     DO j=1,Ny
        x = ext(1) + (ext(2)-ext(1))*(i-1.)/(Nx-1.)
        y = ext(3) + (ext(4)-ext(3))*(j-1.)/(Ny-1.)
        z0 = dcmplx(x,y)
        z=0
        DO itt=1,max_steps
           IF (abs(z)>2.) THEN
              data(i,j) = itt-1 !1./itt         ! result is number of iterations
              EXIT
           ENDIF
           z = z**2 + z0             ! f(z) = z**2+z0 -> z
        ENDDO
    ENDDO
  ENDDO
  !$OMP END PARALLEL DO
  RETURN
END SUBROUTINE Mandelb
```

Improving Python with fortran (f2py)

We can compile fortran mandel.f90 with:

```
f2py -c mandel.f90 -f90flags='-fopenmp' -m mandel
```

which should produce mandel.so

Note: -fopenmp switches on openMP parallelization
To use openMP we need to set OMP_NUM_THREADS, for example

```
export OMP_NUM_THREADS=4
```

Finally, we write short python script and import the module like it was Python module

```
#!/usr/bin/env python
from scipy import *  # for arrays
from pylab import *  # for plotting
import mandel  # importing module created by f2py
import time

# The range of the mandelbrot plot [x0,x1,y0,y1]
ext=[-2,1,-1,1]

tc = time.process_time() # cpu time
tw = time.time()  # wall time
data = mandel.mandelb(ext,1000,1000).transpose()

print('# wall time : ', time.time()-tw, 's  clock time : ', time.process_time() - tc, 's')

# Using python's pylab, we display pixels to the screen!
imshow(data, interpolation='bilinear', origin='lower', extent=ext, aspect=1.)
show()
```

Wall time essentially the same as for fortran native code: wall time : 0.273 s clock time : 3.901 s

Improving Python with C++ (pybind11)

Normal C++ code, but needs some extra header files “pybind11/“

This is how to access numpy arrays in C++ through pybind11
dat = data.mutable_unckecked<dim>();

This code is instead of main()
It is specific to pybind11 and needs some learning from pybind11 manual.

```cpp
#include "pybind11/pybind11.h"
#include "pybind11/numpy.h"
#include "pybind11/stl.h"
#include <cstdint>

namespace py = pybind11;
using namespace std;

void mand(py::array_t<double>& data, int Nx, int Ny, int max_steps, const vector<int>& ext)
{
  auto dat = data.mutable_unchecked<2>();
  #pragma omp parallel for
  for (int i=0; i<Nx; i++){
    for (int j=0; j<Ny; j++){
      dat(j,i) = max_steps;
      double x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.);
      double y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.);
      complex<double> z0(x,y);
      complex<double> z=0;
      for (int itr=0; itr<max_steps; itr++){
         if (norm(z)>4.){
            dat(j,i) = itr;
            break;
         }
         z = z*z + z0;
      }
    }
  }
}
PYBIND11_MODULE(imanc,m){
  m.doc() = "pybind11 wrap for mandelbrot";
  m.def("mand", &mand);
}
```

Improving Python with C++ (pybind11)

To create python module from C++ code, we type:

```
g++-10 `python3 -m pybind11 --includes` -undefined dynamic_lookup -O3
-fopenmp -shared -std=c++11 -fPIC imanc.cc -o imanc.so
```

g++-10 must be replaced by your C++ compiler.
Notice that "python3 -m pybind11 —includes" should give correct include files of your python installation, provided pybind11 was properly installed. Otherwise one needs to find python include files manually.

Notice also that "-undefined dynamic_lookup" is needed only in mac (not linux). -fopenmp is for openMP parallelization

Improving Python with C++ (pybind11)

Here we import C++ module imanc.so

This is old Numba code

Comparing pybind11 and Numba:

This executes C++ module

```
pybind11: walltime:  0.153 cputime:  0.852
numba:    walltime:  1.241 cputime:  1.212
```

C++ with pybind11 is 8-times faster,
mostly because we use multiple cores

Call to C++ module

On a single core:

```
pybind11: walltime:  0.776 cputime:  0.776
numba:    walltime:  1.252 cputime:  1.220
```

Call to Numba

C++ with pybind11 is still 60% faster, sometimes more.

```
from scipy import *
from pylab import *
import time
from numba import jit
import imanc

@jit(nopython=True)
def MandNumba(ext, max_steps, Nx, Ny):
    data = ones( (Nx,Ny) )*max_steps
    for i in range(Nx):
        for j in range(Ny):
            x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.)
            y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.)
            z0 = complex(x,y) #z0 = x+y*1j
            z = 0j
            for itr in range(max_steps):
                if z.real*z.real + z.imag*z.imag > 4.:
                    data[j,i]=itr
                    break
                z = z*z + z0
    return data

def MandPybind11(ext, max_steps, Nx, Ny):
    data = ones((Ny,Nx));
    imanc.mand(data, Nx, Ny, max_steps, ext)
    return data

if __name__ == '__main__':
    Nx = 1000
    Ny = 1000
    max_steps = 1000 # 50
    ext = [-2,1,-1,1]
    t0 = time.time()
    t0_ = time.process_time() # cpu time
    data = MandPybind11(ext, max_steps, Nx, Ny)
    t1 = time.time()
    t1_ = time.process_time() # cpu time
    print('pybind11: walltime: ', t1-t0, 'cputime: ', t1_-t0_)
    imshow(data, extent=ext)
    show()

    t0 = time.time()
    t0_ = time.process_time() # cpu time
    data = MandNumba(array(ext), max_steps, Nx, Ny)
    t1 = time.time()
    t1_ = time.process_time() # cpu time
    print('numba: walltime: ', t1-t0, 'cputime: ', t1_-t0_)
    imshow(data, extent=ext)
    show()
```

Homework:

Speed up the implement mandelbrot with f2py or with pybind11.

Compilation and Linking Instructions + creating Makefiles

C/C++ and fortran code needs to be compiled before it can be run.
The compilation takes two steps: producing object (machine) code from the source code, and linking objects into executable.
The commands are:

- compile: `g++ [options] -c <source1>.cc`
  compile: `g++ [options] -c <source2>.cc`
- link: `g++ [options] -o <executable> <source1>.o <source2>.o`
- execute: `./<executable>`

If compiling a single source file, we can achieve both steps with one command

compile&link: `g++ [options] -o <executable> <source>.cc`
execute: `./<executable>`

Options can be omitted, but we will many times use options for optimization (`-O`, or `-O3`)
adding debugging information (`-g`), or additig profiling information (`-p` or `-pg`)

For fotran, code we can use identical process, except `g++` is replaced by fortran compiler, i.e., either gnu-fortram `gfortran` or intel's `ifort`.

Compilation and Linking Instructions + creating Makefiles

Python is interpreter. The code does not need explicit compilation. By invoking Python interpreter, the code is compiled on the fly and executed at the same time

compile&execute: `python <script>.py`

If we want to avoid invoking python interpreter explicitly, we need to do the following:

- change script permission: `chmod +x <script>.py`
- the first line needs to be: `#!/usr/bin/env python`
- execute: `./<script>.py`

Creating Makefiles

It is a good practice to write a makefile for every project. Makefile typically contains information about the default compilers, location of necessary include files and necessary libraries to link to the executable.

There are many nice tutorials available on the Web including

https://cs.colby.edu/maxwell/courses/tutorials/maketutor/

https://www.tutorialspoint.com/makefile/index.htm

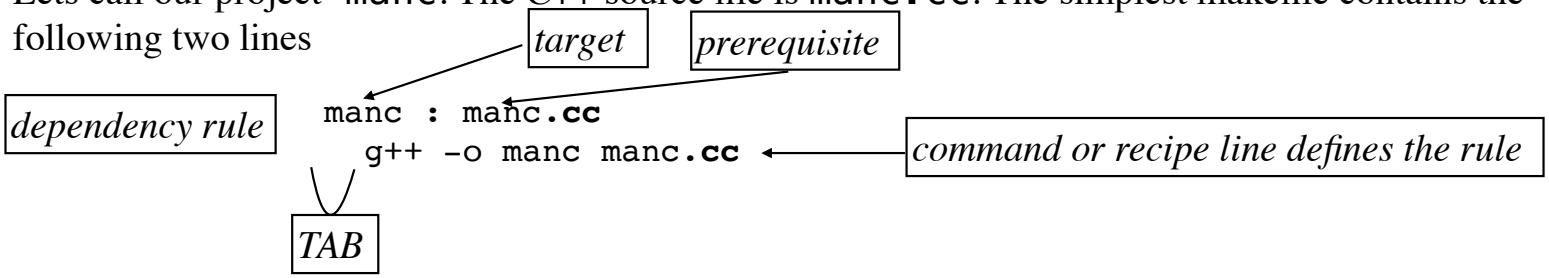
https://www.gnu.org/software/make/manual/

We will briefly describe the steps in writing simple makefiles.
But first remember:

- The name of the makefile can be ”Makefile” or ”makefile” and is typically located in the same directory as other source files.
- User types ”make” in the source directory and makefile is executed producing the executable file.

Creating Makefiles

Lets call our project `manc`. The C++ source file is `manc.cc`. The simplest makefile contains the following two lines



Note: Each line in the commands list must begin with a TAB character!

The dependency rule defines under what conditions a given file needs to be recompiled, and how to compile it.

The above rule states that the executable `manc` (is a target) has to be recompiled whenever `manc.cc` (prerequisite) is modified. The rule tells us that `manc` can be obtained by the command `g++ -o manc manc.cc` (the recipe).

We can have multiple rules, which are executed recursively.
By default, make always executes the first rule in the makefile. The other rules are executed, if they are called by some other rule (starting from the first rule).
The exception is the case when we give an argument to the make command, make will start at the rule with such name.

Creating Makefiles

Here is an example with multiple rules

```
all : manc manf # if all does not exists, manc and manf are envoked

manc : manc.cc # target : dependencies // time1 > time2 -> execute
  g++ -o manc manc.cc # commands

manf : manf.f90 # target : dependencies
  gfortran -o manf manf.f90 # command
```

The first rule is `all`, and make will start evaluating it.

The first lines says that `all` depends on `manc` and `manf`. If the two files do not exist, make will create them by finding and executing rules for `manc` and `manf`. Even if the two files (`manc` & `manf`) exist, make will check if they are up to date, otherwise it will evaluate the rules. Up to date means that prerequisites (on the right) are older than targets (on the left). For example, if `manc.cc` is newer than `manc`, the rule for `manc` will be evaluated even though `manc` exists. We could say that if the file does not exists, it is equivalent to be very old for the purpose of makefile rules evaluation.

Creating Makefiles

Next we could define some constants for compiler names and compiler flags (optimization).
For example

```
C++ = g++          # define variable C++
FORT = gfortran    # define variable FORT
CFLAGS = -O3
FFLAGS = -O3

# rules below

all : manc manf # target : prerequisite

manc : manc.cc          # target : prerequisite // time1 > time2 -> execute
  $(C++) $(CFLAGS) -o manc manc.cc # commands

manf : manf.f90         # target : prerequisite
  $(FORT) $(FFLAGS) -o manf manf.f90 # command
```

This is useful for porting makefiles to different computer/operating system, as only a few variables needs to be changed on different system.

Creating Makefiles

Most makefiles have a rule named `clean`. This will remove all object files and all executables, so that a fresh compilation can be started after clean is invoked. We would add a rule like that

```
clean :
  rm -f manc manf
```

Notice that the dependency list is empty, hence the rule is always executed when invoked.

To invoke the `clean` rule, we need to call make with the argument: `make clean`

Make also defined many special variables, such as `$@, $<, $*`. The variable `$@` stands for the target on the left hand side, and `$<` is the first item in the prerequisites list.

We could rewrite the `manc` and `manf` rules in the following way:

```
manc : manc.cc          # target : prerequisite // time1 > time2 -> execute
  $(C++) $(CFLAGS) -o $@ $< # commands

manf : manf.f90         # target : prerequisite
  $(FORT) $(FFLAGS) -o $@ $< # command
```

Notice how the two commands become almost identical when using special variables.

We can exploit this similarity of commands by writing generic rules for any pair of target:prerequisite.

Creating Makefiles

When we have many C++ and fortran files, which need to be compiled in a similar way, we can define generic rule.
For example, we can define a rule that produces `xxx.o` from a corresponding `xxx.f90` file.
We can achieve that by so called pattern rules, which can be added at the end of the makefile.

```
#..............
# Patter rules
#..............
%.o : %.cc
  $(C++) $(CFLAGS) -c $<
%.o : %.f90
  $(FORT) $(CFLAGS) -c $<
```

Now we do not need to write a rule for obtaining `xxx.o` from `xxx.f90` or xxx.cc. The pattern rule will find such files in the current directory and execute the commands.

Note that if we have multiple files with the same name, for example `xxx.f90` and also `xxx.cc`, makefile will get confused of which file to use in order to generate `xxx.o`. It will just use one of the two source files. Therefore always avoid naming multiple files with the same name.

Why parallelization?

Top 500 computers in the world: www.top500.org

Kilo 10^3
Meta 10^6
Giga 10^9
Tera 10^{12}
Peta 10^{15}
Exa 10^{18}

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371

Fast computers have several million cores, which need to be used efficiently & simultaneously

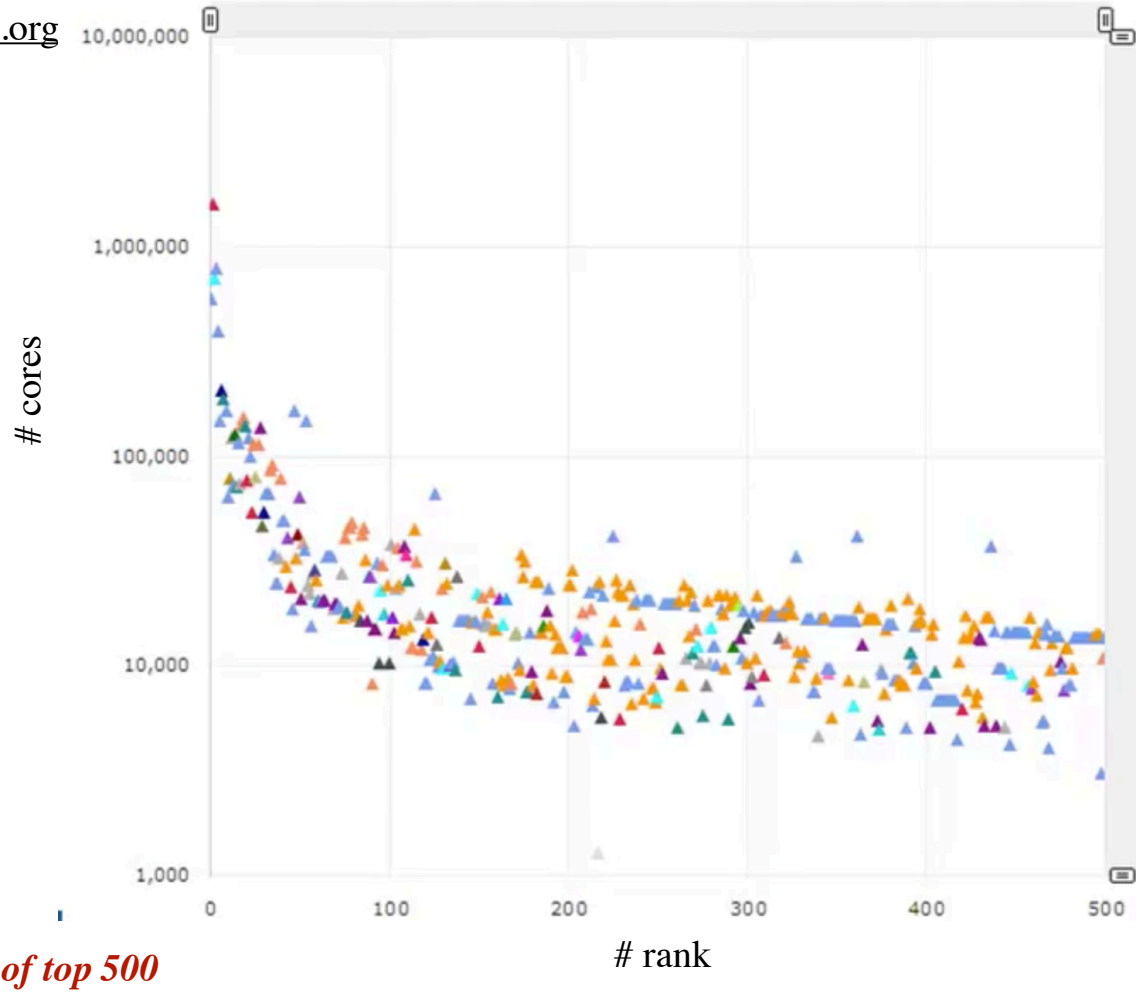
my laptop: 8 cores, 2.4 GHz with 8 single-precision FLOPS's per second
hence theoretical performance = 8*2.4GHz*8 = 38.4GFLOPS/s=0.0384TFLOPS/s

This is theoretical not actual speed, the list contains actual TFLOPS by running LINPACK benchmark

Why parallelization?

Top 500 computers in the world: www.top500.org

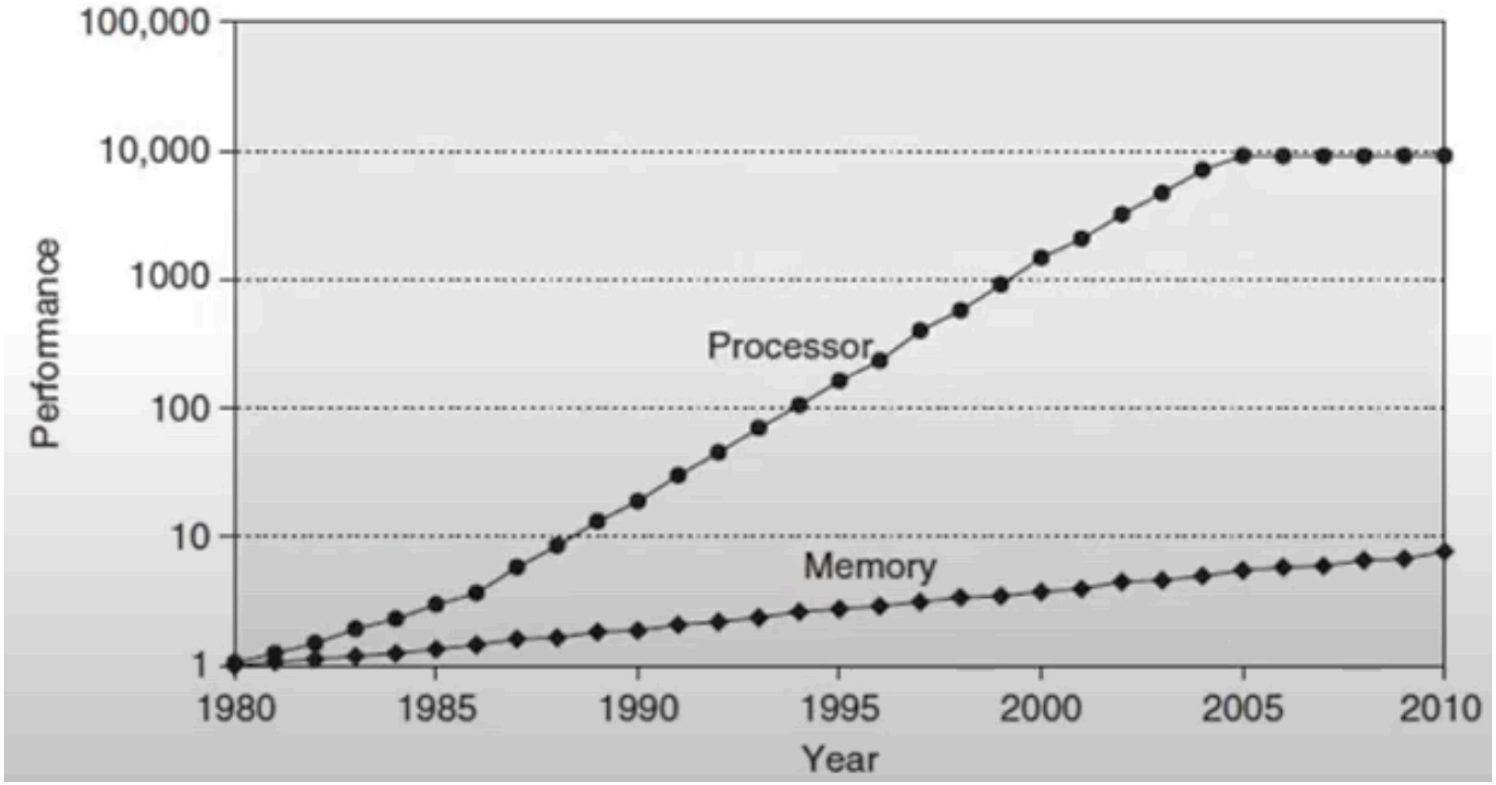
Kilo 10^3
Mega 10^6
Giga 10^9
Tera 10^{12}
Peta 10^{15}
Exa 10^{18}



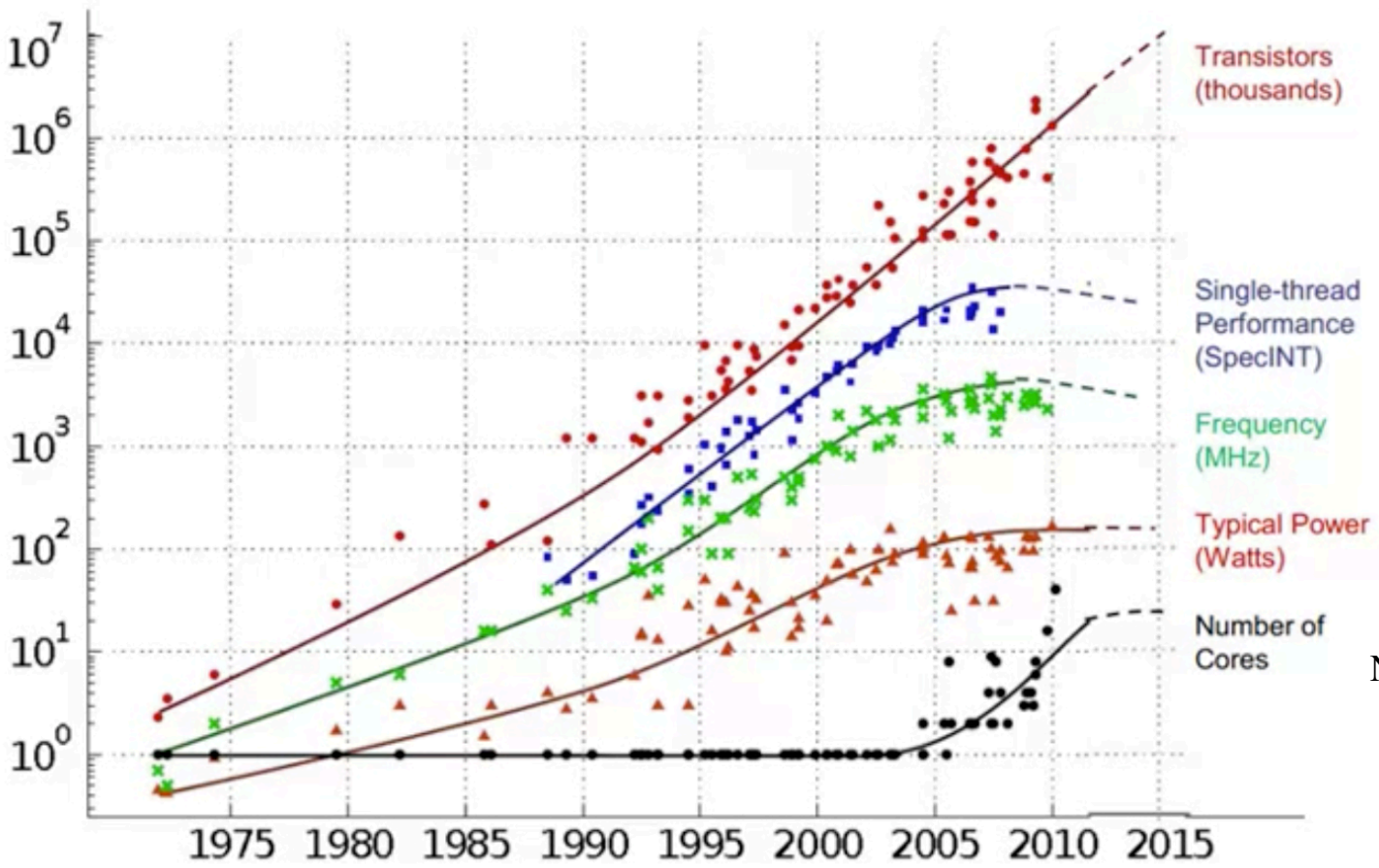
The number of cores is exploding in the list of top 500

Why parallelization?

Processor's speed increased linearly with small slope between 1980-1985 (1.25/year), and larger slope between 1985-2000 (1.52/year)
Processor's speed plateaued in 2005 (people were predicting Moor's law to break).
Instead of increasing the speed of single processor, number of processors and cores is now increasing exponentially



Moore's law still works!



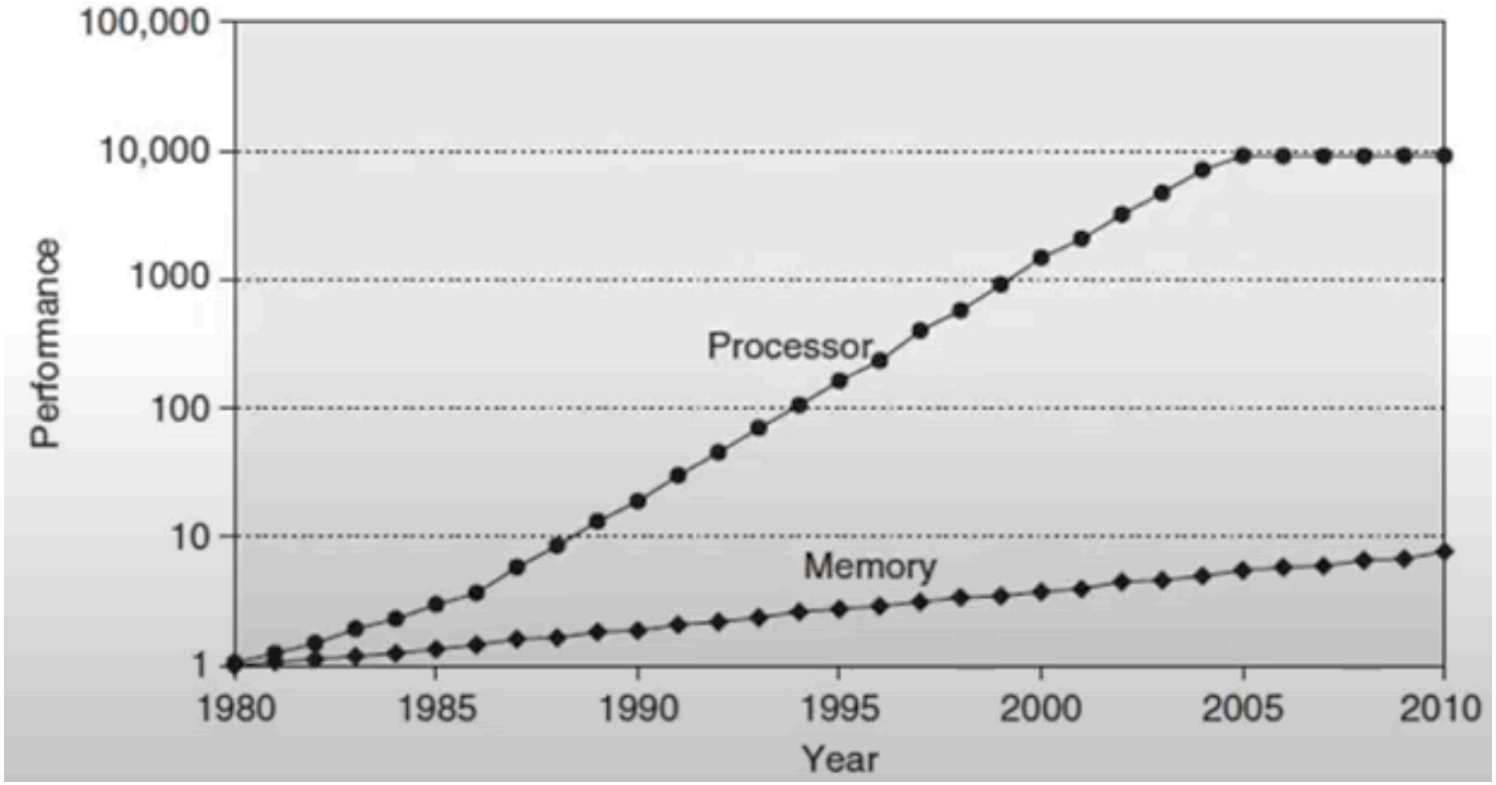
Number of transistors is still exploding, which defines Moore's law.

Quantum limit for single core, it can not be too small, because it stops behaving classically

Number of cores is exploding

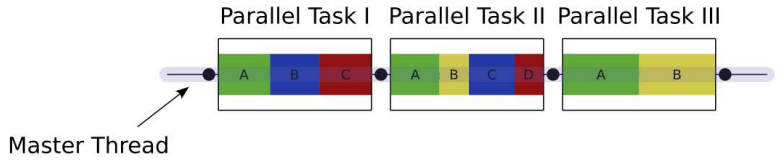
Why parallelization?

Also important is memory latency, which is improving slowly with 1.07/year. Hence memory speed is substantially slower than processor speed, and it will remain so for foreseeable future.

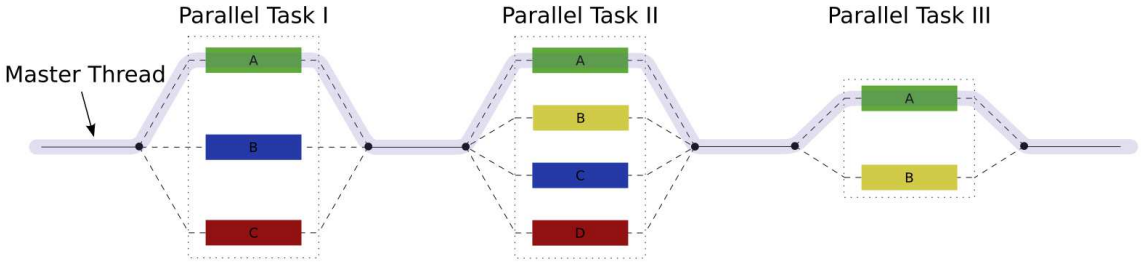


openMP and multicore execution

Usual serial execution



openMP multicore execution



- OpenMP is designed for multi-processor/core to run a program on several cores (using several ”threads”)
- OpenMP programs accomplish parallelism exclusively through the use of threads. Typically, the number of threads match the number of machine processors/cores. However, the actual use of threads is up to the application.
- OpenMP is a shared memory programming model, most variables in OpenMP code are visible to all threads by default.
- But sometimes private variables are necessary to avoid race conditions
- OpenMP is an explicit (not automatic) programming model, offering the programmer full control over parallelization.
- Parallelization can be as simple as taking a serial program and inserting compiler directives.... Or as complex as inserting subroutines to set multiple levels of parallelism, locks and even nested locks.

openMP and multicore execution

The simplest case of parallel mandelbrot calculation:

```
#pragma omp parallel for
for (int i=0; i<Nx; i++){
  for (int j=0; j<Ny; j++){
    double x = ext[0] + (ext[1]-ext[0])*i/(Nx-1.);
    double y = ext[2] + (ext[3]-ext[2])*j/(Ny-1.);
    mand[i*Ny+j] = Mandelb(complex<double>(x,y), max_steps);
  }
}
```

The loop over `i` is parallelized. Each core is calculating different `i` term.

Note that `mand` array is shared across all cores, because all cores have access to the entire array, but each core is changing only its own slice of the array.

Note that `x` and `y` must be different on each core. As they are declared inside the loop, compiler makes them private to each core.

In more general case, the `omp parallel` statement is

```
#pragma omp parallel shared(mand,ax,ay) private(beta,pi)
```

By default all variables are shared, hence `shared` statement is not really needed.

openMP and multicore execution

The same loop in fortran is:

```
!$OMP PARALLEL DO  PRIVATE(j,x,y,z0)
do i=1,Nx
   do j=1,Ny
      x = ext(1) + (ext(2)-ext(1))*(i-1.)/(Nx-1.)
      y = ext(3) + (ext(4)-ext(3))*(j-1.)/(Ny-1.)
      z0 = dcmplx(x,y)
      mande(i,j) = Mandelb(z0, max_steps)
   enddo
enddo
!$OMP END PARALLEL DO
```

Note that in fortran all variables are declared at the top of the program, hence `x, y, z0, j` need to be declared private. Also `i` is private, but the first loop counter does not need to be added to the private list, as compiler will add it automatically.

The code is compiled by adding a flag `-fopenmp`:

```
g++ -fopenmp -O3 -o mandc mandc.cc
```

or

```
gfortran -fopenmp -O3 -o mandf mandf.f90
```

Also the environment variable `OMP_NUM_THREADS` should be set to the number of cores (threads) we want to use. We can issue a command

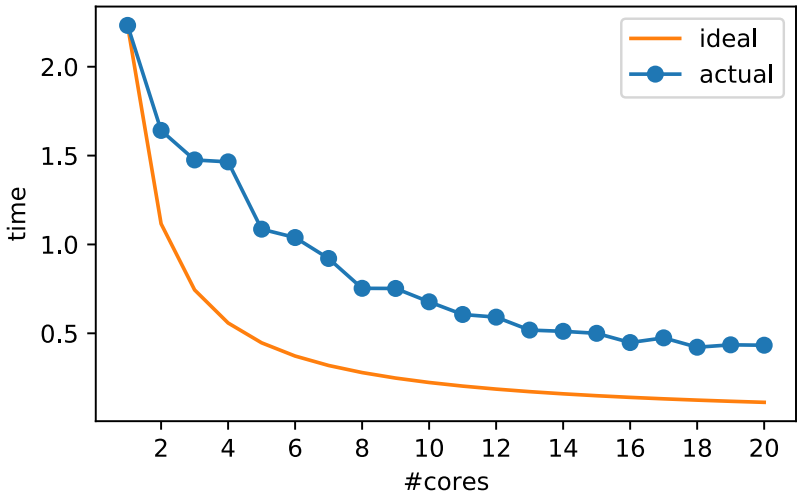
```
export OMP_NUM_THREAS=4
```

openMP and multicore execution

Example of time for mandelbrot set on multiple cores for Intel Core i9 processor:

speed improves, but not close to theoretical (1/core) estimate. Why?

speed improves even beyond 8 threads, even though we have 8 cores. Why?



One more openMP example

$$\pi = \int_0^1 \frac{4}{1+x^2} dx$$

1/n is spacing for trapezoid rule

reduction: We not only make the loop parallel, but we need to tell the compiler that fSum is neither private not shared, but variable to be reduced.

reduction operators are:

`+, -, *, min, max, &, |, ^, &&, ||`

```
#include <iostream>
#include <ctime>
#include <cmath>
#include <omp.h>
using namespace std;

double f(double x){
  return 4.0/(1.0+x*x);
}
double calcPi(int n)
{
  const double dx = 1.0/n;
  double fSum = 0.0;
  #pragma omp parallel for reduction(+:fSum)
  for (int i=0; i<n; ++i){
    double x = (i+0.5)*dx;
    fSum += f(x);
  }
  return fSum*dx;
}
```

One more openMP example

The alternative, but worse implementation: We do not specify that fSum is obtained by reduction, but we specify that a particular line "fSum+=df" should be done without parallelization.

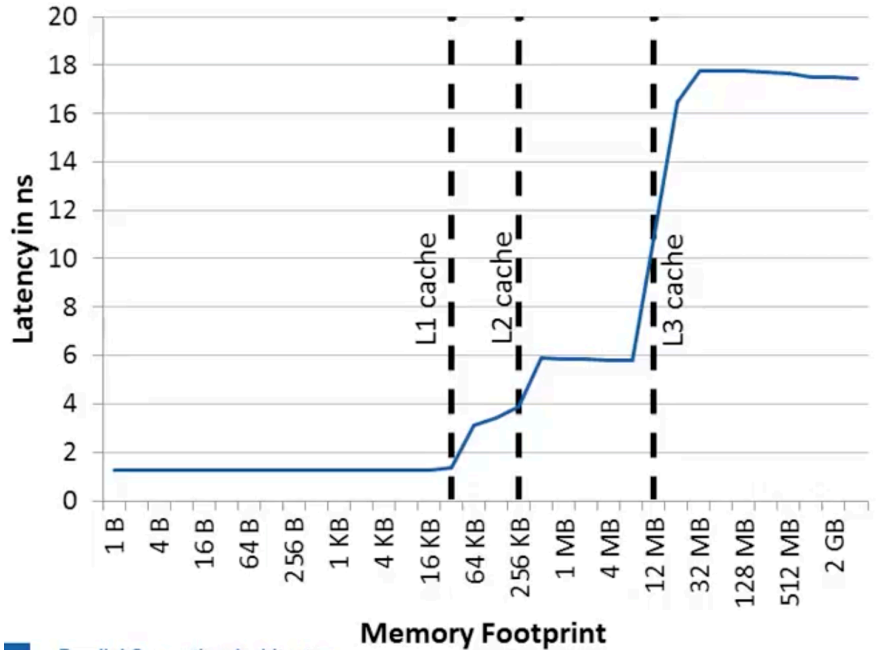
omp critical can be used for any line that can not be parallelized.

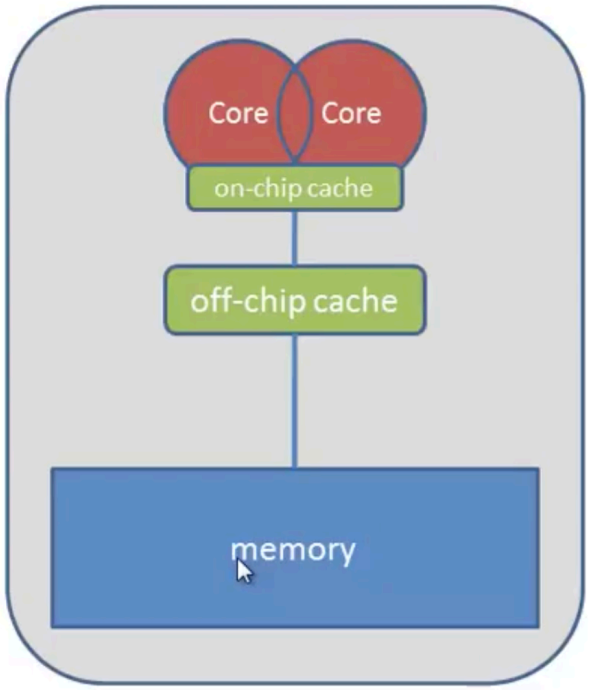
```
#include <iostream>
#include <ctime>
#include <cmath>
#include <omp.h>
using namespace std;

double f(double x){
  return 4.0/(1.0+x*x);
}

double calcPi_bad(int n)
{
  const double dx = 1.0/n;
  double fSum = 0.0;
  #pragma omp parallel for
  for (int i=0; i<n; ++i){
    double x = (i+0.5)*dx;
    double df = f(x);
    #pragma omp critical
    fSum += df;
  }
  return fSum*dx;
}
```

openMP and multicore execution

Memory access is slow. When several cores need to manipulate few MB of data, several cores compete for the bandwidth/access to RAM and L3 cache.

CPU: ~3GHz ~ 0.3ns per tick ~ 0.04ns for floating point operation (8FP per tick)
L1 cache: latency~ 1ns, size ~16KB
L2 cache: latency~ 3ns, size ~256KB
L3 cache: latency~ 6ns, size ~2MB
RAM : latency~20ns, size ~GB, bandwidth~0.3GHz, corresponding to 3.3ns



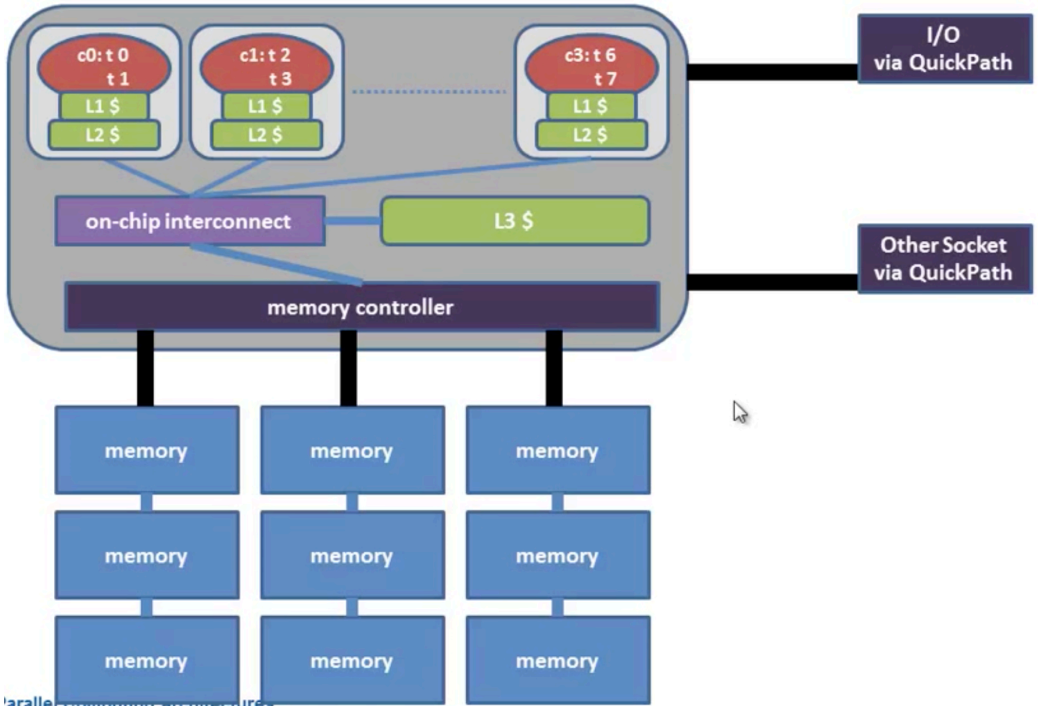


Latency: Delay incurred when a processor accesses data inside the memory (even when reading just one number)

Bandwidth: Rate at which data can be read from or stored into memory by a processor

More realistic multicore architecture

~32KB L1 cache per core
~256KB L2 cache per core
~2MB L3 cache per core, but shared by all cores
several GB RAM

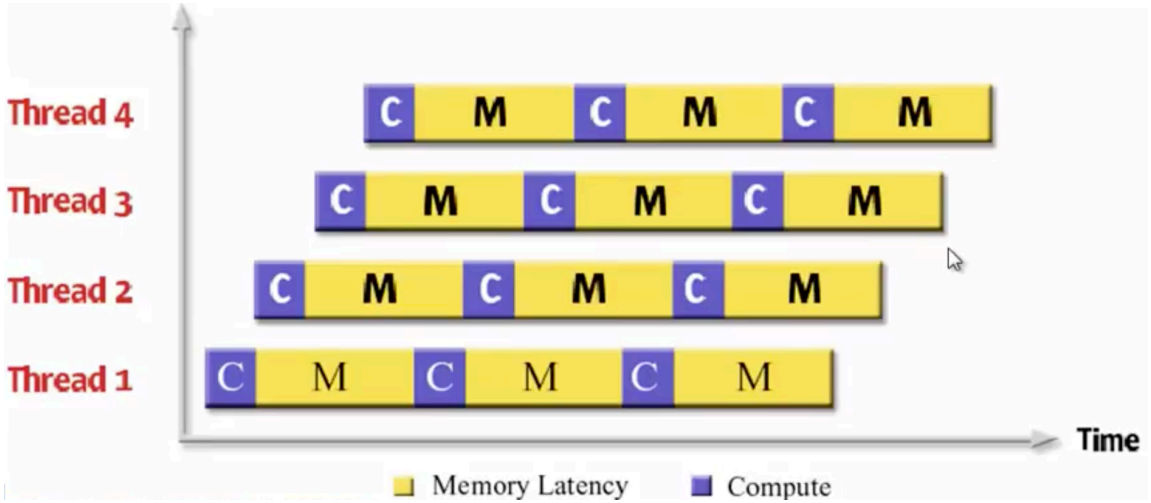


Since we write data into common variable, speed is limited by memory access and not computation, hence we do not get theoretical performance.

Why do we get speedup when using more threads than cores?

Design of modern CPU

Access to memory is arranged to be staggered: some threads are doing computation and some are writing, so we can squeeze out a bit of performance by floading CPU with threads. Notice that this is not necessary the case. Sometimes the execution is slowed down when number of threads exceeeds number of cores.



If you want to learn more about `openMP`, consult these resources

https://www.openmp.org
https://www.openmp.org/resources/tutorials-articles/
https://www.youtube.com/channel/UCtdrEoe46tD2IvJJRs_JH1A/videos

How to improve memory management?

To squeeze out best performance can be a very hard software engineering problem, which is handled by compiler, and user does not have complete overview how memory access is handled.

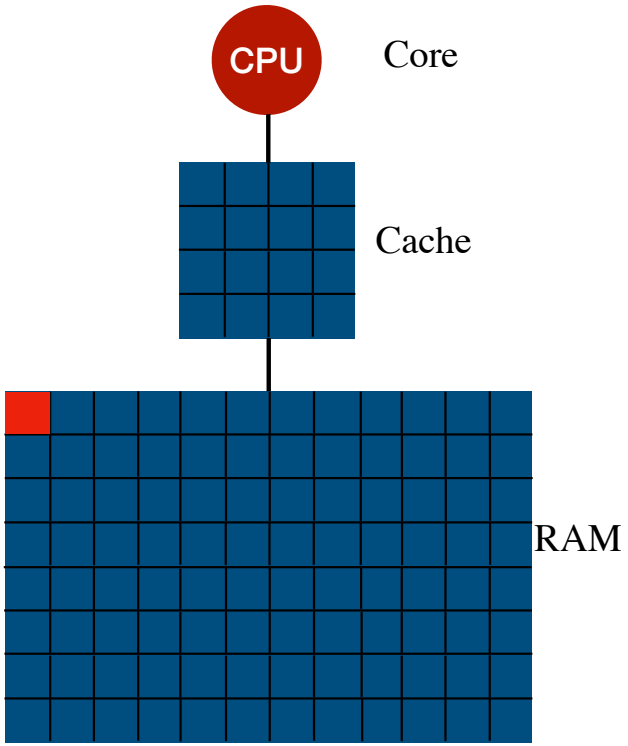
However, there are some general ideas tips of how to access memory to allow compiler well optimize the code.

- Do not use hard-disc for data manipulation if possible. Keep data in RAM. If you need a lot of RAM, estimate whether it fits into RAM. Rethink your algorithm before you start writing data to hard-disc.
- Try avoiding random access of data in RAM to reduce cache misses.
- The data which you need in the innermost loop should be stored in a way that the access is maximally continuous.

Why should we access memory continuously?
Because CPU does not load a single number, but a page, which is 64 byte (8 double's).
We can use data already present.

How does memory work?

For reading or writing one element in the memory, a complete page of memory has to be loaded into cache



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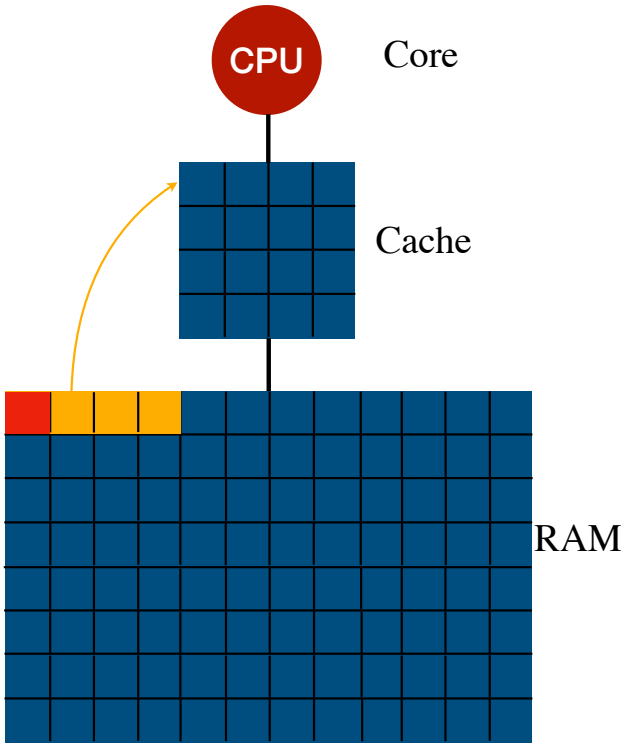
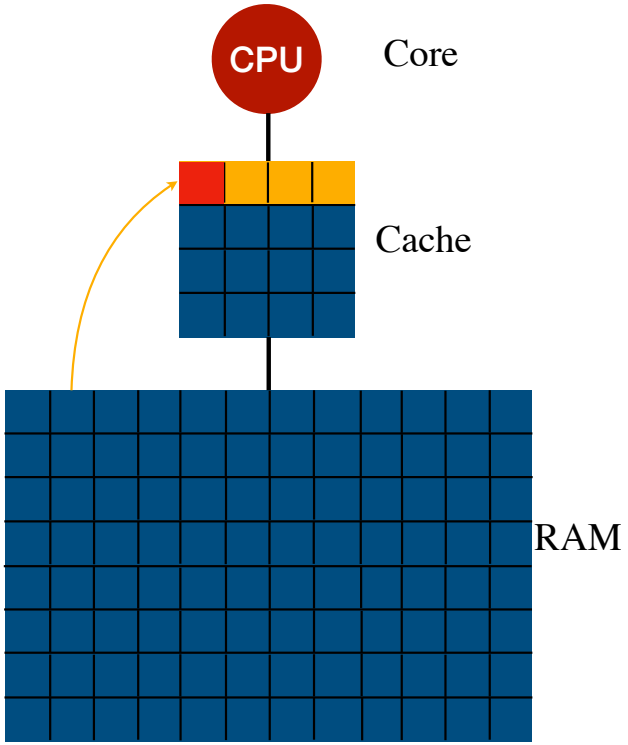


How does memory work?

For reading or writing one element in the memory, a complete page of memory has to be loaded into cache

Now the processor can read and write the elements

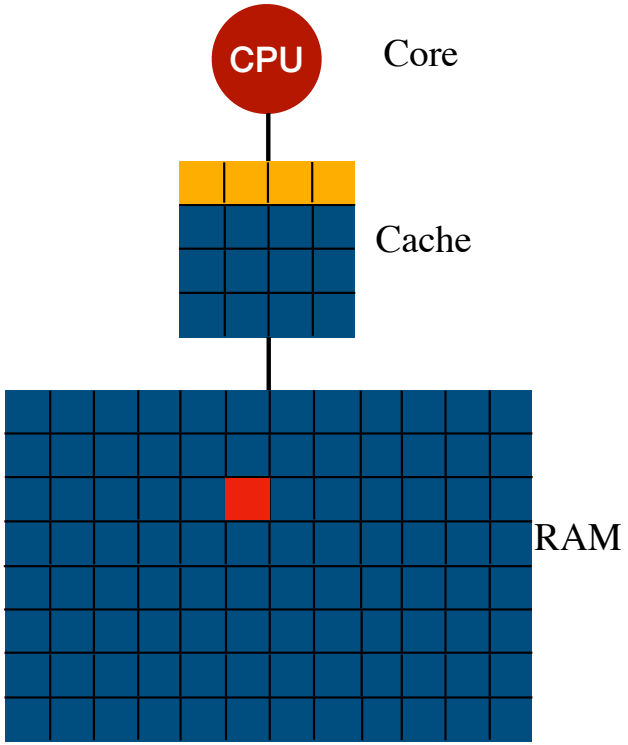


How does memory work?

For reading or writing one element in the memory, a complete page of memory has to be loaded into cache

Now the processor can read and write the elements

If the next element is outside the loaded cache pages, another page needs to be loaded.



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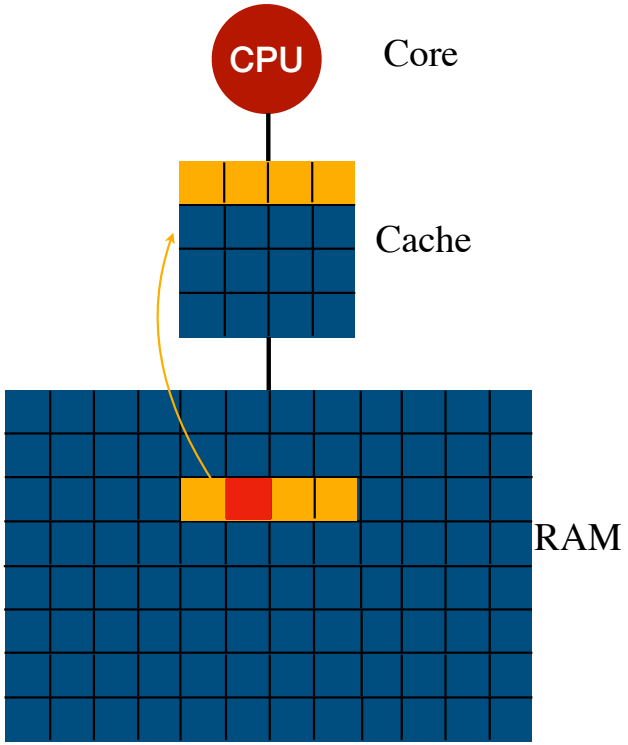

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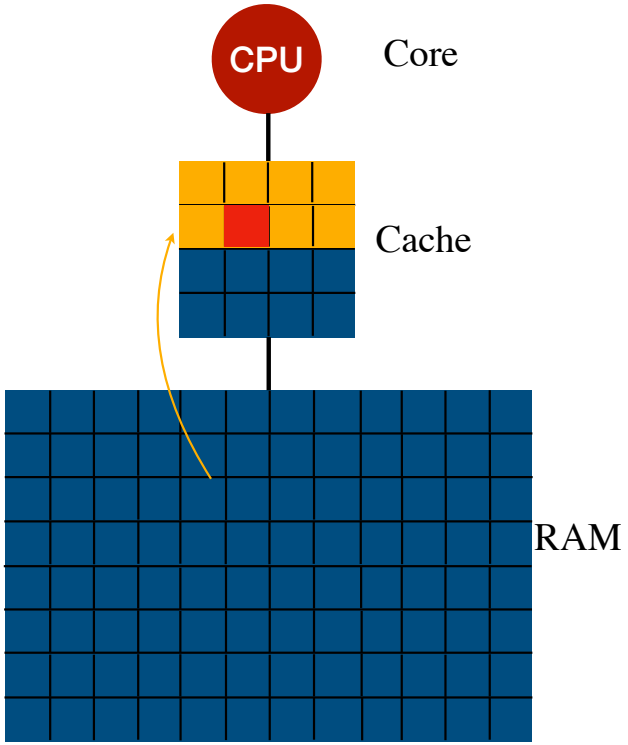

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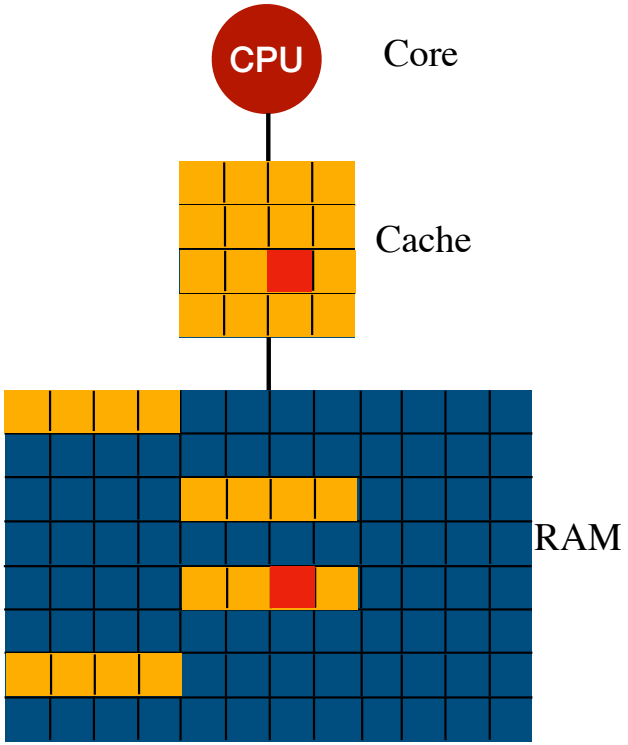
Now the processor can read and write the elements

If the next element is outside the loaded cache pages, another page needs to be loaded.

Accessing an element already loaded in cache is very fast and does not cost extra cycles.



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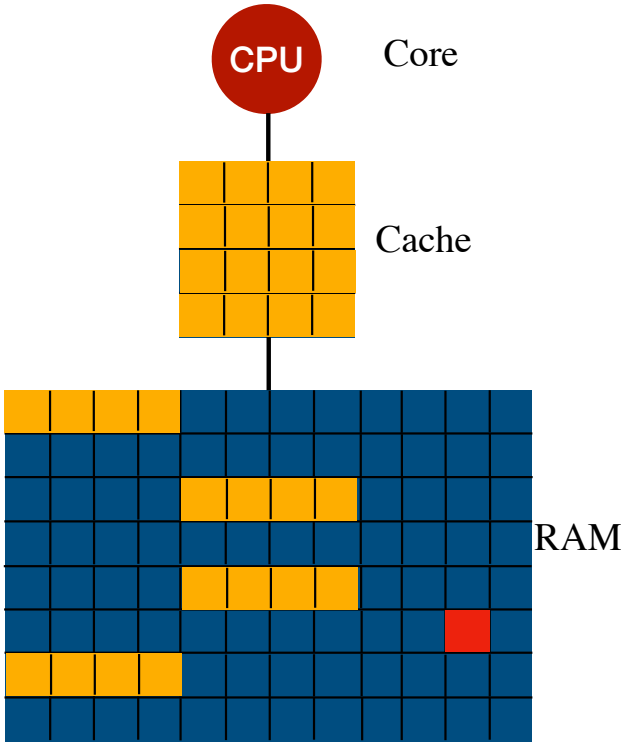
Accessing an element already loaded in cache is very fast and does not cost extra cycles.

If the cache is full and a new cache page should be loaded, an old one must be dropped, which costs several hundred cycles, and is called cache miss.



How to improve memory management?

Typical example is a matrix manipulation.
In C or C++, one needs to access multidimensional arrays in the following order

since the data is stored in a row major order.

```
for (int i=0; i<size; i++)
    for (int j=0; j<size; j++)
            A[i][j] = .....
```

In Fortran, the same loop should be written in the following way

```
do i=1, size
    do j=1, size
           A(j,i) = .....
    enddo
enddo
```

This is because Fortran (C) uses column (row) major storage. The figure explains it all.

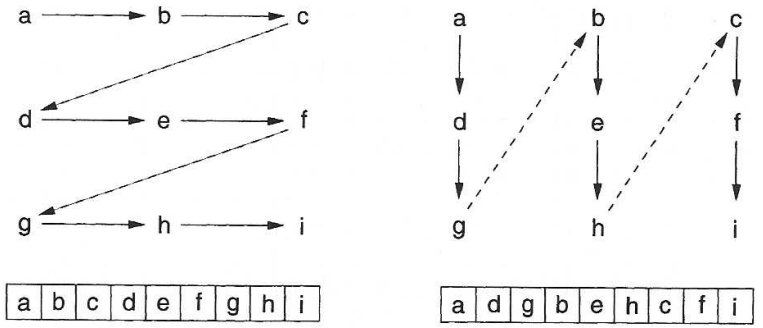


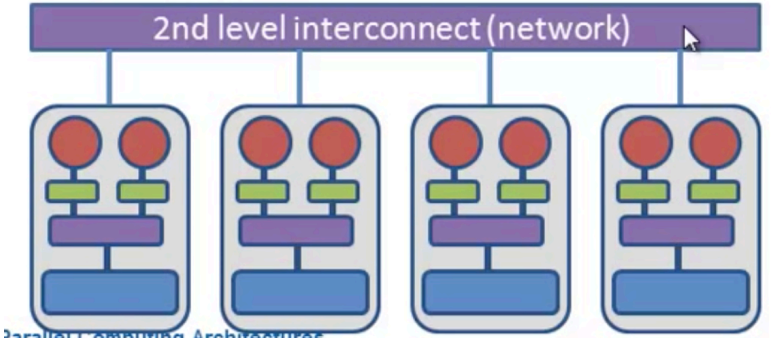
Fig. 15.2 (*Left*) Row-major order used for matrix storage in C and Pascal; (*right*) column-major order used for matrix storage in Fortran. On the bottom is shown how successive matrix elements are stored in a linear fashion in memory.

Multi-node parallelization : MPI

When parallel execution uses several nodes (not just several cores on a single node), we need to use MPI parallelization.
MPI requires one to call specialized MPI routines to communicate and exchange data. This is more technically involved programing.

Inter-node (2nd level interconnect) speed:

- InfiniBand: latency ~5μs, bandwidth ~1Gb/s
- GigaBit Ethernet: latency 60μs, bandwidth ~0.1Gb/s



Latency: Time required to send a message of size zero (time to set up communication)

Bandwidth: Rate at which large messages (>=2Mb) are transfered

Virtual box from past years (which should work if other installations fail):

If you do not want/succeed to install the necessary software, you should download the file :
http://hauleweb.rutgers.edu/downloads/509/509.ova

(warning: 4.8GB file, it might take a while)

Then you should install VirtualBox to run the provided virtual machine:
https://www.virtualbox.org

Finally, start the VirtualBox and navigate to *File/Import Appliance*, and choose the downloaded 509.ova file.

Then click *Start* and wait for the linux to start. Once linux is running, you can start a terminal *Konsole* and start *emacs* in the terminal. You can navigate to

```
cd ~/ComputationalPhysics/mandelbroat
```

and examine the files we will discuss in the first lecture. If you need username, use *student*, and passwd *student123*.

Learning Python

Next learning python from the following lectures:

https://github.com/jrjohansson/scientific-python-lectures

If you prefer video, this might be very good one:

https://www.youtube.com/watch?v=xCKfR80E8ZA