INF3380: Parallel Programming for Natural Sciences

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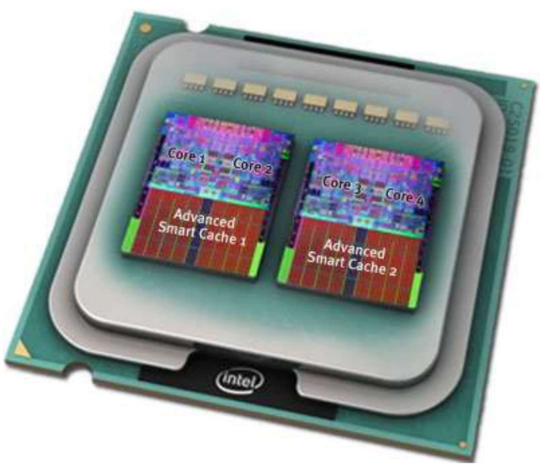
Lecture 1: Overview & recap of serial programming

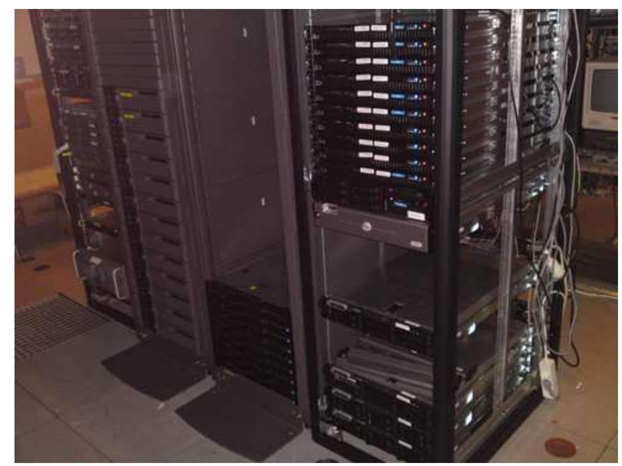
Motivations (1)

- Many problems in natural scienes can benefit from large-scale computations
  - more details
  - better accuracy
  - more advanced models
- Example of huge computations: Weather simulation of the entire globe
  - surface area: $510,072,000$ km^2
  - spatial resolution 1×1km$^2 \rightarrow 5.1 \times 10^8$ small patches
  - spatial resolution 100×100m$^2 \rightarrow 5.1 \times 10^{10}$ small patches
  - additional layers in the vertical direction
  - high resolution in the time direction
- Traditional single-CPU computers are limited in capacity
  - typical clock frequency $2 \sim 5$ GHz
  - typical memory size $2 \sim 8$ GB

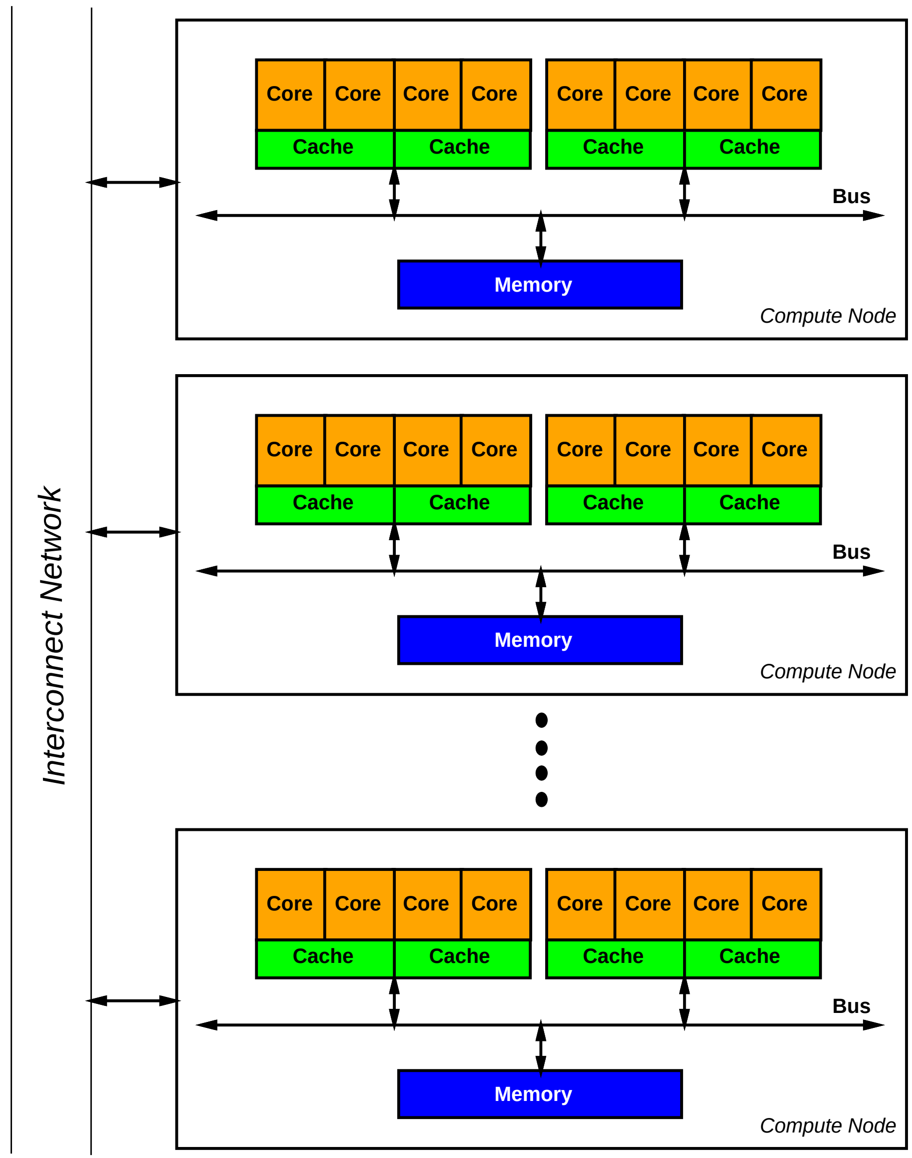
Motivations (2)

- Parallel computers are now everywhere!
  - CPUs may have more than one core on a chip
  - One computer may have several multicore chips
  - There are also accelerator-based parallel architectures — CellBE & GPGPU
  - Clusters of different kinds





An example of multicore-based cluster



Why parallel programming?

- Parallel computing – a form of parallel processing by utilizing multiple computing units (cores) concurrently for one computational problem
  - shortening computing time
  - solving larger problems
- Modern multicore-based computers are good at multi-tasking, but not good at automatically computing one problem in parallel
- Automatic parallelization compilers have had little success
- Special parallel programming languages have had little success
- Serial computer programs have to be modified or rewritten to utilize parallel computers
- Programming parallel codes is thus important!

What will you learn?

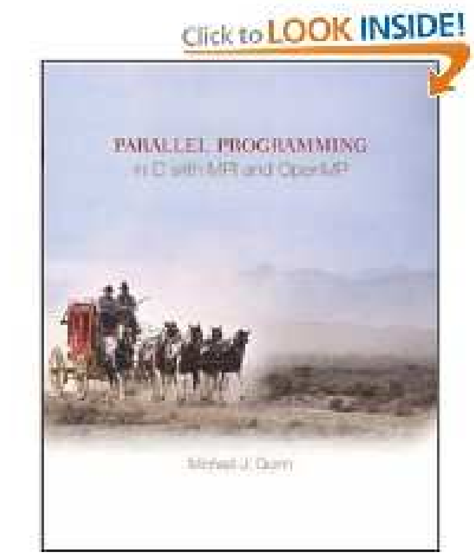
- An introduction to parallel programming
  - important concepts
  - basic parallel programming skills (MPI and OpenMP)
  - use of multicore PCs and PC clusters
  - a peek into GPU computing
- After finishing the course, you should be able to write simple parallel programs
- You should also be able to learn more about advanced parallel progamming on your own later

Teaching approaches

- Focus on fundamental issues
  - parallel programming = serial programming + finding parallelism + enforcing work division and collaboration
- Use of examples relevant for natural sciences
  - mathematical details are not required
  - understanding basic numerical algorithms is needed
  - implementing basic numerical algorithms is essential
- Hands-on programming exercises and tutoring

Some important info

- Textbook: *Michael J. Quinn*, **Parallel Programming in C with MPI and OpenMP**, McGraw Hill Higher Education, 2003



- Lecture slides ready for download at least one week in advance
- Two mandatory assignments
- Written exam with grades A–F

Recapitulation of serial programming

What is serial programming?

- Roughly, a computer program consists of a sequence of operations applied to data structures
- Example of programming languages:
  - C & Java – statically typed
  - Python – dynamically typed
- Data structures:
  - variables of primitive data types (`char, int, float, double` etc.)
  - variables of composite and abstract data types (`struct` in C, `class` in Java & Python)
  - array variables
- Operations:
  - statements and expressions
  - functions

Variables

- In a dynamically typed programming language (e.g. Python) variables can be used without declaration beforehand

```
a = 1.0
b = 2.5
c = a + b
```

- In statically typed langauges (e.g. Java and C) declaration of variables must be done first

```
double a, b, c;

a = 1.0;
b = 2.5;
c = a + b;
```

Simple example

- Suppose we have temperature measurement for each hour during a day
- t_1 is the temperature at 1:00 o'clock, t_2 is the temperature at 2:00 o'clock, and so on.
- How to find the average temperature of the day?
- We need to first add up all the 24 temperature measurements:

$$T = t_1 + t_2 + \ldots + t_{24} = \sum_{i=1}^{24} t_i$$

- The average temperature can then be calculated as $\frac{T}{24}$.

Simple example (cont'd)

How to implement the calculations as a computer program?

- First, create an array of 24 floating-point numbers to store the 24 temperatures. That is, `t[0]` stores t_1, `t[1]` stores t_2 and so on. Note that array index starts from 0!
- Sum up all the values in the array `t`
  - Same syntax for the computational loop in Java & C:

    ```
    T = 0;
    for (i=0; i<24; i++)
      T = T + t[i];
    ```

  - Syntax for Python:

    ```
    T = 0
    for i in range(0,24):
      T = T + t[i]
    ```

- Finally, `t_average = T/24;`

Similarities and differences between languages

- For scientific applications, arrays of numerical values are the most important basic building blocks of data structures
- Extensive use of `for`-loops for doing computations
- Different syntax details
  - allocation and deallocation of arrays
    - Java: `double[] v=new double[n];`
    - C: `double *v=malloc(n*sizeof(double));`
    - Python: `v=zeros(n,dtype=float64)` (using NumPy)
  - definition of composite and abstract data types
  - I/O

C as the main choice of programming language

- C is one of the dominant programming languages in computational sciences
- Syntax of C inspired many newer languages (C++, Java, Python)
- Good computational efficiency
- C is ideal for using MPI and OpenMP (also GPU programming)
- We will thus choose C as the main programming language
- This lecture will give a crash course on scientific programming, with syntax details in C

Some words about pointers in C

- A variable in a program has a name and type, its value is stored somewhere in memory
- `Type *p` declares a pointer to a variable of datatype `Type`
- A pointer is actually a special type of variable, used to hold the memory address of a variable
- From a variable to its pointer: `int a; int *p; p = &a;`
- We can use a pointer to change the variable value `*p = 2;`
- A pointer can also be used to hold the memory address of the first entry of an array (such as returned by `malloc`)
- Array indexing: `p[0], p[1]` ...
- Pointer arithmetic:

```
int *p = (int*)malloc(10*sizeof(int));
int *p2 = p + 3;  /* p2 is now pointing to p[3] */
```

Allocating multi-dimensional arrays (1)

Let's allocate a 2D array for representing a $m \times n$ matrix

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

- Java:

```
double[][] A = new double[m][n];
```

- C:

```
double **A = (double**)malloc(m*sizeof(double*));
for (i=0; i<m; i++)
   A[i] = (double*)malloc(n*sizeof(double));
```

- Same syntax in Java and C for indexing and traversing a 2D array

```
for (i=0; i<m; i++)
  for (j=0; j<n; j++)
    A[i][j] = i+j;
```

Allocating multi-dimensional arrays (2)

- Use of NumPy makes array allocation very simple in Python

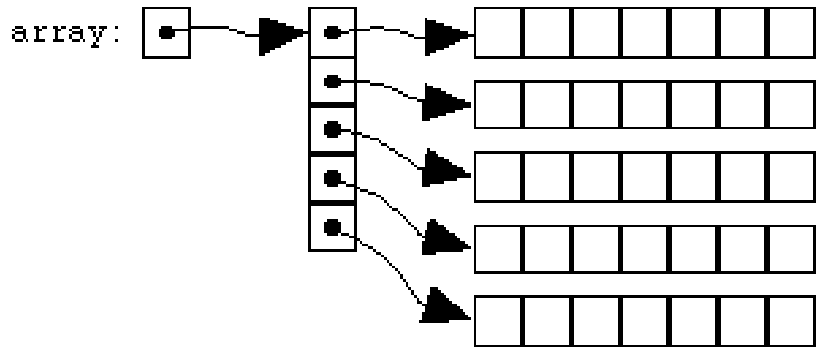
```
from numpy import *
A = zeros((m,n), dtype=float64)
```

- Indexing and traversing a 2D array in Python

```
for i in range(0,m):
  for j in range(0,n):
    A[i,j] = i+j;
```

More about two-dimensional arrays in C (1)

- C doesn’t have true multi-dimensional arrays, a 2D array is actually an array of 1D arrays (like Java)



- `A[i]` is a pointer to row number i+1
- It is also possible to use static memory allocation of fix-sized 2D arrays, for example:

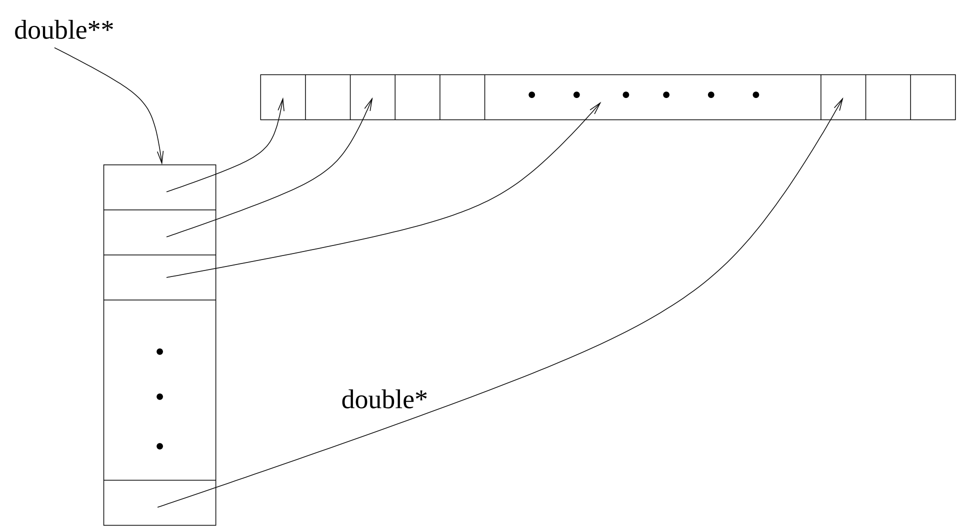
  ```
  double A[10][8];
  ```

  However, the size of the array is decided at compiler time (not runtime)

More about two-dimensional arrays in C (2)

- Dynamic memory allocation of 2D arrays through e.g. `malloc`
- Another way of dynamic allocation, to ensure contiguous underlying data storage (for good use of cache):

```
double *A_storage=(double*)malloc(n*n*sizeof(double));
double **A = (double**)malloc(n*sizeof(double*));
for (i=0; i<n; i++)
  A[i] = &(A_storage[i*n]);
```



Deallocation of arrays in C

- If an array is dynamically allocated, it is important to free the storage when the array is not used any more
- Example 1

```
int *p = (int*)malloc(n*sizeof(int));
/* ... */
free(p);
```

- Example 2

```
double **A = (double**)malloc(m*sizeof(double*));
for (i=0; i<m; i++)
   A[i] = (double*)malloc(n*sizeof(double));
/* ... */
for (i=0; i<m; i++)
  free(A[i]);
free(A);
```

- Be careful! Memory allocation and deallocation can easily lead to errors

The form of a C progam

- A program in C is made up of functions
- A stand-alone C program must at least implement function `main`, which will be executed by the operating system
- Functions are made up of statements and declarations
- Variables must be declared before usage
- Possible to use functions and variables declared in libraries

Some syntax details in C

- Semicolon (`;`) terminates a statement
- Braces ({}) are used to group statements into a block
- Square brackets (`[]`) are used in connection with arrays
- Comments can be added between `/*` and `*/`

Functions in C

- Function declaration specifies name, type of return value, and (optionally) a list of parameters
- Function definition consists of declaration and a block of code, which encapsulates some operation and/or computation

```
return_type function_name (parameter declarations)
{
  declarations of local variables
  statements
}
```

Function arguments

- All arguments to a C function are passed by value
- That is, a copy of each argument is passed to the function

  ```
  void function test (int i) {
    i = 10;
  }
  ```

  The change of `i` inside `test` has no effect when the function returns
- Passing pointers as function arguments can be used to get output

  ```
  void function test (int *i) {
    *i = 10;
  }
  ```

  The change of `i` inside `test` now has effect

Function example 1: swapping two values

```
void swap (int *a, int *b)
{
  int tmp;
  tmp = *a;
  *a = *b;
  *b = tmp;
}
```

Function example 2: smoothing a vector

We want to smooth the values of a vector $\mathbf{v}$ by the following formula:

$$v_i^{\text{new}} = v_i + c\left(v_{i-1} - 2v_i + v_{i+1}\right), \quad 2 \leq i \leq n-1$$

where c is a constant

```
void smooth (double *v_new, double *v, int n, double c)
{
  int i;
  for (i=1; i<n-1; i++)
    v_new[i] = v[i] + c*(v[i-1]-2*v[i]+v[i+1]);
  v_new[0] = v[0];
  v_new[n-1] = v[n-1];
}
```

Similar computations occur frequently in numerical computations, e.g., solving the heat equation

Function example 3: matrix-vector multiplication

We want to compute $\mathbf{y} = \mathbf{A}\mathbf{x}$, where $\mathbf{A}$ is a $m \times n$ matrix, $\mathbf{y}$ is a vector of length m and $\mathbf{x}$ is a vector of length n:

$$y_i = \sum_{j=1}^{n} A_{ij} x_j, \quad 1 \leq i \leq m$$

```
void mat_vec_prod (double **A, double *y, double *x,
                   int m, int n)
{
  int i,j;
  for (i=0; i<m; i++) {
    y[i] = 0.0;
    for (j=0; j<n; j++)
      y[i] += A[i][j]*x[j];
  }
}
```

Example of a complete C program

```
#include <stdio.h>    /* import standard I/O functions */

int myfunction(int x) /* define a function */
{
  int r;
  r = x*x + 2*x + 3;
  return r;
}

int main (int nargs, char** args)
{
  int x,y;
  x = atoi(args[1]);  /* read x from command line */
  y = myfunction(x);  /* invoke myfunction */
  printf("x=%d, y=%d\n",x,y);
  return 0;
}
```

Compilation

- Suppose a file named `first.c` contains the C program
- Suppose we use GNU C compiler `gcc`
- Step 1: Creation of a file of object code:

  ```
  gcc -c first.c
  ```

  An object file named `first.o` will be produced.
- Step 2: Creation of the executable:

  ```
  gcc -o run first.o
  ```

  The executable will have name `run`.
- Alternatively (two steps in one),

  ```
  gcc -o run first.c
  ```
- Better to use the 2-step approach for complex examples

Some important compiler options

- During compilation:
  - Option `-O` turns on optimization flag of the compiler
  - Option `-c` produces an object file for each source file listed
  - Option `-Ixxx` suggests directory `xxx` for search of header files
- During linkage:
  - Option `-lxxx` links with a specified library with name `libxxx.a` or `libxxx.so`
  - Option `-Lxxx` suggests directory `xxx` for search of library files
  - Option `-o` specifies the name of the resulting executable

Exercises (1)

- Write a C program to verify that the limit of $1 - \frac{1}{2^2} + \frac{1}{2^4} - \frac{1}{2^6} + \ldots$ is $\frac{4}{5}$.
- Write a C program that allocates a 1D array of runtime-prescribed length n, assigns the values of the array with random numbers, and finds the maximum and minimum values. (You can use e.g. the `rand` function from `stdlib.h`.)
- When assigning values to the entries of a $m \times n$ matrix, it is common to use a nested `for`-loop with the outer index looping over the rows and the inner index looping over the columns. Does it matter if the sequence of these two loops is swapped?
- Write a C program that allocates a 3D array of dimension (n_x, n_y, n_z). A 1D underlying contiguous storage should be used. Assign some values to the entries of the 3D array. Deallocate the 3D array at the end of the program.

Exercises (2)

- Write a C program that reads from a data file containing one day's temperature measurements of the following format:

  ```
  00:05  -0.1
  00:21   0.1
  00:29  -0.2
  ...
  ```

  Find out the highest and lowest temperatures and when they occurred. Compute also the average temperature and the associated standard deviation.

- Extend the `smooth` function to be applicable to a 2D array, for which the numerical formula is

$$v_{i,j}^{\text{new}} = v_{i,j} + c\left(v_{i-1,j} + v_{i,j-1} - 4v_{i,j} + v_{i,j+1} + v_{i+1,j}\right)$$

Exercises (3)

- The following two functions implement the famous quicksort (see `http://alienryderflex.com/quicksort/`):

```
void swap(int *a, int *b)
{
  int t=*a; *a=*b; *b=t;
}
void sort(int arr[], int beg, int end)
{
  if (end > beg + 1) {
    int piv = arr[beg], l = beg + 1, r = end;
    while (l < r) {
      if (arr[l] <= piv)
        l++;
      else
        swap(&arr[l], &arr[--r]);
    }
    swap(&arr[--l], &arr[beg]);
    sort(arr, beg, l);
    sort(arr, r, end);
  }
}
```

Modify the `sort` function such that instead of directly sorting the array `arr`, we keep it as is but produce a so-called permutation vector `perm`. The purpose is that `arr[perm[0]]`, `arr[perm[1]]`, ..., `arr[perm[n-1]]` is an ordered series.