IN3200/IN4200: High-Performance Computing & Numerical Projects

Course overview & quick recap of serial programming

Xing Cai

Simula Research Laboratory & University of Oslo, Norway

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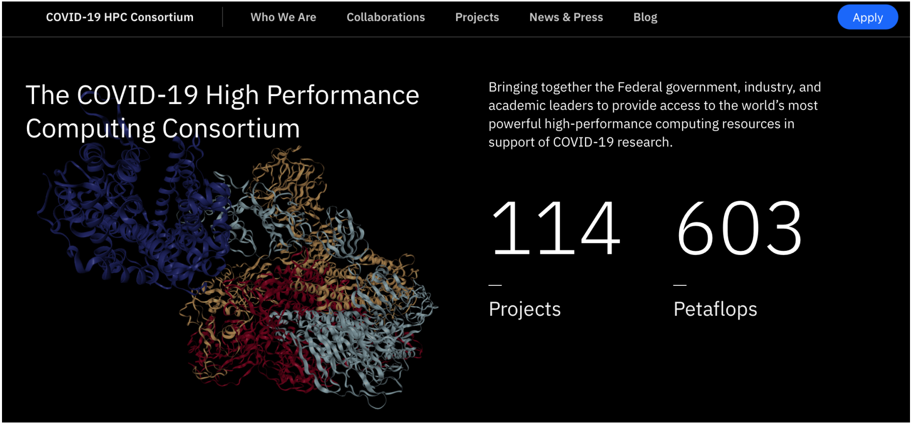
Motivation from the real life



https://covid19-hpc-consortium.org (website last visited on 2022.01.17)

Motivation from the real life (2)

https://www.ukri.org/ (website last visited on 2022.01.17)

Real-life example 1

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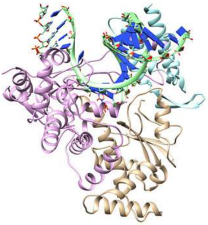
SEPTEMBER 19, 2020

Pulling the plug on the coronavirus copy machine

by Jorge Salazar, Texas Advanced Computing Center



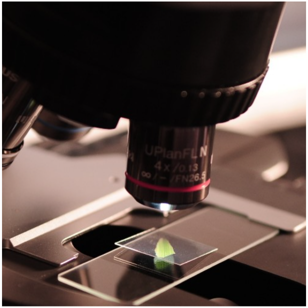
https://phys.org/news/2020-09-coronavirus-machine.html

Real-life example 1 (cont'd)

- To model key proteins used by coronavirus for its reproduction
- Use basic math and physics of Newton's equations and quantum mechanics to calculate the properties of these proteins
- HPC & supercomputers allow much faster simulations
- Goal: Finding ways to improve COVID-19 drugs
- Research team from University of North Texas

Simulations done on Frontera: No. 9 supercomputer in the world (according to TOP500 ranking in Nov. 2020)

https://phys.org/news/2020-09-coronavirus-machine.html



FEATURES

Fighting COVID-19 With the Power of Genomics and HPC

By Janet Morss | June 17, 2020

Researchers at Cardiff University are using the power of genomic sequencing and high performance computing to unlock the secrets of COVID-19.

In scientific laboratories around the world, efforts are under way to put the power of genomic sequencing and high performance computing (HPC) to work in the fight against COVID-19. At Cardiff University in Wales, a team of scientists is working with the COVID-19 Genomics UK Consortium (COG-UK), to unlock the secrets of the coronavirus that causes COVID-19.

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FEATURES

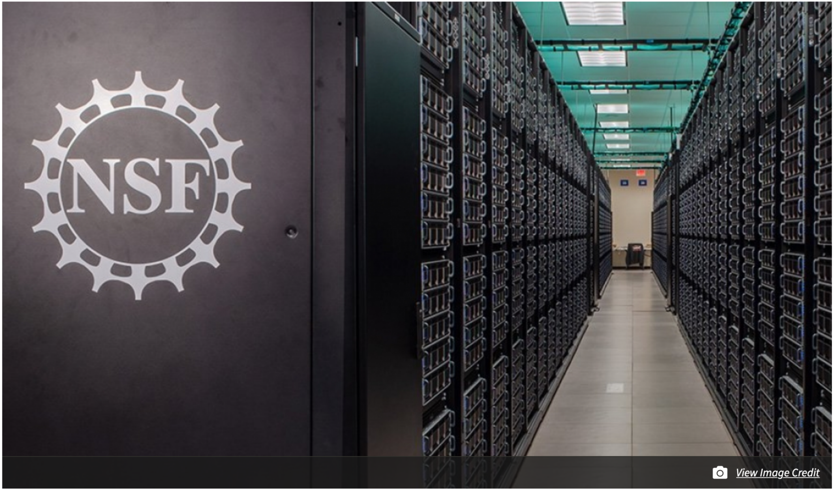
https://www.delltechnologies.com/en-us/blog/fighting-covid-19-with-the-power-of-genomics-and-hpc/

Real-life example 2 (cont'd)

- Large-scale, rapid genomic sequencing and analysis of the coronavirus
- Relying on a large shared system that provides 2.5 petabytes of HPC data storage, also a huge amount of memory (78 terabytes)
- Goal: Unlocking the secrets of the coronavirus
- Research team from Cardiff University in Wales

https://www.delltechnologies.com/en-us/blog/fighting-covid-19-with-the-power-of-genomics-and-hpc/

More about fighting COVID19 with HPC



Why are supercomputers so important for COVID-19 research?

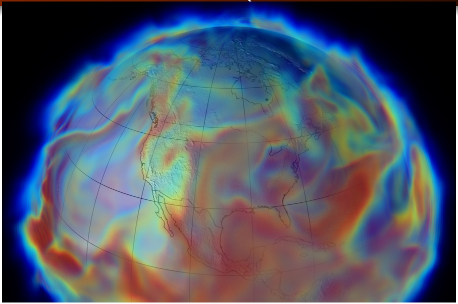
Spread the Word

https://beta.nsf.gov/science-matters/why-are-supercomputers-so-important-covid-19-research?linkId=86826125

General motivations for HPC

- Many problems in natural sciences can benefit from large-scale or huge-scale computations
  - more details
  - better accuracy
  - more advanced models
- The need for computing is ever-increasing
- However, standard laptop PCs or desktop computers are not powerful enough!

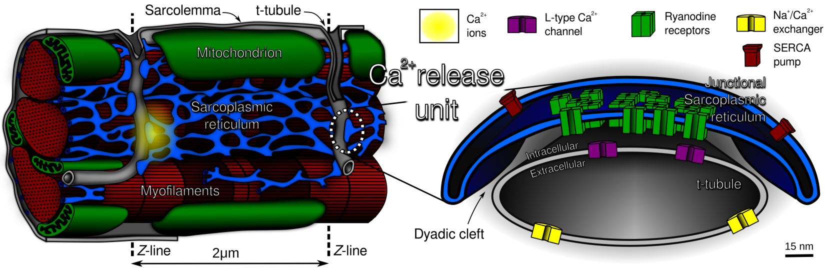
Huge computation example 1 (Climate Simulation)



NASA Center for Climate Simulation

- Earth surface area: $510,072,000$ km^2
- If a spatial resolution of 1×1km^2 is adopted $\rightarrow 5.1 \times 10^8$ (510 million) small patches
- If a spatial resolution 100×100m^2 is adopted $\rightarrow 5.1 \times 10^{10}$ (51 billion) small patches
- Additional layers in the vertical direction
- High resolution in the time direction

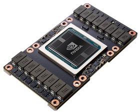
Example 2 (Subcellular Calcium Dynamics Simulation)

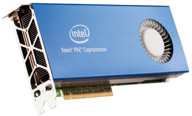


- Size of one cardiac muscle cell: $100\mu m \times 10\mu m \times 10\mu m$
- Width of calcium release channels: 1 nanomater (nm)
- Ideal computational mesh resolution: 1 nm
- Computational mesh required: $10^5 \times 10^4 \times 10^4$ (in total 10^{13} computational voxels)
- Number of simulation time steps needed: $\sim 10^6$

Motivations (cont'd)

- Parallel computers are now everywhere!
  - CPUs nowadays have multiple "cores" on a chip
  - One computer may have several multicore chips
  - There are also accelerator-based parallel architectures — GPGPU (general-purpose graphics processing unit)
  - Clusters of different kinds





What do we learn in IN3200/IN4200?

High-performance computing (HPC) – an introduction

- Proper implementation of numerical algorithms
- Effective use of the hardware for numerical computations

After finishing the course, you should

- be able to write simple parallel programs with sufficiently good performance
- be able to learn more about advanced computing later on your own

Part 1 of the course: Serial programming

- A brief architectural overview of modern cache-based microprocessors
- Inherent performance limitations of microprocessors
- Basic C programming
- Optimization strategies of serial code

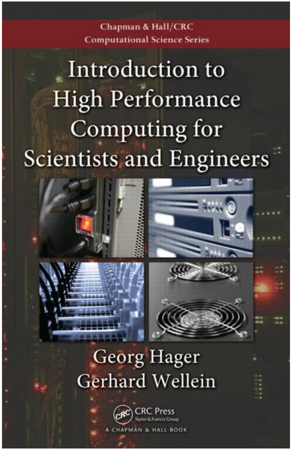
Part 2 of the course: Parallel programming

- Parallel computer architecture
- Theoretical considerations of parallel computing
- Shared-memory parallel programming (OpenMP)
- Distributed-memory parallel programming (MPI)

Why learning parallel programming?

- Parallel computing – a form of parallel processing by concurrently utilizing multiple computing units for one computational problem
  - shortening computing time
  - solving larger problems
- However . . .
  - 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 completely rewritten to utilize parallel computers
- Learning parallel programming is thus important!

Textbook



Georg Hager, Gerhard Wellein

Introduction to High Performance Computing for Scientists and Engineers

1st Edition, CRC Press, ISBN 9781439811924

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
- English is the "official language" of the course, but students should feel free to ask questions, write emails/reports in Norwegian

Recapitulation of serial programming
+
some difficult issues in C programming

A tutorial in C programming will be given in the next lecture

What is serial programming?

- Roughly speaking, a computer program executes a sequence of operations applied to data structures
- A program is normally written in a programming language
- 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 languages (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/24.0;`

Similarities and differences between languages

- For scientific applications, arrays of numerical values are the most important basic building blocks of data structure
- 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 has 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
- (Most of the textbook's coding examples are in Fortran, but many of the "performance-engineering" principles are the same.)

Some words about pointers in C

- A variable in a program has a name and type, its value is stored somewhere in the memory of a computer
- `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;` (The value of a is now 2.)
- We can use several pointers (if needed) to work with an array:

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

Allocating multi-dimensional arrays

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

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

- Java:

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

- C:

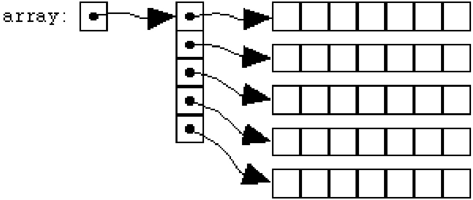
```
double **A = (double**)malloc(m*sizeof(double*));
for (i=0; i<m; i++)
   A[i] = (double*)malloc(n*sizeof(double));
```

- 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;
```

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



- `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:

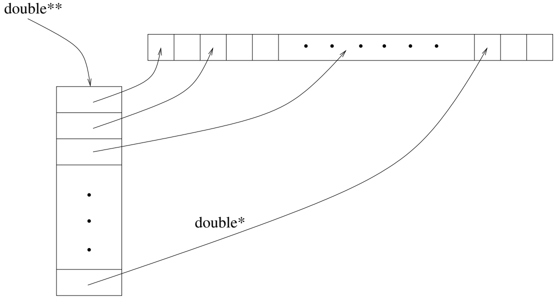
  `double A[10][8];`

  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

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 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 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 **v** by the following formula:

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

  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

Function example 3: matrix-vector multiplication

- We want to compute $\mathbf{y} = \mathbf{Ax}$, 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:

$$y_i = A_{i1}x_1 + A_{i2}x_2 + \ldots A_{in}x_n = \sum_{j=1}^{n} A_{ij}x_j, \quad 1 \leq i \leq m$$

```
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];
  }
}
```