# Quiz 3 - Computational Physics II

**NAME:** Alan Palma Travez **SCORE:** 18,5/20

**Date:** Tuesday 6 May 2025 **Duration:** 45 minutes

**Credits:** 20 points (4 questions) **Type of evaluation:** LAB

**Provide clear and concise answers to the following items.**

1. **(5 points) High-performance computing**
   (a) List and briefly explain 3 key architectural differences between CPUs and GPUs.
   (b) Provide 1 example of an application more suited for CPUs and 1 more suited for GPUs.

a) 1. The CPUs have less cores than the GPUs.

2. The CPUs cores are more powerfull than the GPU cores.

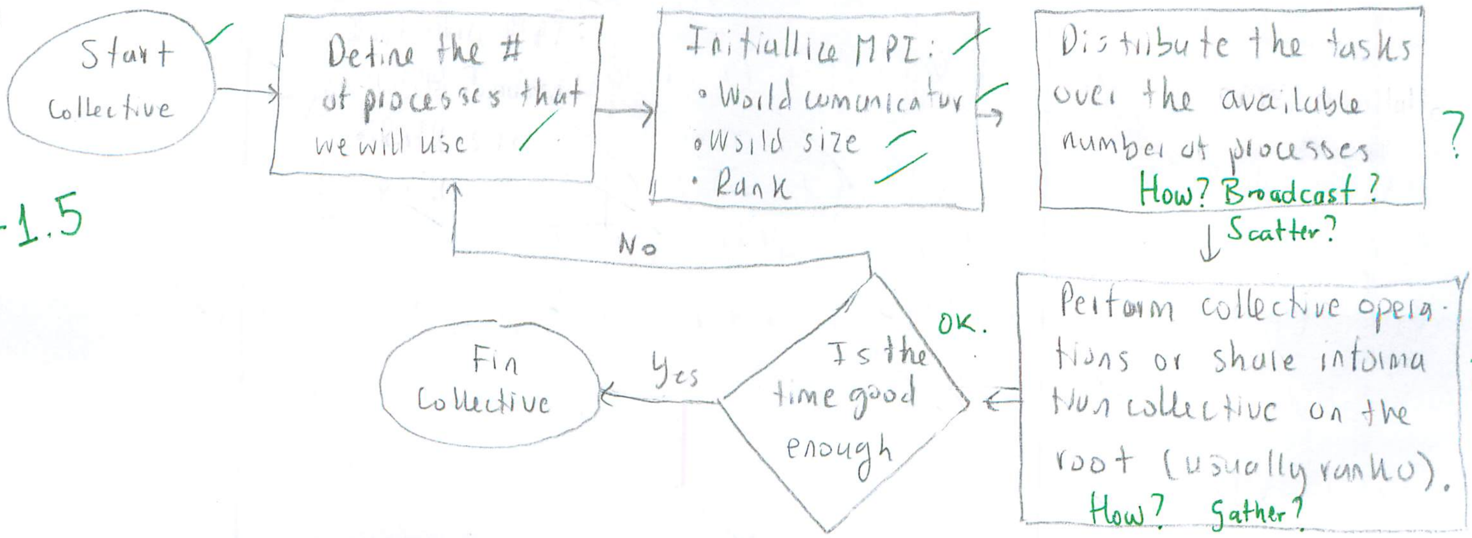
3. The CPUs generally have virtual cores while GPUs does not have virtual cores.

b) The CPUs are used to parallelisation when the task is more complicated and it is needed power than number, e.g., matrix multiplication, making complex operations than can be divided in 2 or more processes. The GPUs are more suited for repetitive tasks that does not need so much computational power, e.g. rendering images.

2. **(5 points) MPI parallelisation**
   (a) Describe 1 difference between point-to-point and collective MPI communication.
   (b) Sketch a workflow that clearly shows the main steps needed to parallelise python code using collective MPI communication.

a) Point-to-point communication consists in sharing information between processes once at a time, from a sender to a reciever. Usually rank 0 is used as the reciever. (receiver) ~~In~~ On the other hand, collective comunication made operations or distribute information in all ranks in one way. All the processes in world communicator works collectively.

b)

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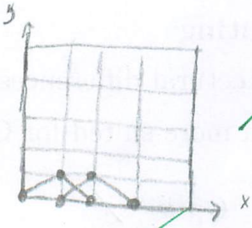
3. **(5 points) Partial Differential Equations (PDEs)**

   (a) Explain the concept of a stencil in the context of numerically solving PDEs.

   (b) Mathematically explain why the heat equation is used to study diffusion processes.

a) The concept of stencil is related with the geometrical shape that is created in the grid by solving the PDE. This take in account the points used to compute the solution $\emptyset_{i,j+1}$.




b) The heat equation $\frac{\partial \emptyset}{\partial t} = -c\nabla^2\emptyset$ relates the evolution of time with the curvature of the "quatity", in this case temperature. In this way, a initial shape will spread out as time evolves. This shows diffusion of some property that will be faster at higher curvature.

4. **(5 points) Discretisation and numerical stability**
   Consider the one-dimensional heat equation with a positive thermal diffusivity ($c > 0$).

   (a) Write down the discrete equation that results from applying an implicit numerical scheme (first order in time, second order in space) on a uniform grid to the heat equation.

   (b) Derive the stability condition for the above implicit scheme based on the amplification factor obtained from the von Neumann analysis.

Heat equation: $\frac{\partial \emptyset}{\partial t} = c\,\frac{\partial^2 \emptyset}{\partial x^2}$

a) Explicit

$$\frac{\partial \emptyset}{\partial t} = \frac{\emptyset_{i,j+1} - \emptyset_{i,j}}{\Delta t} + O(\Delta t); \quad \frac{\partial^2 \emptyset}{\partial x^2} = \frac{\emptyset_{i-1,j} - 2\emptyset_{i,j} + \emptyset_{i+1,j}}{\Delta x^2} + O(\Delta x^2)$$

$$\Rightarrow \frac{\emptyset_{i,j+1} - \emptyset_{i,j}}{\Delta t} = \frac{c}{\Delta x^2}\left(\emptyset_{i-1,j} - 2\emptyset_{i,j} + \emptyset_{i+1,j}\right)$$

$$\Rightarrow \emptyset_{i,j+1} = \overbrace{\frac{c\Delta t}{\Delta x}}^{r}\left(\emptyset_{i-1,j} - 2\emptyset_{i,j} + \emptyset_{i+1,j}\right) + \emptyset_{i,j}$$

$$\Rightarrow \boxed{\emptyset_{i,j+1} = r\,\emptyset_{i-1,j} + (1-2r)\,\emptyset_{i,j} + r\,\emptyset_{i+1,j}}$$

b) Let the solution be $\emptyset = A_j e^{Ii\theta}$ $(I = \sqrt{-1})$:

$$\Rightarrow A_{j+1} e^{Ii\theta} = r A_j e^{I(i-1)\theta} + (1-2r) A_j e^{Ii\theta} + r A_j e^{I(i+1)\theta}$$

$$\Rightarrow \frac{A_{j+1}}{A_j} = r e^{-I\theta} + (1-2r) + r e^{I\theta} = 1 - 2r + r\cos(\hat{\theta}) \Rightarrow \boxed{\left|\frac{A_{j+1}}{A_j}\right| \le |1-r|}$$

To be stable $\left|\frac{A_{j+1}}{A_j}\right| \le 1$, then:

$$\Rightarrow |1-r| \le 1 \qquad 0 \le r \le \frac{1}{2}$$