

Numerical Techniques 2023–2024

7. Parallel computing and implications in NWP

Daan Degrauwe

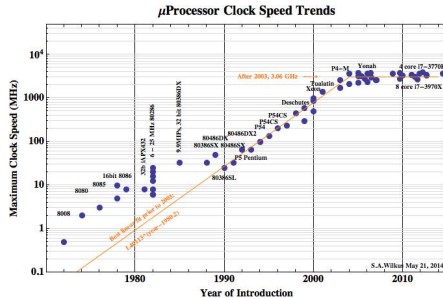
`daan.degrauwe@meteo.be`

Postgraduate Studies in Weather and Climate Modeling

Ghent University

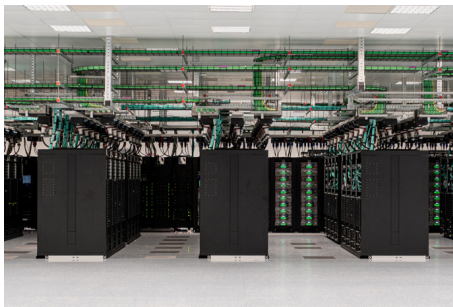
- General aspects of parallel computing:
 - ▶ Introduction
 - ▶ Amdahl's law
 - ▶ Shared and distributed memory
- NWP-specificities
 - ▶ Design of an NWP model; 'physics' and 'dynamics'
 - ▶ Parallelization in physics
 - ▶ Parallelization in dynamics
 - ▶ The future?

- We want to run forecasts as quickly as possible. . .
- Until ~ 2003 , performance was increased by making processors *faster*



- It seems that increasing the clock frequency above 3GHz isn't beneficial (power consumption!)

- So we'll just use *more* processors instead of faster ones.
- For example: ECMWF's Atos machine



with 1,040,384 cores, or RMI's machine with 2688 cores

- There's a trend to share resources between European countries (e.g. EuroHPC)

- Not everything goes faster when you use more processors!
- For instance: Newton-Raphson iterative method to find a root of a function $f(x)$:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

x_i is required for the calculation of x_{i+1} , so the different iterations cannot be performed by different processors.

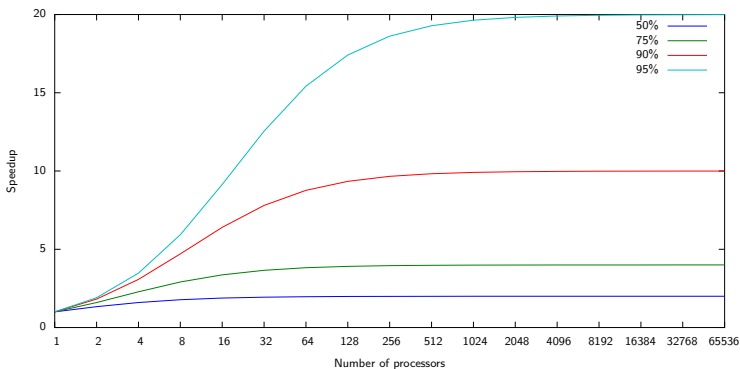
- Consider a program consisting of two parts
 - ① a part that cannot be parallelized: the *serial* part S . This part is responsible for a fraction σ of the total time T_1 on a single processor.
 - ② a parallelizable part P . This part is responsible for a fraction $1 - \sigma$ of the total time on a single processor.
- Then in a parallel environment with n processors, the total time will be

$$T_n = \sigma T_1 + \frac{1 - \sigma}{n} T_1$$

So the speed-up is

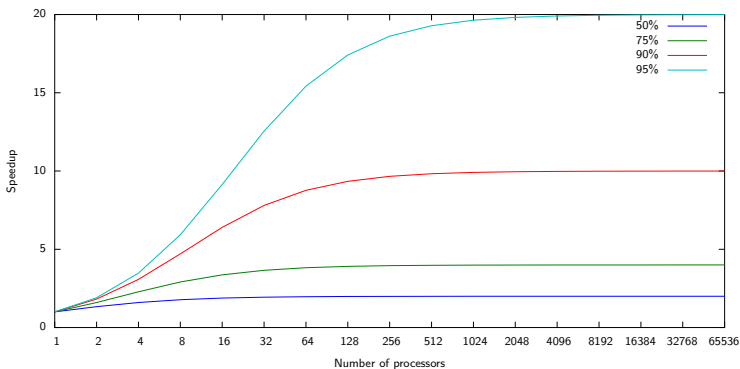
$$\frac{T_1}{T_n} = \frac{1}{\sigma + \frac{1 - \sigma}{n}}$$

- Speedup as a function of the number of processors:



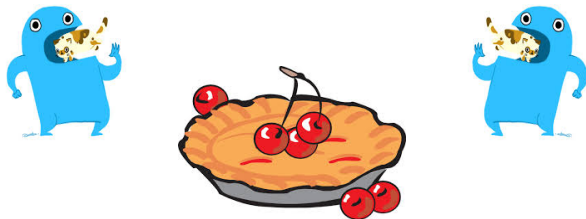
- So there's a limit to the speed-up that can be achieved by parallelizing! We call this the *scalability* of a program.

- Speedup as a function of the number of processors:



- So there's a limit to the speed-up that can be achieved by parallelizing! We call this the *scalability* of a program.
- But in fact, this isn't even the biggest challenge in NWP/Climate on high-performance systems.

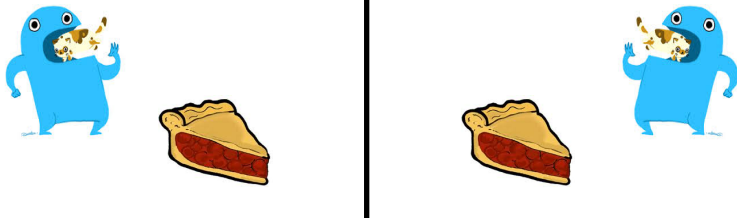
- Memory is the part of a computer where data are stored temporarily, right before/after the numerical operations.
- The most convenient setup is where all processors can access some central memory, and divide the work



- We call this a *shared* memory environment
- The standard for shared-memory parallelization is *OpenMP*

Shared and distributed memory

- Due to hardware constraints, shared memory becomes unfeasible for large systems
- In such systems, every processor is attributed his own piece of memory, and other processors cannot access it.

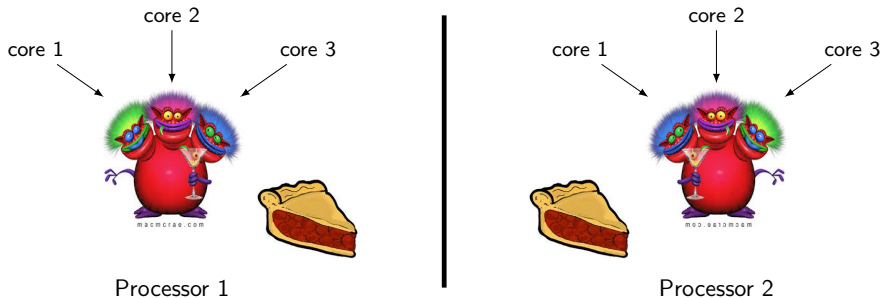


- We call this a *distributed* memory environment

- In a distributed memory environment, communication between processors has to be coded explicitly through *messages*.
- For instance:
 - ① Processor 1 reads some data from a file;
 - ② Processor 1 *sends* (pieces of) the data to the other processors 2 – n ;
 - ③ Processors 1 – n process their piece of data;
 - ④ Processors 2 – n *send* their result back to processor 1;
 - ⑤ Processor 1 writes the results to a file.
- The standard for distributed memory parallelization is *MPI* (Message Passing Interface).
- The cost of communications (slowly) *increases* with the number of processors:
 - ▶ number of messages increases
 - ▶ message sizes decrease
 - ▶ processors are further apart

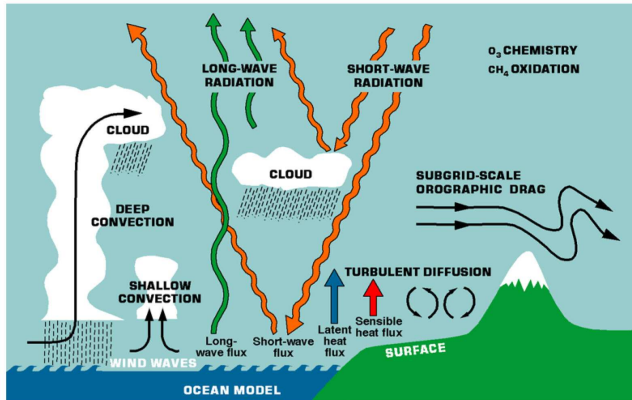
- Multicore processors allow for hybrid systems:

- ▶ *within* a processor (i.e. between different cores of the same processor), memory is shared, and OpenMP is used for parallelization
- ▶ *between* processors, memory is distributed, and MPI is used for communication



- Almost all NWP models consist of a 'dynamical part' and a 'physical part'.
- Dynamics (3D) are conservation of mass, energy, momentum; perfect gas law.
- The dynamics of the ACCORD/ARPEGE/IFS model are
 - ▶ spectral
 - ▶ semi-implicit
 - ▶ semi-Lagrangian
 - ▶ for LAM: Davies coupling to global model (ARPEGE/IFS)
 - ▶ terrain-following hybrid pressure coordinate
 - ▶ hydrostatic and nonhydrostatic

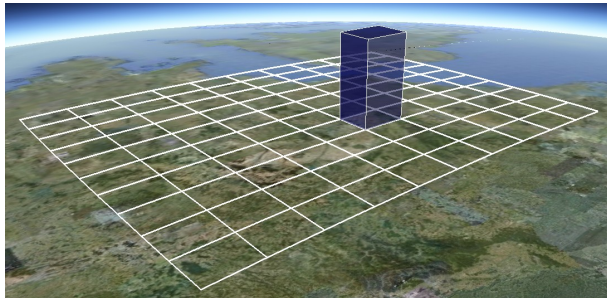
- The physics part models the *unresolved* or *subscale* phenomena: turbulence, radiation, diffusion, clouds, precipitation, surface, ...



A single timestep of the spectral ACCORD model looks like:

- 1 calculate derivatives in spectral space
- 2 apply explicit part of *dynamics*
- 3 Fourier transform to gridpoint space
- 4 semi-Lagrangian interpolations and nonlinear dynamical terms
- 5 calculate *physics* contributions to energy and momentum equations
- 6 apply *boundary conditions*
- 7 Fourier transform to spectral space
- 8 solve implicit operator (*dynamics*)

- Most physics phenomena act mainly in the vertical (e.g. precipitation, stability, ...)
- The physics are computed in vertical columns



- There's no interaction (so no communication!) between the columns
- So the physics scale very well (quasi-perfectly!).
- (the column-approach may become problematic for very high resolutions)

- The spectral dynamics are parallelized by distributing the wavelengths over the processors.
- The Fourier transforms are quite communication-intensive!

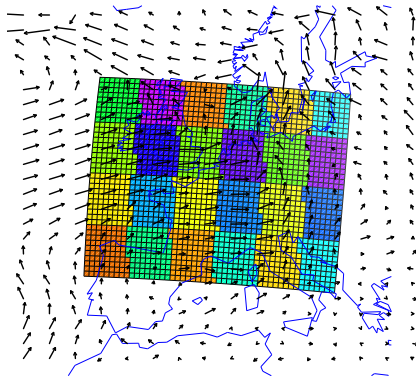
$$f(x_j) = \sum_{k=-N/2}^{k=N/2} \alpha_k \exp(ikx_j)$$
$$\alpha_k = \frac{1}{N} \sum_{j=1}^N f(x_j) \exp(-ikx_j)$$

So a wave amplitude depends on *all* gridpoints, and vice versa; a gridpoint value is the combination of *all* composing waves.

- We say that the Fourier transform is *not local* (as opposed to finite differences)
- **Note:** this nonlocality is also the key to the high accuracy of spectral methods.

Dynamics parallelization: semi-Lagrangian advection

- Semi-Lagrangian calculations require interaction with nearby processors: the trajectory departure points may well belong to another processor.



- Implicit timestepping is also not local, even when using finite differences.
- For example, the trapezium scheme for the advection equation

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{c}{2} \left(\frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x} + \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} \right) = 0$$

leads to a tridiagonal linear system that needs to be solved every timestep:

$$\mathbf{T}\phi^{n+1} = \mathbf{R}$$

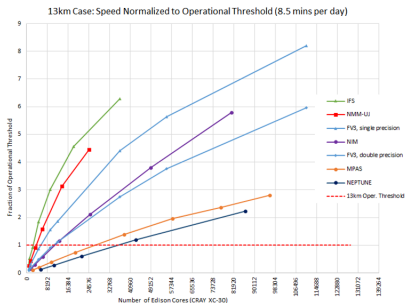
where \mathbf{T} is a tridiagonal matrix, and \mathbf{R} is the right-hand side (depending on ϕ^n).

- So the next timestep's solution is obtained as

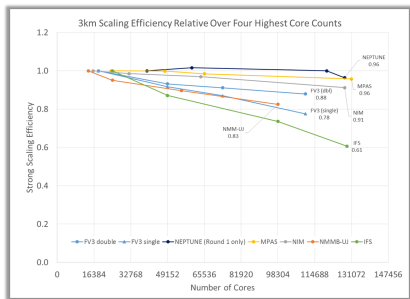
$$\phi^{n+1} = \mathbf{T}^{-1}\mathbf{R}$$

- But the inverse of a tridiagonal matrix is a full matrix!
- So the solution in a point at $t + \Delta t$ depends on the values of *all* gridpoints at t , meaning you need communications between all processors.

- Both efficiency and scalability of a scheme are important
- Spectral semi-implicit semi-Lagrangian is quite efficient (since it allows very large timesteps and has a good accuracy), but it doesn't scale very well



IFS speed



IFS scaling

- As machines get larger, there's a trend towards methods requiring less communications:
 - ▶ spectral → finite differences
 - ▶ implicit (trapezium) → explicit (Runge-Kutta)
 - ▶ Lagrangian → Eulerian
- Maybe intermediate solutions such as HEVI (Horizontal Explicit, Vertical Implicit) are the future?
- There's always a tradeoff between accuracy and computational cost
- Power consumption may become a bigger challenge than communications
- New (energy-efficient) hardware architectures like Graphical Processing Units (GPUs) are finding their way to NWP.