Parallelizing The Hydro Code

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High Performance Computing

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Contents

Hydro Code Explained

The hydro code is a simulation of a fluid or gas in an enclosed system. The initial conditions are set as to generate an unperturbed, homogeneous environment. Then, one can introduce points of higher or lower pressure or density to imitate an explosion or jet. The code then calculates the propagation of this perturbation using Godunov's method and outputs each frame as a single file, which can be used to create an animation.

There are five main components with different functionality to this Fortran based code. They are:

- `main.f90`
  - calls `init_hydro` to initialize the grid with the initial conditions
  - executes the main time loop by calling
    - `output` to generate output data
    - `cmpdt` to compute the time step
    - `godunov` to calculate the fluid dynamics
- `module_hydro_principal.f90` contains the subroutines
  - `init_hydro`
  - `cmpdt`
  - `godunov` which calls
    - `make_boundary` to set the upper, lower, left and right boundaries of the grid
    - `allocate_work_space`/`deallocate_work_space` to (de)allocate space in the memory
    - other subroutines for calculation purposes
- `module_hydro_utils.f90` contains
  - `make_boundary`
  - other subroutines
- `module_hydro_IO.f90` contains the subroutines
  - `read_params` to read the parameters from the `input.nml` file
  - `output`
- `module_hydro_commun.f90` contains
  - `allocate_work_space`/`deallocate_work_space`
  - various other subroutines, mainly to define the variables used elsewhere in the code

Additionally, there are several input files to set the grid size, initial condictions, etc.

Parallelization Techniques

MPI

Introduction

MPI stands for *message passing interface*. This refers to the fact that parallel computing occupies multiple CPUs to fasten up the execution of a code. As these CPUs work independently and with their own associated memory, they will have to communicate in some way; this is what MPI does.
The advantage of MPI over other libraries is that one has much more control over how the code is parallelized. The programmer can explicitly choose how the different cores communicate to each other and which information they share.
On the other hand, this freedom makes parallelizing a code a much more complex problem than it could be with other libraires. It requires quite a deep understanding of how the code works to know where and what to adjust.

Parallelization Process

The main idea for parallelizing the code was to split the initial grid horizontally into equally sized parts in assigning each core a certain portion of it. Each process would then calculate the evolution of the fluid in his portion only. Finally, these different parts would be merged together to create a grid of initial size. This merging is where the most complex part of the paralellization process had to be implemented:
For a process to be able to calculate a given pixel of its grid, it needs information of its four neighbouring pixels. Thus, to calculate the values of the lower and upper most pixels within the grid, each process has to have access to the values of the process below or above of it. The communication of these values was implemented in the following way:

Apart from usual MPI formalisms, such as calling `MPI_INIT`, `MPI_FINALIZE` and other syntactically necessary methods, the main components that needed to be adjusted were

- workspace allocation,
- time step computation,
- Godunov boundaries
- Communication between boundaries
- Output formatting

Results

The plots for the respective runtimes of both the strong and weak scaling can be seen below:
The simulation was run from 1 to 36 cores 10 times each.

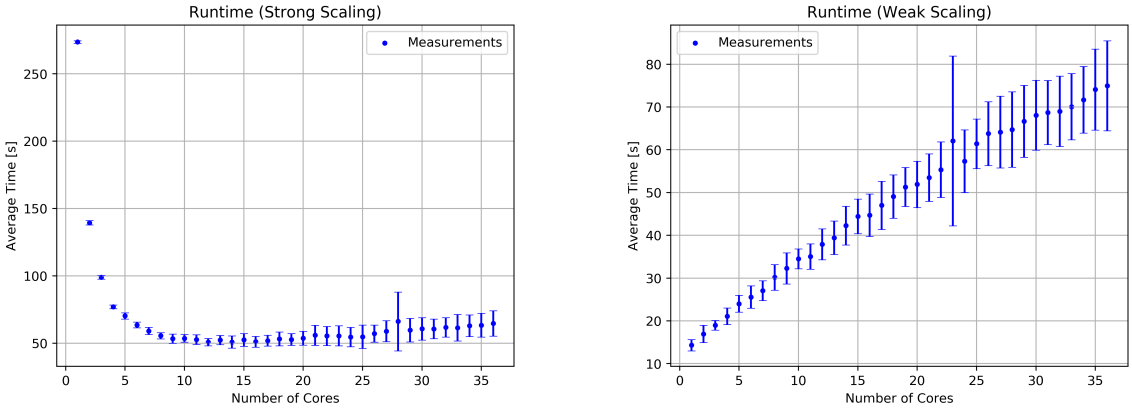

Figure 1: Respective runtimes for strong and weak scaling

The settings for the strong scaling were the following:

t_{end}	nx	ny	dx
50.0	50	9000	0.08

The settings for the weak scaling were the following:

t_{end}	nx	ny	dx
50.0	50	300	0.08

Note that the nx remained unchanged during the weak scaling run, but ny increased linearly with the number of processes involved, $ny = ny\cdot$ (number of processes).
The fit for the strong scaling is done with the following formula (Lecture 5):

$$\frac{1}{\alpha + \frac{1-\alpha}{N}} \tag{1}$$

Where α represents the non-parallelized fraction of the code, and N is the number of processes.
This yields the following value:

$$\alpha = 0.166 \pm 0.006 \tag{2}$$

This indicates that roughly 83.4% of the code is paralel.
The formula for the fit for the weak scaling can be derived quite easily. Again, take α to be the non parallelized fraction of the code. Then, $T_p(N)$, the time needed for the parallel code, is

$$T_p(N) = N \cdot \alpha + (1 - \alpha)$$

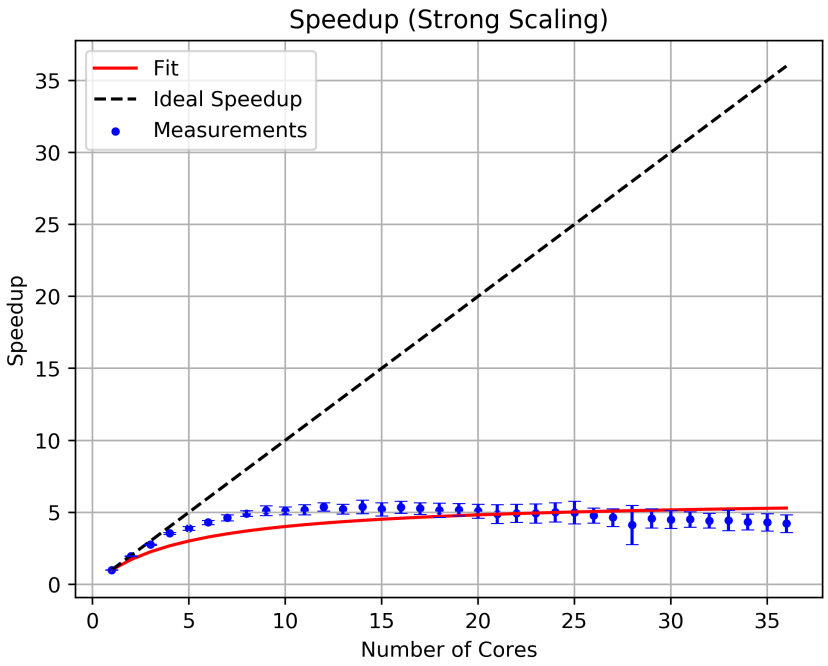

Figure 2: Speedup for strong scaling

So then,

$$\text{Speedup}(N) = \frac{T_s(N)}{T_p(N)} = \frac{T_s}{T_p(N)} = \frac{1}{(\alpha) \cdot N + (1 - \alpha)}$$

Fitting this over the data yields:

$$\alpha = 0.145 \pm 0.002 \tag{3}$$

Again, this indicates that around 85.5% of the code is parallelized.

Other Techniques

OpenMP

OpenMP stands for *open multiprocessing*. The fundamental difference between OpenMP and MPI is the parallelization process. MPI communicates between nodes, whereas with OpenMP the parallelization occurs within one node. The so-called *master thread* spawns several *slave threads* (called forking) to speed up a designated section of the code.
What it may lack in flexibility (can only run on shared-memory computers), it makes up in ease of implementation and communication speed.

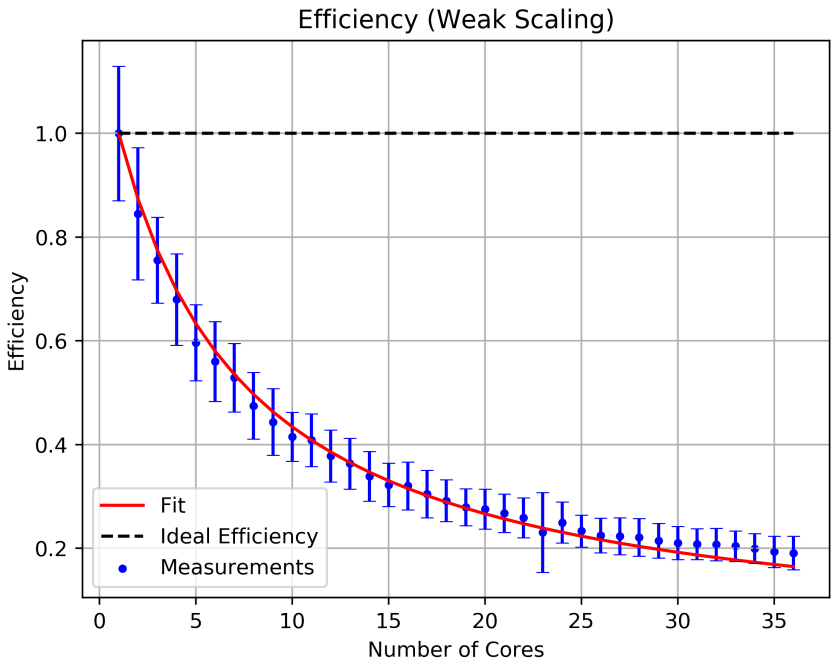

Figure 3: Speedup for weak scaling

MPI - OpenMP Hybrid

Implementing both of these methods can make use of the distributed memory architecture of a supercomputer, while further speeding up the runtime by running multiple threads. This combines the advantages of MPI and OpenMP.

Discussion

As can be seen in Figure 1, the standard deviation on some of the runtimes can be quite big. This is mainly due that the whole run (going from 1 to 36 precesses) was only performed 10 times. If one of these times is abnormally high or low, averaging over only 10 values will not suppress this spike well enough.

Conclusion