Parallelizing The Hydro Code

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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. test

Parallelization Process

The main points that needed to be adjusted were the following:

- 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.

The settings for the strong scaling were the following:

$$t_{\rm end}$$
 nx ny dx 50.0 50 9000 0.08

The settings for the weak scaling were the following:

$$\begin{array}{c|cccc} t_{\rm end} & nx & ny & {\rm d}x \\ \hline 50.0 & 50 & 300 & 0.08 \end{array}$$

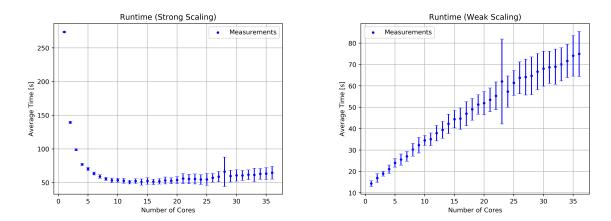


Figure 1: Respective runtimes for strong and weak scaling

Note that the nx remained unchanged during the weak scaling run, but ny increased linearly with the number of processes involved, ny = ny (number of processes).

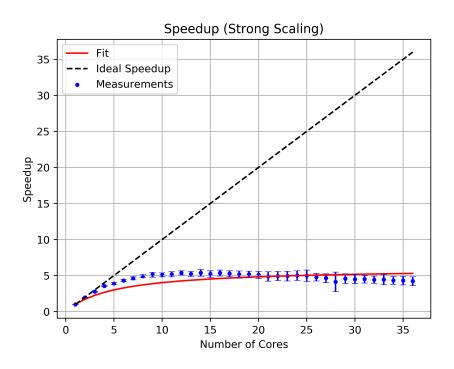


Figure 2: Speedup for strong scaling

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.

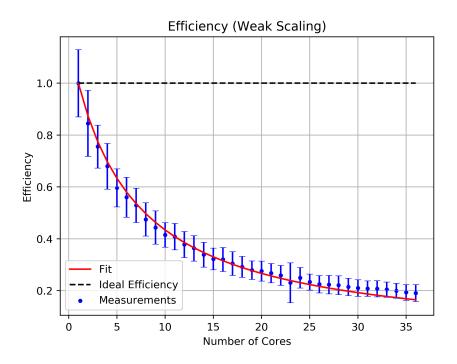


Figure 3: Speedup for weak scaling

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

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

So then,

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.

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