Rule of thumb to parallelize your simulation with Smilei

A. Beck

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This document presents how to pick correct parallelization parameters to make sure you benefit as much as possible from the awesome performances of Smilei.

1 Parameters

- Total number of physical cores: n_c
- OMP_NUM_THREADS: n_t
- Number of MPI process along X: N_x
- Number of MPI process along Y: N_y
- Oversize: o.
- Total number of ghost cells: n_g
- Total number of cells along X: s_x
- Total number of cells along Y: s_y

2 Assumptions

We assume that only one openMP thread is used per physical core (no hyperthreading). This gives

$$n_c = N_x N_y n_t. \tag{1}$$

The total number of ghost cells is given by $n_g = 2o(N_x s_y + N_y s_x)$. We assume that the best performances are reached when we minimize n_g. But we have to take into account that the openMP parallelization is essentially done in the X direction and we have to make sure that all threads are sufficiently "fed". In order to take that into account, we can consider that the number of thread along the X direction is $N_{xt} = N_x n_t$ and we now want to minimize the virtual number of ghost cells

$$n_{vg} = 2o(N_x n_t s_y + N_y s_x). \tag{2}$$

3 Results

Introducing 1 into 2 we get

$$n_{vg}(N_y) = 2o\left(\frac{n_c s_y}{N_y} + N_y s_x\right). \tag{3}$$

A derivation gives

$$\frac{dn_{vg}}{dN_y} = 2o\left(-\frac{n_c s_y}{N_y^2} + s_x\right) \tag{4}$$

The minimum is reached when the derivative becomes 0 and we get the recommended number of MPI process along Y:

$$N_y = \sqrt{\frac{n_c s_y}{s_x}}. \tag{5}$$

It is interesting to note that the recommended N_y does not depend on n_t. The corresponding recommended number of MPI process along X is

$$N_x = \sqrt{\frac{n_c s_x}{s_y n_t^2}}. \tag{6}$$

These number were obtained for a given value of n_t. One has to keep in mind that increasing n_t deacreases the total number of MPI process and therefore decreases the total number of ghost cells while improving the load balancing at the same time. As a consequence, it is generally beneficial to use a large n_t, typically equal to the number of physical cores of the processors of your system.

4 Disclaimer

These rules are simple considerations in order to help newcomers to get reasonably good performances. In reality, the best set of parameters is, of course, case and system dependant. Please let us know if you find your optimal setup to be completely different from the one suggested here.