Code update: from SP6 towards the Blue Gene architecture

On computational level, the first task is to modify the data distribution among the CPU. In this moment only one direction is distributed and this limits the maximum number of CPU which can be used to the grid resolution N . Consequently, only architectures with fast CPUs and a large memory per CPU, like IBM Sp6, can be efficiently used. Iâll modify the code by distributing two directions in order to allow to increase the maximum number of CPU that can be used up to N^2 , thus allowing to run the code also on machines like IBM Blue-Gene. This requires to rewrite the computation of non-linear terms, where the FFT/inverse FFT computation is performed by a data transposition routine. The new scheme to compute the non-linear convective terms $C_ij = u_iu_i$ is detailed in the scheme below. In the following x_a, represents the $a-th$ physical direction. Data are stored in three-dimensional arrays ordered as (x_1, x_2, x_3). Directions 2 and 3 of the array, which correspond to the physical directions x_1 and x_3, are distributed among the CPUs.

At the end of the procedure, data are stored again as (x_1, x_2, x_3) in the wavenumber space. To improve the code optimization, my second task is to review of the input/output routines, and to modify the FFT/iFFT routine interface in order to allow to link different FFT libraries, different than NAG, to try to reduce the computational time.

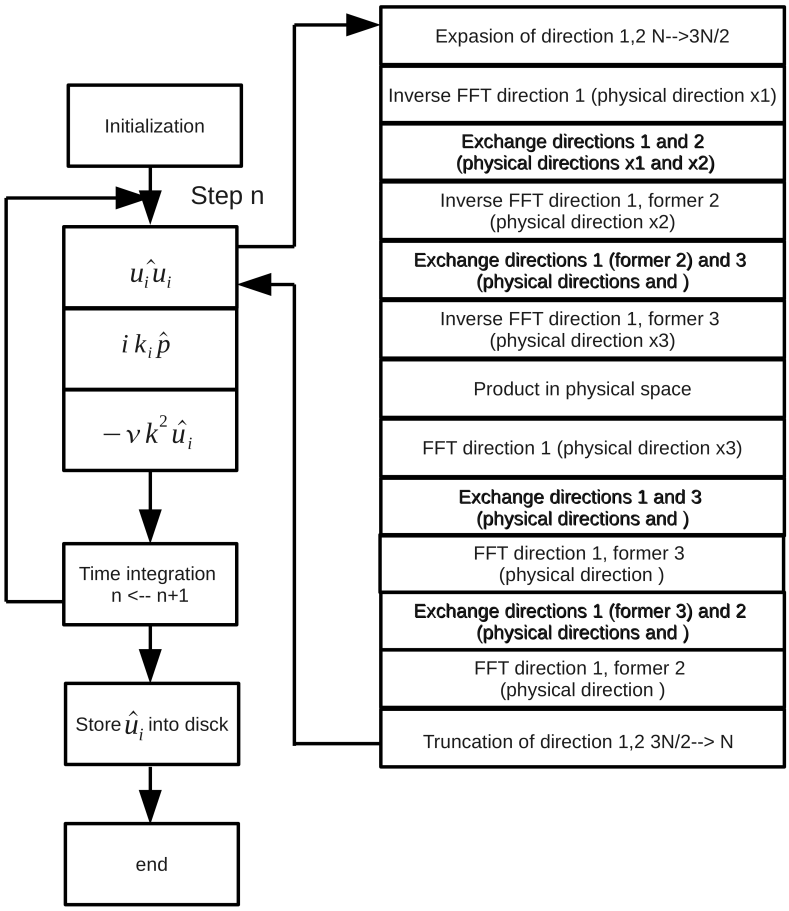

Figura 1: Distributed code scheme in two directions