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Seismic waves modeling with the Fourier pseudo-spectral method on massively parallel machines.

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The Fourier pseudo-spectral method (FPSM) is an approach for the 3D numerical modeling of the wave propagation, which is based on the discretization of the spatial domain in a structured grid and relies on global spatial differential operators for the solution of the wave equation. This last peculiarity is advantageous from the accuracy point of view but poses difficulties for an efficient implementation of the method to be run on parallel computers with distributed memory architecture.
The 1D spatial domain decomposition approach has been so far commonly adopted in the parallel implementations of the FPSM, but it implies an intensive data exchange among all the processors involved in the computation, which can degrade the performance because of communication latencies. Moreover, the scalability of the 1D domain decomposition is limited, since the number of processors can not exceed the number of grid points along the directions in which the domain is partitioned. This limitation inhibits an efficient exploitation of the computational environments with a very large number of processors.
In order to overcome the limitations of the 1D domain decomposition we implemented a parallel version of the FPSM based on a 2D domain decomposition, which allows to achieve a higher degree of parallelism and scalability on massively parallel machines with several thousands of processing elements. The parallel programming is essentially achieved using the MPI protocol but OpenMP parts are also included in order to exploit the single processor multi - threading capabilities, when available. The developed tool is aimed at the numerical simulation of the seismic waves propagation and in particular is intended for earthquake ground motion research. We show the scalability tests performed up to 16k processing elements on the IBM Blue Gene/Q computer at CINECA (Italy), as well as the application to the simulation of the earthquake ground motion in the alluvial plain of the Po river (Italy).