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Tapas4Grid: a grid tool for performing parametric studies based on complex workflows

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One typical problem to be solved by fusion codes, which is suitable for grid and parallel computing, is the parameter scan. There are several codes whose main purpose is to get results for wide parameter range. So it makes sense to build a tool that allows one to perform this parameter scan in an automated way. We have build and used a new tool suitable for solving this kind of problems: TAPaS. This tool is, in principle, and thanks to its layer based design, suitable for both HPC s and grid computing, although it has only been used on the grid.

Detailed analysis

TAPaS itself is able to manage a complex workflow that implies running the main code automatically with a wide variation of its input parameters and managing the results.

"TAPaS4grid" (Tool for Automatic Parameter Studies for Grid) provides a workflow for preparation and submission of extensive parameter studies for running on the grid (s.t.a.r.t.). As a case example, EMC3_EIRENE and BIT1 have been taken to test this tool, but it is possible to run other codes using this tool. Internally TAPaS4grid provides a workflow including all steps to run intensive parameter studies using any suitable code on the grid.

EMC3-EIRENE is a package of two coupled Monte Carlo codes, the 3D fluid edge plasma code EMC3 and the 3D neutral particle kinetic transport code EIRENE. An iterative procedure is applied to obtain a self-consistent solution for all plasma and neutral particle parameters.

BIT1 is an application to perform Particle-in-Cell (PIC) simulations. This application represents a powerful tool for plasma studies having a number of advantages like the fully kinetic description of high-dimensional plasma and the ability to incorporate complicated atomic and plasma-surface interactions.

Conclusions and Future Work

We have developed a tool for automatic parameter studies that is being used to perform different tests with different applications in the nuclear fusion field. The application hides all the interaction with the grid environment, allowing the scientist to define the tests that he wants to run via a parameter's file and launch the tool. The obtained results show a set of relevant results for fusion community, and this tool opens a wide range of possibilities to perform more detailed tests.

Impact

Even though TAPaS4grid has been initially developed to use the grid infrastructure, it could be ported to other infrastructures like HPC. The tool can be divided into two different layers:

- Parametric studies. This layer takes the parameter file and the input file of the application used for the studies, and generates a set of valid input files that will be used to run the application. This layer is standard and does not need to be changed.

- Infrastructure interaction. This layer is the responsible for the interaction with the grid. It creates the job, submits it, retrieves the results,... This layer should be ported to different infrastructures in order to use the tool.

Before starting TAPaS4grid it is needed to create a parameter file including the necessary input data for every job. In this file there can be added an unlimited number of different variables. During the workflow they will be replaced by the values specified in the parameter file.

With this parameter scan process we show how we can perform a deep study of the configuration parameters of a fusion device, modelling the behaviour of this device in many different ways.

Keywords

Parametric, Grid, Automatic, START

URL for further information

https://wiki.eu-euforia.eu/index.php/TAPaS4grid

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