

CalCul: A Python-based Workspace for High-Performance Parameters-Survey in Scientific Legacy Codes

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Abstract. Scientific legacy codes are usually holding large numbers of physical arrays which have been used and updated by the code routines, and the code parameters are set using a simple textual data file. Therefore, in cases when there is a need to perform a parallel large scale parameters-survey, the user needs to manually replicate the code multiple times, change the data file to its needs, run the code and control its performances - at each working directory separately. This task is practicable when there is a need to create several computations, but impossible when there is a need to run a large-scale parallel parameters-survey on a cluster with thousands of calculations. In this work we present CalCul - A Python-based Workspace for High-Performance Legacy Scientific Codes, which is able to automatically render most of legacy codes data files into a python object, allowing the user – using many other functionalities – to control and handle all the needs of a parameters-survey using the simplicity and sophistication of Python libraries, and thus allowing the conversion of work with software from manual to automatic. Also, in order to not damage the way legacy software work, and in order to abstain from replacing existing work modules for these software, the CalCul system provides a mirror between the changes done using the Python object and the legacy data files, and thus allows working dually on the software – either from CalCul or from the data files itself. CalCul also interfaces with IPython interactive command shell, and in this way, the user can manage all of his scientific actions entirely in one hermetic workspace.

Keywords. High-Performance Computing, Python Workspace, Legacy Computational Scientific Codes, Parallel Tools, Parameters-Survey.

1. Introduction

Scientific computation is a central tool in computerized simulation planning, which runs on a powerful, parallel computer [1]. In order to perform their research jobs, physicists at NRCN use software developed by the computational groups (such as LEEOR2D-3D [2] [3] [4]), and other software such as OCTAVE [5] visualize and analyze results. In this paper, we will examine the workspace in which the physicist work while using the scientific software and the parallel computing, and provide a software system that will significantly improve the physicist's working processes.

In order to demonstrate the essence of the improvement, there is a need to understand first the workflow of a physicist in a computational group. Usually, the physicist has