ExaQUte

Exascale Quantification of Uncertainties for Technology and Science Simulation

D1.2 First release of the softwares

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Executive summary

This deliverable presents the software release of the Kratos Multiphysics software [3], "a framework for building parallel, multi-disciplinary simulation software, aiming at modularity, extensibility, and high performance. Kratos is written in C++, and counts with an extensive Python interface". In this deliverable we focus on the development of Uncertainty Quantification inside Kratos. This takes place in the MultilevelMonteCarloApplication, a recent development inside the software that allows to deal with uncertainty quantification.

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Nomenclature / Acronym list

Acronym	Meaning
Kratos	Kratos MultiPhysics
MC	Monte Carlo
MLMC	Multi Level Monte Carlo
CMLMC	Continuation Multi Level Monte Carlo
UQ	Uncertainty Quantification
CFD	Computational Fluid Dynamics

1 Introduction

The Kratos software is capable to deal with many different engineering fields, from CFD and convection diffusion to structural and solid mechanics problems. In all these fields it may be very important the necessity of dealing with uncertainties in some data, and to see how these affect the final results. The purpose of the Multi Level Monte Carlo application is exactly this: to study the uncertainty propagation in physical problems.

2 Methods

2.1 Algorithms

Different algorithms [2, 6, 8] are presented in the software:

- Monte Carlo,
- Multi Level Monte Carlo,
- Continuation Multi Level Monte Carlo.

MC is the simplest algorithm and deals only with one accuracy level, i.e. one mesh; on the other hand MLMC and CMLMC work with different accuracy levels. These levels present an increasing quality of the results and of the computational cost.

2.2 Adaptive refinement

In the application this increasing accuracy is achieved through a solution-oriented space refinement. The software presents a geometric error estimate [5] in order to perform the adaptive refinement. The metric is evaluated computing the hessian of the numerical solution, and this is given as input to the refinement software Mmg [4].

2.3 High efficiency

The necessity of running multiple simulations leads to the fundamental requirement of high efficiency. To achieve such result, there is a direct integration between Kratos and the chosen distributed software COMPSs [1, 7, 9]. The integration takes place at very high level, employing a Python layer. There is a direct integration between Kratos and PyCOMPSs, the COMPSs python library, and this allows to run many Kratos simulations independently and concurrently. A remarkable computational time efficiency is currently achieved.

2.4 Current results

The application presents a benchmark test case, that is a Poisson equation, and a more challenging engineering problem. This last studies the lift coefficient behavior of a compressible flow around an airfoil with random Mach number and random angle of attack. The application is currently capable to run in distributed environment, and has been tested that with 25 worker nodes (1200 cores) and 130000 simulations it fills all the hardware nodes.

3 Softwares

A release of the Kratos software with DOI (10.5281/zenodo.3235261) can be found at the following link: `https://zenodo.org/record/3235261`.

The PyCOMPSs library can be found at this link: `https://github.com/bsc-wdc/compss.git`.

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