Conference in Numerical Analysis 2014 (NumAn 2014)
September 2-5, 2014
Chania,Greece

Software Platforms for Multi-Domain Multi-Physics Simulations[1]

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Abstract

Advances in hardware and software technologies in the 1980s led to the modern era of scientific modeling and simulation. This era seems to come to an end. The simulation needs in both industry and academia mismatch with the existing software platforms and practices, which to a great extent have remained unchanged for the past several decades. We foresee that this mismatch, together with the emerging ICT advances and the cultural changes in scientific approaches will lead to a new generation of modeling and simulation.

This paper proposes approaches for designing, analyzing, implementing and evaluating new simulation frameworks particularly suited to multi-domain and multi-physics (MDMP) problems that have Partial Differential Equations (PDEs) in their foundations. We focus on introducing software platforms that facilitate the numerical solution of PDEs associated with MDMP mathematical models.

In particular, we propose an enhanced meta-computing environment which is based on: (a) scripting languages (like python) and their practices, and (b) on the Service Oriented Architecture (SOA) paradigm and the associated web services technologies.

The proposed environment has been designed and engineered having in mind a set of characteristics particularly suited for MDMP problems. More specifically, it:

- Allows domain experts to focus on expressing the models, rather than delving into implementation details.
- Fully utilizes the plethora of PDE solving modules available.
- Allows the programmer to effectively select the most appropriate available software module for the particular component of the problem, as this is defined by its associated single physics model and its simple/single domain
- Transparently benefits from recent algorithmic advances (e.g. domain decomposition)
- Allows users to efficiently deploy and run the MDMP computations on loosely coupled distributed and heterogeneous compute engines.

Although our design is generic, covering a wide range of problems, our proof of concept implementation is restricted to elliptic PDEs in two or three dimensions. Furthermore, it clearly shows that our tool can easily exploit state of the art numerical solvers like those available in FENICS and deal.II, domain decomposition methods with or without overlapping, Monte Carlo based hybrid solvers, rectangular or curvilinear domains and interfaces and beyond.

Key words: Numerical Solution of PDEs, Multi-domain, Multi-physics, Problem Solving Environments.

[1]The present research work has been co-financed by the European Union (European Social Fund ESF) and Greek national funds through the Operational Program *Education and Lifelong Learning* of the National Strategic Reference Framework (NSRF) - Research Funding Program: THALIS. Investing in knowledge society through the European Social Fund.