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Interoperable executive library for the simulation of biomedical processes

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ABSTRACT

We present an Interoperable Executive Library (IEL) built to run, in parallel, a collection of multi-component tasks focusing on simulating complex biomedical phenomena of the heart. The IEL is a light-weight software integrator designed for managing the distribution of data and memory, coordinates communication among parallel processes, and directs execution of a set of loosely coupled numerical and physics tasks or modules. The dynamical process of the heart uses computing modules of electrical generation, physiological signal propagation, mechanics deformation, and fluid flow transportation. The cardiac electro-physiology is represented by a reaction–diffusion equations using the Beeler–Reuter model. The contracting motion of the heart is described by the continuum mechanical equilibrium equations. At the end of a heart beat, the fluid flow pattern inside the ventricle is computed by solving the incompressible Navier–Stokes equations. The finite element method is used to solve these loosely coupled sets of equations. Simulations are performed on two simplified heart models as well as a dog ventricle. The functionality and performance of the IEL framework on a distributed computing system are demonstrated and shown.

1. Introduction

The complexity of simulating any system-wide processes in the human body represents a daunting challenge to unravel. Often in many of these numerical simulations the interplay of various biological, chemical, and physical models goes beyond the reach of a single set of computer code.

A multitude of multiphysics solver frameworks have been developed over the years, each using different techniques and methods with multiple purposes in mind. ROCCOM [1] is one of the first frameworks developed to handle complex calculations for rocket motor designs. ROCCOM organizes its data into objects called windows which can then be split into panes for parallel computation. The physics modules then perform data communication through windows [1]. COMSOL [2] is a finite element commercial software package capable of solving a large variety of engineering problems. The software framework is composed of many applications libraries and tools in a modular fashion tailored to multiphysics simulations. DEAL.II [3] is a tightly coupled parallel finite element package that features some functionalities similar to COMSOL. A fluid structure interaction study involving cardiovascular blood flow of the heart was performed by the Karlsruhe Institute of Technology using the Fluent fluid solver from ANSYS and the finite element structural solver ABAQUS. This simulation utilizes an external communication program to transfer boundary information [4]. As illustrated by these software packages,

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the common approach to solve a multiphysics problem is a loosely coupled methodology which eliminates the burden to build a code limited for a single application. A monolithic code is often difficult to maintain and adapt to new software and hardware technologies but is essential for some specific applications to produce converging solutions.

In this paper we introduce the Interoperable Executive Library (IEL) which is a software framework built in a loosely coupled approach and also has the flexibility to admit any monolithic code. We demonstrate the effectiveness of the IEL in a heart simulation. In this simulation the tasks in the IEL are designed in a modular fashion and provide a simple application programming interface, or API, for handling data communication. The interacting cardiac chemistry, physiology, and mechanics are encapsulated in computing modules managed by the IEL. The IEL provides a number of commonly used scientific libraries such as Trilinos [5], PETSc [6], MAGMA [7], and ScaLAPACK [8], to represent the systems of differential equations often used in the multiphysics models and solve the resulting large system of linear equations in parallel. Other tools for pre-processing and post-processing, such as performing I/O using HDF5 [9], decomposition of the grid generated by Pointwise [10] or Cubit [11], and visualization of computed results using Paraview [12], are also available. A feature of this interoperable framework involves the use of shared boundary conditions, that act as points of data exchange between the two different modules. This modular approach in conjunction with a set of users' defined input files allows the IEL to run multiple simulations either concurrently or in a designated sequence. Hence it can then be implemented in various ways well suited for scaling and parametric studies.

Cardiovascular disease is the leading cause of death in America [13]. Computer simulation of complicated dynamics of the heart has great potential to provide quantitative guidance for diagnosis and treatment of heart problems. The heart is a complex electromechanical system. It weighs 11 ounces and has the size of a first. The heart beats 100,000 times per day or 2.5 billion times in a lifetime. There have been intensive research efforts on developing accurate computer models to advance the understanding on the mechanisms of cardiovascular dynamics. Heart beats are the result of a sequence of electrochemical excitation waves that are initiated from the sinoatrial node. The electrical impulses induce intracellular calcium cycling, which in turn causes heart muscles to contract. This process, known as excitation–contraction coupling (ECC), is essential to the functioning of a healthy heart. On the other hand, mechanical changes that responds to neural and hormonal influences also impact the electrical properties of the heart. A variety of mathematical models for electromechanical simulations have been proposed. Nash and Panfilov [14] presented a computational framework which integrated a three-variable FitzHugh–Nagumo-type (FHN) [15] excitation–tension model to the governing equations of the non-linear stress in the electromechanical and mechanoelectric feedback mechanisms. Goktepe and Kuhl [16] presented a FHN model to study the electro-physiology of the heart. Doyle et al. [17] applied parallel computing to the simulation of heart mechanics and Lafortune et al. [18] developed a parallel electromechanical model of the heart.

The presented simulation focuses on the ventricle section of the heart. When a part of the heart tissue is stimulated, the induced action-potential propagates out, making the tissue contract. Such action is controlled by a given set of Kirchoff stress parameters and stress activated ion channels. The incompressible Navier–Stokes equations is then solved for fluid flow pattern in the deformed ventricle. These sets of equations are numerically solved by an implicit, finite element-based approach. The simulations of two simplified heart models and a dog ventricle are performed to demonstrate the functionality and performance of the IEL framework on a distributed computing system. The ability of the IEL to schedule multiple physics tasks in parallel allows these simulations to be computed on supercomputers such as Darter and Kraken at the National Institute for Computational Sciences (NICS).

Section 2 of this paper illustrates the details of the IEL. The electro-physiology and the mechanical models are presented in Section 3. The fluid flow calculation is shown in Section 5 preceded by the description of the mesh regeneration. Section 6 details the results and discussions.

2. The interoperable executive library

The IEL is a software framework used for multi-component simulations and is designed to execute and schedule in parallel a series of solvers or modules. Often in multiphysics simulations coupling interaction in a section of the physical domain is a common occurrence and therefore requires data and information exchange on points called shared boundaries. Beyond its scheduling and data managing capabilities the IEL also provides a number of scientific libraries and tools to extend its capabilities in solving a system of differential equations and processing I/O data.

The IEL is composed of three major components: the configuration file, the communicator library, and the executive. The configuration file defines the functionality of each simulation, the number of shared boundary conditions between different modules, and the number of processors that are assigned for the parallel computation. The second component is the communicator library (COMMLIB) which is built as a wrapper for the Message Passing Interface (MPI) and handles the transfer of the data on the shared boundaries between modules. The third component is the executive which schedules and manages the workflow of a set of tasks prescribed in the configuration file. A user specific driver program initiates the computation by passing a configuration file to the executive which organizes the sequence of a simulation. A great asset of the IEL is its ability to schedule multiple computational tasks in parallel, allowing a number of simulations to be conducted either concurrently or in sequence on large scale computing platforms such as Darter or Kraken, which consists of over 100,000 computing cores.