SUPPORTING INFORMATION

A Validated Multiscale In-silico Model for Mechano-sensitive Tumour Angiogenesis and Growth

Vasileios Vavourakis, Peter A. Wijeratne, Rebecca Shipley, Marilena Loizidou, Triantafyllos Stylianopoulos, David J. Hawkes

FE implementation of the tumour angiogenesis and growth model

The coupled mechano-biological multiscale finite element procedure has been implemented in a scalable C++ code, and incorporated into the existing in-house numerical analysis framework [FEB3]. FEB3 has been designed in an object-oriented manner and facilitates parallel computation using the message passing interface technology of the [MPICH] library, while it is founded on the following high-performance, open-source numerical libraries:

- blitz++ is a meta-template library in C++ which was utilised in FEB3 for tensor algebra and multi-dimensional tensor manipulation [1].
- GNU Scientific Library is an ANSI-C library that contains an wide range of mathematical routines (over 1000 in total) such as random number generators, special functions, statistics, numerical differentiation, data fitting, etc. (see online documentation: [https://www.gnu.org/software/gsl/manual/html_node/]) [2].
- METIS and ParMETIS is a pair of libraries containing established algorithms for partitioning graphs, partitioning finite element meshes and producing fill-reducing orderings for sparse matrices, in serial and in parallel computing respectively [3].
- MPICH is a standardized and portable message-passing system which is a communication protocol for programming parallel computers.
- PETSc is a suite of data structures and routines for the solution of scientific applications, and is been used within FEB3 in solving linear and nonlinear systems [4, 5]. PETSc is also integrated with MPICH to facilitate parallel computations, while it communicates with METIS and ParMETIS for sparse system partitioning.
- libMesh is the top-level library used by FEB3. libMesh is an object-oriented C++ framework for the numerical simulation of partial differential equations using arbitrary unstructured discretisations on serial and parallel platforms [6], while it integrates with high-performance computing libraries such as PETSc.

FEB3 is freely available upon request from: [https://bitbucket.org/vasvav/feb3-finite-element-bioengineering-in-3d/wiki/Home].

The three-dimensional FE tissue mesh and the one-dimensional vascular network mesh was decomposed and parallelised across multiple processors using the [ParMETIS] libraries.

References:

1. [http://glaros.dtc.umn.edu/gkhome/metis/metis/overview]
2. [http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview]
3. [http://libmesh.github.io/]
library. All simulations presented in this work were carried out on a desktop machine having an Intel Xeon E5-2620 CPU (2.0 GHz × 6) and 15.6 GB RAM memory, operating Linux (kernel version: 3.13.0-71-generic).

References


