Bio-Numerical Simulations with SimBio

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ABSTRACT The central objective of the SimBio§ project is the improvement of clinical and medical practices by the use of large-scale numerical simulation for bio-medical problems. SimBio provides a generic simulation environment running on parallel and distributed computing systems. An innovative key feature is the input of patient specific data to the modelling and simulation process. While future SimBio users will be able to develop application specific tools to improve practices in many areas, the project evaluation & validation will demonstrate improvements in: non-invasive diagnosis and pre-operative planning and the design of prostheses. The SimBio environment consists of components for the discrete representation of the physical problem, the numerical solution system, inverse problem solving, optimization and visualization. The core of the environment is the numerical solution system comprising parallel Finite Element solvers and advanced numerical library routines. The compute-intensive components are implemented on high performance computing (HPC) platforms. The following article explains the HPC requirements of the bio-medical project applications and presents the SimBio solutions for the project validation examples: electromagnetic source localization within the human brain, bio-mechanical simulations of the human head and the design of knee joint menisci replacements. Results include performance measurements of the parallel solvers in the SimBio environment. The paper concludes with an outlook on future Grid-computing activities based on SimBio developments.

KEYWORDS Bio-medical, Bio-numerics, Simulation, Finite Elements, Distributed computing, HPC (High Performance Computing)

1. INTRODUCTION

The objective of the SimBio project, financed by the European Commission's Information Societies Technology (IST) programme1, is the improvement of clinical and medical practices by the use of numerical simulation. This goal is achieved by developing a generic distributed simulation environment that enables users to develop application specific tools for a variety of medical areas (see Fig. 1). The potential impact is demonstrated for specific areas through the SimBio evaluation & validation applications: electromagnetic source localization in the brain, analysis of time-series data, maxillo-facial mechanics, knee-mechanics and prosthesis design. A key feature in the SimBio project is the possibility to use individual patient data as input to the modelling and simulation process - in contrast to simulation based on generic computational models. In order to meet the computational demands of the SimBio applications, the compute-intensive components are implemented on high performance computing (HPC) platforms. In addition to combining medical imaging and finite element analyses with HPC technology, the whole environment is integrated using CORBA‖ to allow remote-site computing, thus creating an Internet-based clinical and medical support tool.

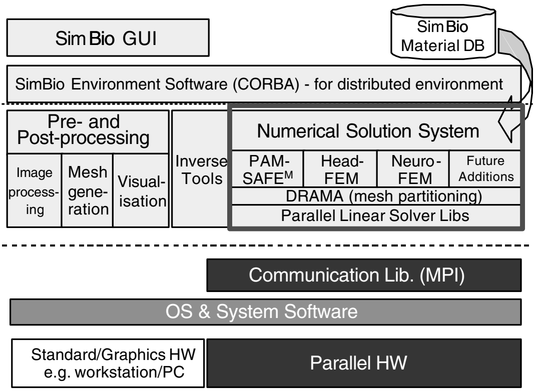

Fig. 1 The SimBio software and hardware.

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§"SimBio — a generic environment for bio-numerical simulation," project number IST-1999-10378, is a 3-year project which commenced in April 2000.

‖CORBA is a registered trademark of the Object Management Group.

2. MODELLING APPROACH

The SimBio environment includes a complete chain of tools necessary for the entire process from geometric model generation from medical scan data (import from DICOM or other proprietary format, segmentation, mesh generation and mesh manipulation) to computer simulation and visualization. Computer tomography (CT) and magnetic resonance imaging (MRI) provide a 3-dimensional description of internal structures by non-invasive measurements. The resultant images permit different types of tissue to be differentiated.

2.1 Segmentation

General segmentation involves the definition of anatomical structures by borders corresponding to signal intensity transitions at tissue interfaces. Here we use an intensity-based algorithm (AFCM, adaptive fuzzy C-means algorithm[1]), which is able to correct intensity inhomogeneities and provide good quality segmentations simultaneously for structures of the human head. However, finding a generally applicable and fully automatic procedure is still an unresolved problem.

2.2 Mesh Generation

Next follows the geometric modelling of the structures identified in the previous step. The VGrid algorithm[2] is based on an adaptive OCTREE data structure exploiting the Cartesian grid structure inherent in medical scan data. VGrid allows the fast generation of uniform and non-uniform (adaptive) tetrahedral and hexahedral meshes suitable for Finite Element simulations (see Fig. 2).

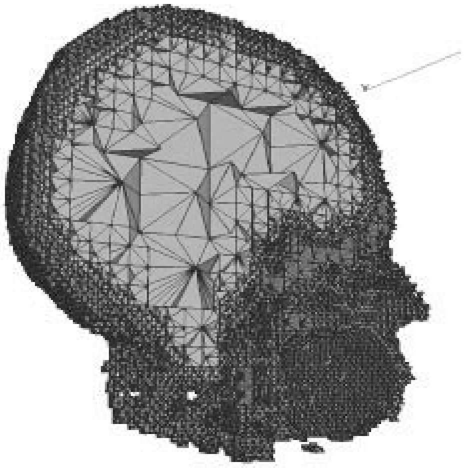

Fig. 2 Material-dependent mesh resolution.

2.3 Model Preparation and Validation

After segmentation and mesh generation a useful model for the simulation of the patient's anatomy has been created. The modelling requirements are:

- Topologically correct volumetric grid.
- Regularly shaped elements.
- Suitable material model for each tissue type.
- Suitably defined boundary and initial conditions.

In order to supply a model with these properties, additional tools have been designed to complement the mesh generation process, for example a mesh quality checker, connected component filtering, and semi-automatic boundary condition specification (see also Fig. 8 below).

3. NUMERICAL SOLUTION

3.1 Source Localization with NeuroFEM

A common clinical task in neurology and neuropsychology is to find realistic electromagnetic source distributions in the human brain. This search is based on EEG measurements that yield electrical potentials on the surface of the head. The data analysis requires in a first step the repeated (up to 10,000 times) solution of a large linear equation system (usually much more than 1 million unknowns). Thus, source localization becomes a supercomputer application. NeuroFEM is a software tool enabling the parallel solution of the large number of forward simulations using a multigrid equation solver. Figures 3 and 4

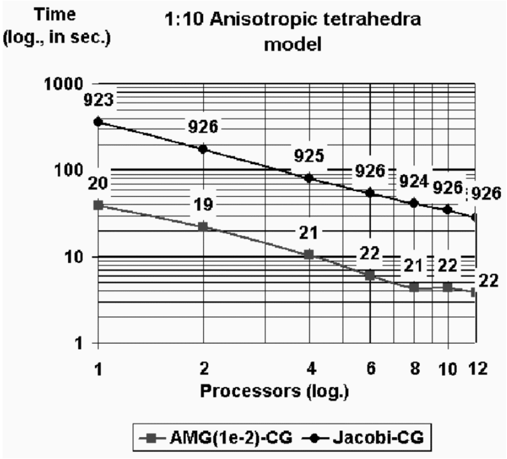

Fig. 3 Timings on SGI Origin for a realistic tetrahedra head model with 147,287 nodes. The number of iterations are depicted next to the curves.

show comparisons between an algebraic multigrid preconditioned conjugate gradient method (AMG-CG) and a Jacobi-CG solver for a head mesh consisting of tetrahedral elements with 147,287 nodes. The AMG-CG solver is about seven times faster than the Jacobi-CG method. The calculations have been carried out on a SGI Origin2000 with 16 MIPS 10000 processors of 195MHz. In Fig. 4 we observe an almost linear speedup that even becomes superlinear for the Jacobi-CG method due to cache effects[3]. The NeuroFEM software has been recently ported to CCRLE's PC cluster, consisting of 32×2 AMD Athlon MP 1900+ processors running at 1.6GHz, interconnected with Myrinet. The 3D potential distribution was calculated in 1.5 sec on twelve processors with the parallel AMG-CG method. Corresponding speedup results are shown in Fig. 5.

3.2 Knee Simulation with PAM-SAFE

The commercial code PAM-SAFE (ESI, Paris) is used for the bio-mechanical modelling of the human knee in order to analyze the dynamics of the knee joint highly. An accurate and smooth finite element mesh of the human knee (see Fig. 6) has been generated from high (0.35×0.35mm in-plane) resolution MRI images to form a template mesh. Patient-specific pre- and post-operative MR images have been acquired from which patient-specific meshes are being generated via morphing the template mesh[9], and are being used to investigate normal and pathologic knee kinematics in addition to the requirements for a meniscal implant. The kinematic behaviour of the knee meshes is being validated by using tools, developed under Simbio, to register the high-resolution MR knee volume to sparse pseudo-dynamic MR slices and to calculate the transformation matrix automatically[10]. Development of an improved material model to model the orthotropic nature of the menisci has been achieved and is being evaluated currently. The parallel version of the finite element code PAM-SAFE runs with its typically high scalability[4].

3.3 Finite Element Analysis with HeadFEM

HeadFEM is designed for the pre-operative planning of maxillo-facial surgery. It is a fully parallel code for the solution of non-linear, finite deformation, large strain finite element problems employing neo-Hookean hyperelastic compressible and incompressible (for soft tissue modelling) constitutive equations. The solution to the non-linear equations is achieved using the non-linear Newton-Raphson iterative method.

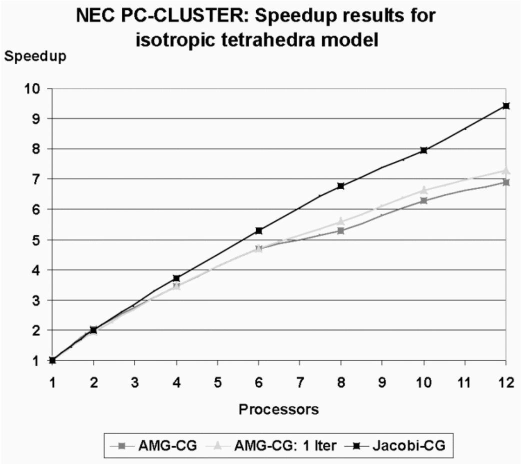

Fig. 5 Scaling on NEC PC cluster.

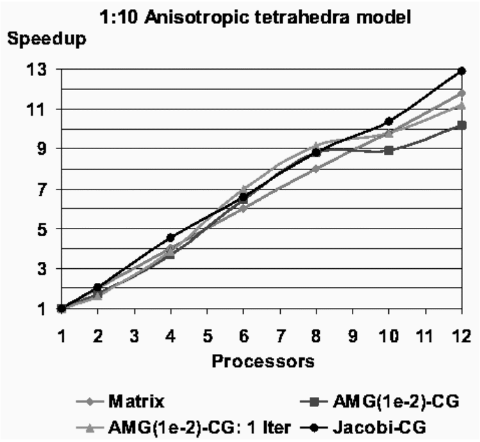

Fig. 4 Scaling on SGI Origin.

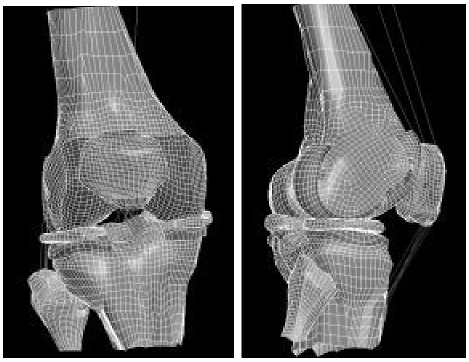

Fig. 6 FE mesh of human knee.

The HeadFEM implementation uses the Finite Element Interface (FEI) definition from Sandia National Laboratories[5], which serves as an abstraction layer between finite element routines managing matrix-assembly and linear-solver modules. Via FEI, HeadFEM is linked to the NEC PILUTS linear solver library, which comprises a variety of state of the art parallel iterative solution (CG, BiCGstab, symQMR) and preconditioning procedures ranging from simple diagonal scaling to incomplete Cholesky, threshold and distributed Schur complement methods[6,7]. For improved parallel efficiency, a partitioning tool based on the DRAMA load-balancing library[8] is used. For the scaling of HeadFEM see Fig. 7.

In order to ease model preparation for this specific task, several additional tools had to be implemented. For specifying the forces exerted on the skull, a virtual version of the medical device called a halo was created, which allows a very easy and quick setting of the boundary conditions, see Fig. 8. Also, the automatic segmentation and mesh generation process may result in meshes with disconnected components, which lead to underdetermined problems and have to be cleaned up by a special tool.

4. COMPONENT INTERACTION

Within the project a GUI has been developed to assist users in setting up their own simulation scenarios, which basically consist of a sequence of applications to be executed (see Fig. 1). All required input and output parameters for each application are entered via specialized windows. The complete scenario is then written to a file using a specially designed extensible markup language (XML) format. A driver program parses the XML files and invokes all programs sequentially (see Fig. 9). Output and error messages are kept in log files. The design of the generic environment distinguishes local and remote applications. In the SimBio context all local applications will be executed at the user machine whereas the remote ones are executed at a compute server site. All remote transactions, such as file and parameter transfers, are achieved via small software agents that act upon a CORBA middleware layer. To attain an adequate level of security here, secure socket layer (SSL) based encryption for all remote operations can be employed. At the remote site, CORBA servers insert incoming requests into databases, generate batch scripts and then launch them to the local scheduling system. The information kept in the database is used to re-launch a request in case of error, adds an additional authentication layer to the system and finally serve as the basis for an optional accounting system.

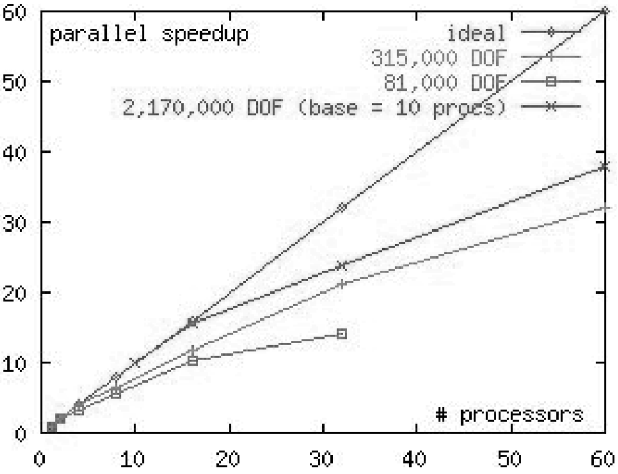

Fig. 7 Scaling of HeadFEM code.

Fig. 8 The virtual halo device.

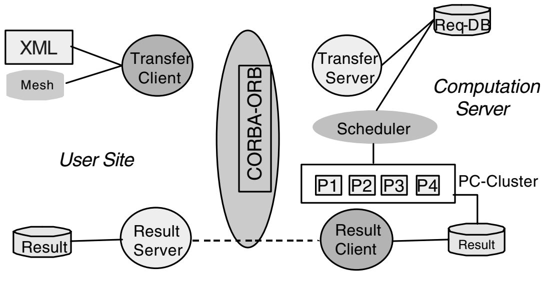

Fig. 9 Corba Component Coupling.

5. CONCLUSION

The SimBio environment combines medical imaging and finite element techniques with up-to-date HPC algorithms and technologies. The SimBio project provides an extensive tool for numerical modelling of human body parts. A major advantage of the SimBio approach is the ability to set up models of body parts of individual human beings based on medical scan data. This concept thus paves the way for the future set-up of virtual models of individuals applicable for the investigation of a wide range of medical problems. The idea of SimBio is taken a step further by the new EC project (GRID-enabled Medical Simulation Services) that started in September 2002. GEMSS will enable medical practitioners and researchers to use SimBio-like simulations via a GRID infrastructure. The motivation is to improve the quality of health service that can be delivered to society by predictive computer simulations and create new business models for such services.

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