



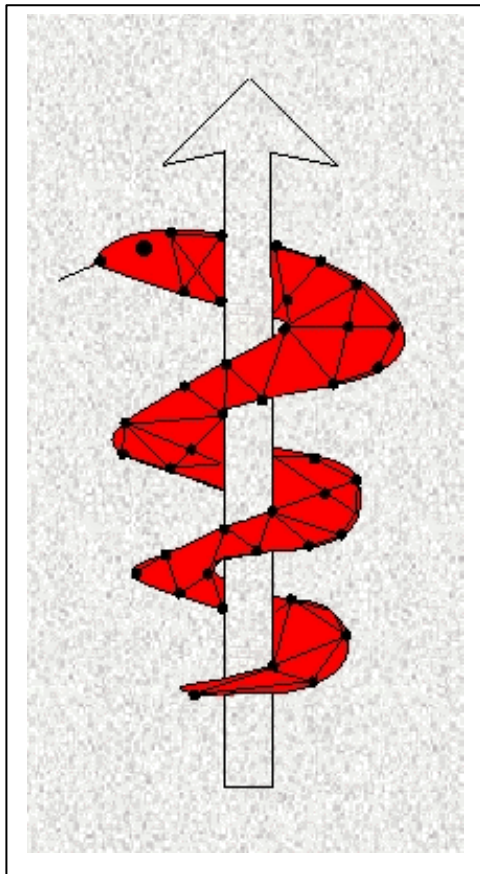
The IST Programme

Project No. 10378

SimBio

SimBio - A Generic Environment for Bio-numerical Simulation

<http://www.simbio.de>



Deliverable 3b

Numerical Solution System

Preliminary Release Notes

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The SimBio Consortium:

NEC Europe Ltd. – UK
A.N.T. Software – The Netherlands
CNRS-DR18 – France
Sheffield University – UK

MPI of Cognitive Neuroscience – Germany
Biomagnetisches Zentrum Jena – Germany
ESI Group – France
Smith & Nephew - UK

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1. Introduction

The numerical solution system (NSS, work-package 3) is a core module of the generic SimBio environment. Figure 1 shows the interaction of the NSS with other modules.

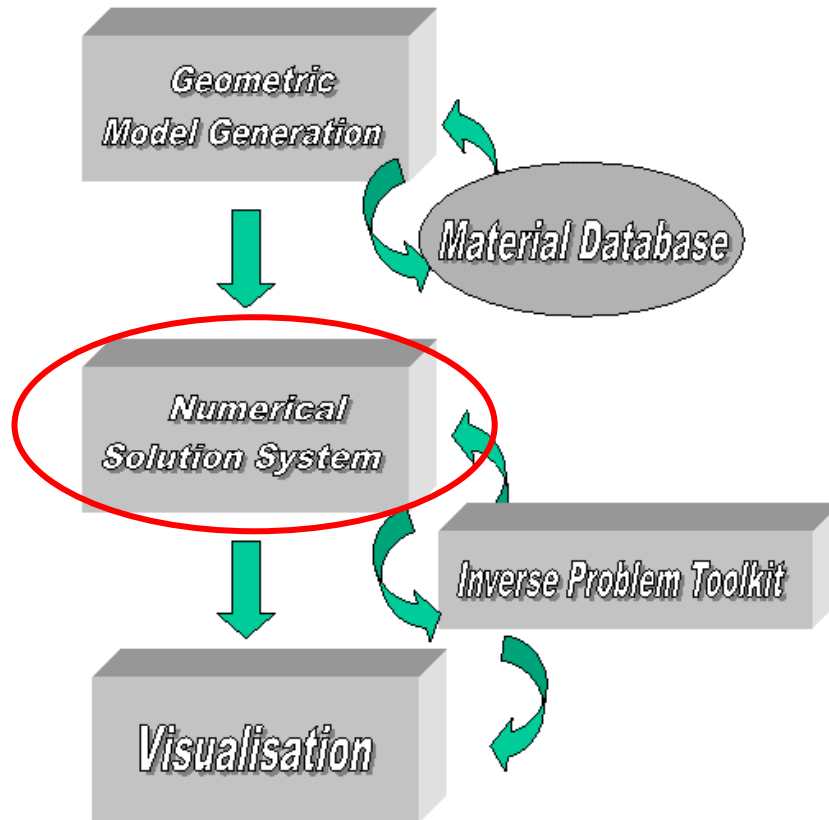


Figure 1: Position of the numerical solution system in the SimBio project.

This document is focused on the description of the present software release. It summarises the technical progress of the NSS components and their integration. The content of the numerical solution system and a detailed explanation of each tool together with preliminary results have been presented in detail in deliverable D3a. The present version of the NSS comprises:

I. Linear Solver Libraries and Partitioning Tool

1. **DRAMA**, a tool for partitioning finite element meshes for efficient parallel execution.
2. **AZTEC/PEBBLES**, public domain libraries for parallel equation solving.
3. **PILUTS**, a highly efficient standalone NEC solver library (**P**arallel **I**ncomplete **L**U with **T**hreshold preconditioned **S**olvers). The routines can be executed as parallel standalone tools or can be called as parallel subprograms in an application code parallelised by domain partitioning.

II. Full Problem Solvers

4. **NeuroFEM (was CAUCHY)**, a full FE code for sequential execution with coupling for parallel solvers provided.
5. An interface for **PAMSAFE**, a fully non-linear FE code for biomechanical applications.
6. **HeadFEM**, a linear fully parallel FE code for special biomechanical applications.

The remainder of this deliverable is organised as follows. For each of the components listed above

- the status of implementation of the software is illustrated by,
 - describing the functionality of its current version,
 - explaining how to access, install and use the tool(s),
- and the plans for the further technical developments are presented.

2. DRAMA Repartitioning Tool

2.1. Introduction

The DRAMA library supports dynamic load balancing for parallel message-passing mesh-based simulation codes. Although the library was originally developed for applications with dynamic, solution-adaptive mechanisms, it can equally well be applied to static problems. Based on a very general cost model, DRAMA provides access to a range of parallel partitioning algorithms through a simple and effective mesh-based interface. The repartitioner tool that is based on the DRAMA library provides load-balancing, matrix partitioning and basic data-migration capabilities to the NSS components.

2.2. Current Status of the Implementation

Recently the repartitioner tool has been extended to enable the use of the VISTA file format for platform independent, compact binary input and output. Also support of material labels has been added. The improved tool consists of the following subroutines (new subroutines are marked in red):

```
drama_simbio_part
├── read_vista_header
├── allocate DRAMA mesh
├── read_vista_mesh
├── repartition
│   ├── read DRAMA options
│   ├── DRAMA_INIT
│   ├── set DRAMA options
│   ├── cost function evaluation
│   ├── DRAMA geometric/graph/mesh migration
│   ├── cost function evaluation
│   ├── migrate data
│   ├── write_pmvis_mesh
│   └── DRAMA_FINALIZE
└── write_vista_mesh
```

The tool is able to exploit the features of the DRAMA library, which give special support to the SimBio applications for the partitioning of sparse symmetric matrices. The repartitioner tool uses file interfaces based on a common ASCII or VISTA format definition. It can be linked with VGrid, NeuroFEM and the PILUTS solver tool in a linear chain (see Fig. 3, 4, 6).

The VISTA mesh file format definition is a platform independent, compact enhancement of the previously defined ASCII file format. It starts with an ASCII header followed by lists of binary data. The details of the format definition are described in D1.2b section 2.1.4.

2.3 How to access, install and use the partitioner tool

The use of the partitioner tool requires that the DRAMA library be installed on the system. The entire software can be obtained in the following two steps:

1. Download the DRAMA library from its homepage: <http://www.ccr1-nece.de/DRAMA/>
2. Download the partitioner tool (`drama_simbio_part.tar.gz`) from the protected part of the SimBio webpage: <http://www.simbio.de/>

The following steps are necessary to install the software:

1. Unpack the release: `tar -xzf drama_simbio_part.tar.gz`
2. Change directory to `drama_simbio_vista`
3. Edit the Makefile and adjust the system dependent information.
4. Build the partitioner: `make`
5. Set appropriate options in the `DRAMA.options` file.

For an implicit solver the file `DRAMA.options` typically should have the following content:

```
!-1-----
! 2 Copyright 2000 by NEC Europe Ltd.
! 3 C&C Res. Lab. Sankt Augustin
! 4 file DRAMA.options,      version date 17.07.2000 JF
!-5-----
 1      number of computational phases
 0      detailed
 4      graph type
10      partitioner type
 0      module type
 1      DRAMA_cost_prediction_choice  0: off 1: on
92      geoinp      91: GEOnodes 92:GEOelements
991     geomod      991:bucket 992:simple
9992    geoversion 9991:DREDUCT 9992:DMOVE
 0      nclags 0: const 1: const+deg. dep. 2: nopn(1:nnodes)
 0 1 0 1 0  costmodel switch
0.0 90.0 0.0  cost model parameters
 0      computing environment
 0      renumbering strategy
```

To run the tool follow the following 3 steps:

1. Create VISTA input file: `input.v`
2. Submit a parallel job: `mpirun -np 4 drama_simbio_part.exe`
3. The partitioned output mesh is found in the file: `output.v`

2.4 Future Planning

To enhance the coupling between the applications it is planned to translate the present ASCII file format to a universal platform independent binary form (VISTA file format). The binary format is more compact and will reduce the communication overhead.

If required by the applications a fine-tuning of the node ordering can be implemented in the DRAMA library to enhance the partitioning quality.

3. AMG-preconditioned CG (PEBBLES-Solver Library)

3.1 Introduction

The kernel of the NeuroFEM-simulator is the FE-solver system. Thousands of large equation systems with symmetric positive definite stiffness matrix have to be solved within the inverse source localisation procedure. Preconditioned conjugate gradient methods are under the most efficient methods for solving such large equation systems. Since the geometry and thus the stiffness matrix stays the same for an inverse source localisation for one patient, the effort for the set-up of the preconditioner can be neglected compared to the solver part. Since a high resolution of the FE-headmodel is necessary with respect to the inclusion of tensor-valued material properties of e.g. skull and white matter, a multigrid-approach seems to be appropriate for the construction of such a preconditioner. An algebraic approach (see [rei00]) is very attractive compared to a purely geometrical multigrid because the generation of a hierarchical grid together with an optimal tuning of the operator and the inclusion of anisotropic tensor-valued material properties within a geometrical approach would be quite difficult. A first comparison between a serial AMG-preconditioner and different serial threshold-factorisation preconditioners in realistic headmodels showed a superior behaviour of the AMG-CG approach especially for very high relative solution accuracy [wol00]. In that paper, the coupling of the solver methods to the FE-code (at that time a pure serial FORTRAN77-code) was realised by means of a "loose" file-coupling, where the files included the stiffness-matrix in compact row format. For these comparisons, no knowledge about the starting vectors was assumed ($\mathbf{0}$ starting vector).

Since it should be possible to calculate better starting vectors through "course-grid-interpolation" techniques and since a final statement about the necessary absolute solver accuracy can only be given after having tested the resolution possibilities of FE-based source localisation and the sensitivity towards the material properties in a later state of the SIMBIO-project, a parallel development/integration of the parallelised algebraic multigrid as well as parallelised threshold-factorisation preconditioners, described in section 4, is important for the NeuroFEM-kernel.

PEBBLES is an external solver library, developed at the SFB F013, "Numerical and Symbolic Scientific Computing", J.Kepler University Linz, Austria. It has a "fee-free" license for non-commercial purposes, which allows a temporary, unrestricted research use of PEBBLES during the SimBio development phase.

3.2 Current Status of the Implementation

The serial version of the algebraic multigrid preconditioned CG method (serPEBBLES, [rei00]) has now been "strongly" integrated into serNeuroFEM by means of an element-wise coupling. This development can be seen as a preparation to a coupling of the parallelised code parNeuroFEM to the parallel AMG-CG parPEBBLES (see [haa00]), described in section 3.2.4. The definition of serPEBBLES basic class within the basic NeuroFEM simulator class, which organises a dynamical memory management of the AMG-CG structures, opens the possibility for the use of deeper PEBBLES-structures, derived from this basic class. In the set-up-phase of serNeuroFEM, the connectivity structure of the FE-geometry (element-nodes list) and in a further step the element stiffness-matrices are handed over to PEBBLES class structures, organising storage in compact row format of the stiffness matrix. After a proper definition of the Dirichlet-node (EEG reference electrode) by means of a penalty-approach, leading to a regular matrix and thus a unique solution for the potential, the hierarchy of stiffness- and prolongation/interpolation-matrices is determined exclusively through the use of the algebraic information in the stiffness-matrix on the finest level (strong neighbour relationship between the nodes). A linear interpolation of the potential for each finer grid node through all neighbouring coarse grid nodes was chosen, which turned out to be most efficient in our simulations compared to more sophisticated interpolation techniques (see

[wol00]). After the calculation of the source load vector (right-hand side of the equation system) and the allocation of a starting vector (currently the $\mathbf{0}$ vector), the solver module is called using one Gauss-Seidel step as Pre- and Post-Smoothing in each iteration. The factorisation on the coarsest grid level is carried out by a LL^T factorisation.

3.3 How to access, install and use the Software

The solver library as kernel of the NeuroFEM-simulator is actually integrated as FE-simulation tool in the ST4.1 release. It can be accessed via the interface functions defined in the release notes of ST4.1. The software is tested and optimised on Linux and SGI-Irix using the Gnu C++ compiler. The ST4.1 release contains libraries and a binary command line tool for Linux and SGI-Irix.

3.4 Future Planning

The parallelisation of the NeuroFEM FE-potential calculation and the integration of the parallel AMG-preconditioned CG solver (parPEBBLES) are in an advanced state. A partitioning of the dual graph of the FE-headmodel is calculated through the use of the public domain METIS *partdmesh*-function. In the future, the software-developments will be coupled directly to the results of the subroutines, described in section 2.2, since the needed dual graph partitioning is also part of the DRAMA-library. The FE-mesh together with the material properties will be distributed element-wise to the processors. The stiffness- and volume-matrices (the latter is needed for head volume and average reference potential calculations in a later phase of the NeuroFEM-simulator) will then be set up fully parallel, following quite closely the descriptions of subsection 3.2.2. The Dirichlet-node information will be sent to all processors which are part of the partition-index-set of that node and implemented in the local sub-matrices as described in 3.2.2. Since the calculation of the source load is extremely fast compared to the local potential computations, the root-process will calculate the right-hand side vector and then distribute it to the processors. In a last step, the speed-up with block-right-hand sides and appropriate starting vectors derived through "course grid interpolation" will be examined and the results will be compared with solver-approaches presented in section 4. With regard to parallel MEG forward solutions, the set-up and storage of the MEG secondary matrix has to be distributed and multiplied with the locally calculated potential distribution. An accumulation then leads to the magnetic flux of the secondary sources, which has to be added to the magnetic flux of the primary source.

4. NEC Solver Library PILUTS

4.1 Introduction

The PILUTS library includes parallel sparse solvers for real symmetric positive definite (spd), general real symmetric and real non-symmetric matrices. As basic iterative methods, the Conjugate Gradient (CG) algorithm, a **sym**metric variant of the **Q**uasi-**M**inimal **R**esidual method (symQMR) and the **Bi**-Conjugate **G**radient **stabilised** (BiCGstab) algorithm are provided [bas00, bas99, bas96, saad96]. CG is applied to equation systems with spd matrices, QMR usually to systems with general symmetric matrix, and BiCGstab usually to systems with non-symmetric matrix. For convergence acceleration of the basic iterations, a selection of preconditioning methods is available. The preconditioners include scaling methods, symmetric or non-symmetric incomplete block factorisations with threshold and **D**istributed **S**chur **C**omplement (DSC) algorithms [bas00, saad99, saad96].

4.2 Current Status of the Implementation

All PILUTS methods are implemented in such a way that the solver routines can be executed as parallel standalone tools or can be called as parallel subprograms in an application code parallelised by domain partitioning. In the former case, the equation system data is read piece-wise from a file and distributed to the processors available. The solution process itself is performed fully in parallel afterwards. In the latter case, the parallel application code provides the distributed equation system data to a local PILUTS subroutine which then solves the matrix problem in parallel.

The DRAMA tool can determine the data distribution of the PILUTS CG solver. The solver can read the partitioning information from a small DRAMA file (“dist.dat”, see Fig. 3) containing the number of nodes in each sub-domain and can distribute the matrix data accordingly. This feature is useful for the current PILUTS-NeuroFEM coupling. For preconditioning CG, simple diagonal scaling, block Incomplete Cholesky decomposition with Threshold (ICT) and block Incomplete LDL^T factorization with Threshold (ILDLT), both with preceding diagonal scaling, are available [bas00, saad96].

Simple diagonal scaling or block ILDLT with preceding diagonal scaling can precondition the current PILUTS symQMR solver.

The PILUTS BiCGstab environment has two additional features: First, the distributed equation system data can be re-partitioned by ParMETIS and re-distributed in order to reduce the couplings between sub-domains and in order to accelerate the convergence of block factorisations or DSC preconditioners. Second, the distributed matrix data can be re-ordered in order to reduce fill-in for incomplete decompositions. For preconditioning, simple diagonal scaling, simple row and column scaling, block Incomplete LU factorisation with Threshold (ILUT), block ILUT with preceding diagonal scaling, block ILUT with preceding row and column scaling, DSC preconditioning using ILUT for local diagonal matrix blocks, DSC preconditioning with preceding row and column scaling using ILUT for local diagonal matrix blocks, and DSC using complete LU decompositions of the local diagonal matrix blocks [bas00, saad99, saad96].

4.3 How to access, install and use the NEC PILUTS library

The PILUTS software can be obtained from the SimBio web page. The following steps are necessary to install the software:

1. Download the PILUTS package (piluts.tar.gz) from the protected part of the SimBio webpage: <http://www.simbio.de/>
2. Unpack the release: `tar -xzf piluts.tar.gz`
3. Change directory to piluts
4. Edit the Makefile and adjust the system dependent information.
5. Build the PILUTS library: `make`
6. To use the library link the object code with `libpiluts.a`

4.4 Future Planning

1. Development of symmetric DSC preconditioners for CG or symQMR.
2. Integration of all PILUTS solvers into the same environment (library: `libpiluts.a`) with support of all features (re-partitioning, re-ordering etc.).
3. Optimisation of the advanced PILUTS interface for HeadFEM and NeuroFEM.
4. Support for efficient execution in the case of multiple right hand sides within the PILUTS routines (use of BLAS routines, useful for NeuroFEM).
5. Further investigation of the effect of matrix re-partitioning and re-ordering on incomplete block factorisation or DSC preconditioning.

5. NeuroFEM

5.1 Introduction

The inverse problem in EEG and MEG amounts to finding a realistic source distribution in the human brain for a given set of field observations on the surface of the head. This requires the repeated simulation of the field propagation for a given dipolar source in the brain using a volume-conduction model of the head. For most realistic modelling, the different tissues have to be segmented and assigned individual conductivity tensor material parameters. As a basis for the development of the NeuroFEM-software, the software package CAUCHY'97, described under

<http://www.rwth-aachen.de/neurologie/Ww/Neurologie/cauchy/CauchyFunctionality.htm>

and in [buc97], [rien97] [wol99], was taken and strongly redesigned.

5.2 Current Status of the Implementation

C++ class-structured software replaces the old FORTRAN77 CAUCHY'97 kernel routines and enables the development of the SIMBIO-software on parallel platforms. The NeuroFEM-simulator has been derived from an abstract simulator class defined in the design report of ST4.1. A hierarchical class structure is used to reduce the number of interfaces and to keep them clean of implementation details. The class structure of the inverse toolbox is described in the release notes of ST 4.1. The toolbox of ST 4.1 provides abstract class interfaces for grid generators, forward simulators using a discrete and continuous search space. NeuroFEM tools are interfaced to classes that are derived from these abstract classes.

The integrated class structure allows future comparisons with boundary-element-based forward simulations and analytical series expansion formulas for spherical shell geometries, which both are also derived from the abstract simulator-class. The goal is an influence-study of tissue anisotropy on the various inverse algorithms of the ST4.1 toolbox. A dynamical memory management has been introduced throughout NeuroFEM, which replaces the former static allocations and enables a user-friendly application on distributed memory platforms. A first test was carried out where the NeuroFEM-simulator was used as forward simulator within an inverse dipole fit method, described in the ST4.1 design report.

In EEG/MEG-source localisation, the source is usually modelled as a mathematical equivalent current dipole, i.e. a current source and a sink, which are infinitesimally close together in the human cortical layer. This point-like equivalent current dipole has been shown to be an adequate model for the synchronous polarisation of a cortical surface of about 30mm^2 . The point-like source directly leads to a singularity in the related potential, which has to be treated numerically. One possibility is the "blurred dipole" where current monopoles are placed at neighbouring FE-mesh nodes around the dipole location such that the resultant moment matches that of the mathematical dipole [buc97]. Another possibility is the subtraction method where the "singularity-potential" for a mathematical dipole in an unbounded homogeneous conductor is calculated analytically and the correction is carried out numerically on the realistic geometry ([rango96], [mar98]). The correction is calculated with the FE method so that the sum of "singularity-" and "correction-", the "total-potential", obeys the charge continuity law within the head and the Neumann boundary conditions at the surface. The subtraction method and the node-shift (ns) mesh generation approach (see ST1.2 report) have been validated in a 4-layer sphere model where a spherical harmonics series expansion of the dipole potential can be derived for anisotropically conducting layers [mun88, mun93].

For the validation of the subtraction method, we assumed the following isotropic conductivities in the 4 layer model: 0.33, 0.0049, 1.0 and 0.34 S/m. Together with node-shifted FE-mesh, the magnification error (optimum 1) was 1.053 and the relative difference measure (optimum 0) 0.023 for 6 electrodes at all extreme sphere surface positions.

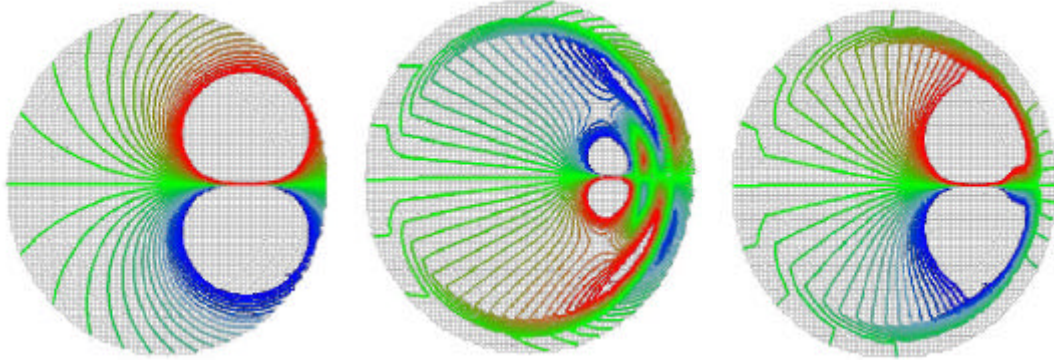


Figure 2: Isopotential lines in ns-models: singularity-potential (left) and FE-correction potential (middle) from -0.5 to 0.5 mV, total-potential from -1 to 1 mV (right).

For the tight coupling between ST4.1 and WP3 in the case of a continuous parameter space for the inverse reconstruction described here, the NeuroFEM tool was extended to provide a source simulation also for dipoles which are not on the discrete grid, but in the continuous space. The simulator is able to simulate several dipoles in the continuous space at the same time. In the case of a discrete parameter space, the coupling between WP3 and ST4.1 is on a simple file level or via close coupling, the leadfield matrix can also be directly handed to the inverse tools if the applications run on the same computer.

Task	Programme Name	seq/par
Meshing	VGrid	seq
	↓	
Re-partitioning	DRAMA tool	seq or par
	↓	
Simulator (forward)	NeuroFEM	seq
	↓ FE matrix written to a file + "dist.dat"	
Linear Solver	PILUTS tool	seq or par
	↓	
Visualisation	VM	seq

Figure 3: The linear software chain based on ASCII-file described in detail in deliverable D3a section 5.2.2.

The activities in this period were focused on the coupling of NeuroFEM to the PEBBLES solver. The coupling to the PILUTS solver library is still based on the matrix/ASCII file coupling described in Fig. 3 and will be changed in the near future (see section 5.4 for details).

5.3 How to access, install and use NeuroFEM

The actual NeuroFEM tool is integrated in the ST4.1 software release. To provide access to NeuroFEM tools, three interface levels are defined in the release notes of ST4.1. The homogeneous interface between the functions of the inverse toolbox and NeuroFEM allows using NeuroFEM as stand-alone application to compute the leadfield matrix and as integrated FEM-simulation tool in the inverse source reconstruction. One level of the interfaces enables the calling of inverse methods on a command line level. This level can be integrated in a complete SimBio application environment.

The software is tested and optimised on Linux and SGI-Irix using the Gnu C++ compiler. The ST4.1 release contains libraries and a binary command line tool for Linux and SGI-Irix.

5.4 Future Planning

NeuroFEM input and output routines will be changed to read and write Vista format files. The FE mesh is stored in a Vista graph file (see D1.2a) that also contains the information about influence nodes. After a partitioning by means of the DRAMA-tool, NeuroFEM reads the partitioned geometry and creates the lead field matrix in binary Vista format. The lead field matrix is stored as a one-dimensional image file in order to avoid compatibility problems between Fortran77 and C++ matrix conventions. The tool will be extended to read a separate surface grid as influence space, extracted from a volume grid by an operator described in the release notes of ST1.2. This surface grid represents the brain surface or the cortex on which the leadfield matrix is computed.

The potential distribution of a dipole source configuration can be written in a vista grid structure and then be visualised with tools from WP5. Figure 4 shows the software chain from mesh-generation to potential distribution visualisation.

Task	Programme Name	seq/par
Meshing	VGrid	seq
	↓	
Re-partitioning	DRAMA tool	seq or par
	↓	
Simulator (forward)	NeuroFEM with integrated PEBBLES and PILUTS interface	seq or par
	↓	
Visualisation	VM	seq

Figure 4: A linear software chain that generates a forward solution with coupling by files in VISTA format.

The coupling of parNeuroFEM to parPEBBLES and PILUTS will be terminated as described in 3.2.4 and section 4. A further parallelisation within NeuroFEM seems to be necessary, especially with regard to a parallelized MEG forward simulation. NeuroFEM will be strongly coupled with the PILUTS library, described in section 4.

The inclusion of anisotropic material properties from the WP's 1 (anisotropic skull conductivity) and 2 (anisotropic conductivities of brain white matter, derived through Diffusion Tensor Imaging, DTI) within NeuroFEM's forward modeling process will get high priority. The coupling between NeuroFEM and the inverse toolbox (ST4.1) will be continued. The toolbox contains a variety of state of the art inverse source reconstruction algorithms. They will be implemented in C++ using a modular class structure.

6. PAMSAFE

6.1. Introduction

The effort of ESI for this task has been reduced by two person-months since the last report. The new time allocation corresponds amongst others to the evaluation of the capability of the new tetrahedral mesh generator of ESI. This mesh generator is currently used in fluid dynamics applications and it can now read voxel data. Two aspects i.e. the pre- / post-processing and the corresponding solver developments are included in the new work plan.

6.2. Current Status of the Implementation

6.2.1 Pre- / Post-Processing

The following figure shows the interaction between the PAM-SAFE™ package and other SimBio components:

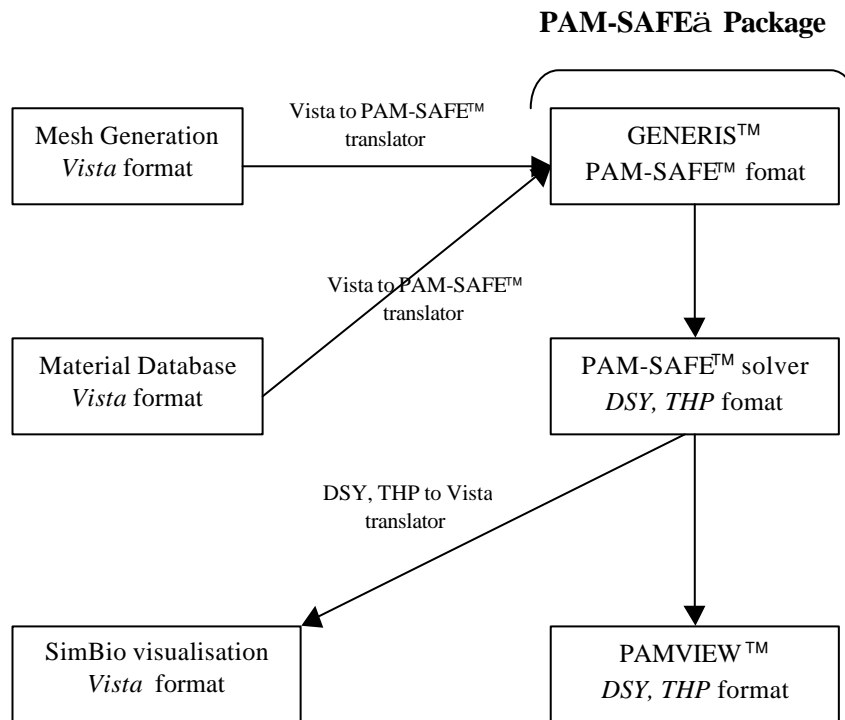


Figure 5: The above diagram shows that the main interaction of the PAM software is to be expected with the mesh generation tool.

In the D3a document, some subtasks were listed to obtain an optimal integration of the ESI tools into the SimBio environment by using the chain (GENERIS™, PAM-SAFE™, and PAMVIEW™) within a biomechanical environment. There has been no modification in this part of the work plan.

Currently, there subtasks, which have already been completed, and others, which have been started. The converter from VISTA mesh format to PAM-SAFE format is finished and its integration in GENERIS has been started. During this task, the Vista tool kit and some components of the SimBio environment like VGrid have been ported (modification of the existing implementation) on the NT platform. The admissible platforms for the converter are

Windows NT and Unix Platforms. Porting to Linux is currently pending. The implementation of the visualisation of the fibre direction within the elements has been completed for shell elements. For the visualisation of the fibre direction and the automatic orientation of the fibre in the local frame of the elements several basic algorithms have been developed. They are related to the mesh management and they have to be completed before the integration in GENERIS. This subtask is still in an initial stage as far as solid elements are concerned. When completed it will be applicable to both hexahedral and tetrahedral meshes of any integration or interpolation order.

6.2.2 Solver improvement

6.2.2.1 Performance evaluation of the current parallel version

An admissible platform for the end user of SimBio is the LINUX cluster. We have chosen this platform in order to improve the parallel version of PAMSAFE for a realistic case in the area of the biomechanical simulations. Its porting to the LINUX platform has been done recently at ESI. Basic tests have already been performed within the context of the SimBio project. However, more realistic tests are required before the LINUX version can be approved for general use.

6.2.2.1 Evaluation of the tetrahedral elements

A series of numerical tests were performed involving the use of the new linear and quadratic tetrahedral elements within a beta version of PAM-CRASH. The evaluation was made using standard NAFEMS benchmarks and compared against the results of equivalent hexahedral meshes at various levels of numerical integration and tetrahedral meshes obtained from degenerate-hexahedral ones. The tests showed interesting new results concerning the accuracy and stability of these new elements.

6.3 Future Planning

As explained in the section about the current status of the PAM-SAFE™ package (section 6.2.1), the next technical developments will concern the pre-processor, GENERIS™, and the PAM-SAFE™ solver.

6.3.1 GENERIS™

1. Visualisation of the fibre direction in elements, in particular solids. (Under way)
2. Automatic orientation of the fibre in the element local frame. (Under way)
3. Reading and writing of the tetrahedron element definition. (To be defined)

6.3.2 PAM-SAFE™ Solver

1. Evaluation of current tetrahedral formulation and its improvement. (Done except the improvements which will be assessed later on within the project)
2. Improvement of some materials in the case of specific parameters of menisci. (Initiated)
3. Performance evaluation of the current parallel version. (Under way)
4. Settings of new (or future) developments necessary for the knee behaviour study in the parallel version. (to be initiated)
5. Setting new features in the splitter tool. (to be initiated)
6. Work on the simulation time reduction for this kind of simulation. (Under way)

6.3.3 Converters

Moreover to permit the interaction with the SimBio environment, translators for SimBio data will be developed:

1. Mesh Vista to Pam-SAFE™ format (Done)
2. PAM-SAFE™ output DSY, THP to Vista format (Under way)
3. Integration of the tool in the SimBio environment (to be initiated)

7. HEAD-FEM

7.1 Introduction

HeadFEM is a parallel FE-code for applications specialized on head-mechanics. The initial implementation (version 1.0) is in C using the AZTEC library [aztec] for the parallel solution of the linear system of equations.

7.2 Current Status of the Implementation

The new code (version 2.0) has been restructured and rewritten in C++ in a modular, object-oriented way. Version 2.0 was designed to allow a clean integration of different solver libraries and to facilitate further enhancements of the software. As a first step of the improvement program described in section 7.4 the NEC PILUTS library has already been integrated in the simulation code.

Task	Programme Name	seq/par
Meshing	VGrid	seq
	↓	
Re-partitioning	DRAMA tool	seq or par
	↓	
Simulator	HeadFEM	seq or par
	↓ with integrated PILUTS call	
Visualisation	VM	seq

Figure 6: SimBio Component interaction for HeadFEM.

HeadFEM is running in parallel with an input mesh generated by VGrid and partitioned by the DRAMA tool. The partitioning information is stored as two additional vectors for elements and nodes separately in the VISTA-file. The results of a linearised static FE-analysis with HeadFEM are vectors of nodal displacements and forces and element based stresses and strains for the mesh. The output is in VISTA format that will be accepted by the SimBio visualisation module VM (see D5b).

To demonstrate the functionality and the successful interaction of the NSS components we present the results of a static FE-analysis of a small test example consisting of 8 hexahedral elements and 27 nodes in parallel on 4 processors of the NEC success PC-cluster. The initial mesh generated by the mesher VGrid (Fig. 7) has a computational imbalance of $21 / 6.75 \approx 3.111$ which is reduced to $8 / 8.75 \approx 1.185$ by the repartitioner tool (Fig. 8). The repartitioner is directed to minimise edge-cut while keeping the imbalance small (perfect balance = 1).

PE	0	1	2	3	
Nodes	21	2	2	2	see Fig. 7 initial mesh generated by VGrid
Elements	5	1	1	1	
Nodes	8	7	7	6	see Fig. 8 output mesh from DRAMA tool (ParMetis k-way)
Elements	2	2	2	2	

Table 1: Node/Element distribution in the initial and re-partitioned mesh.

For the FE-analysis the cube is torn apart in opposite directions at the central node on the top and another one at the bottom. The resulting deformation shown in Fig. 9 has the expected shape.

The structure of the global stiffness matrix with and without re-partitioning is visualised in Figs. 10 and 11 using the public domain MatView tool from Oak Ridge National Laboratory [matview].

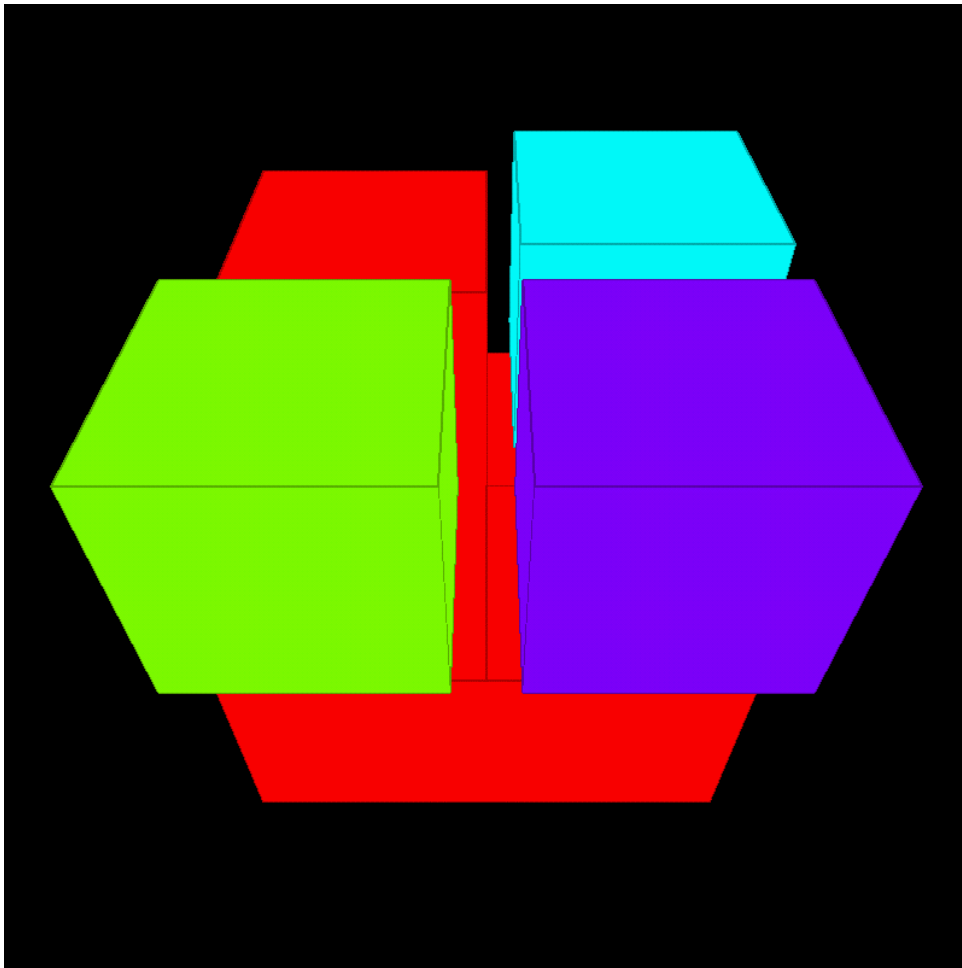


Figure 7: Visualisation of the output mesh from the mesh generator VGrid with the public domain *pmvis* tool from the University of Minnesota [pmvis].

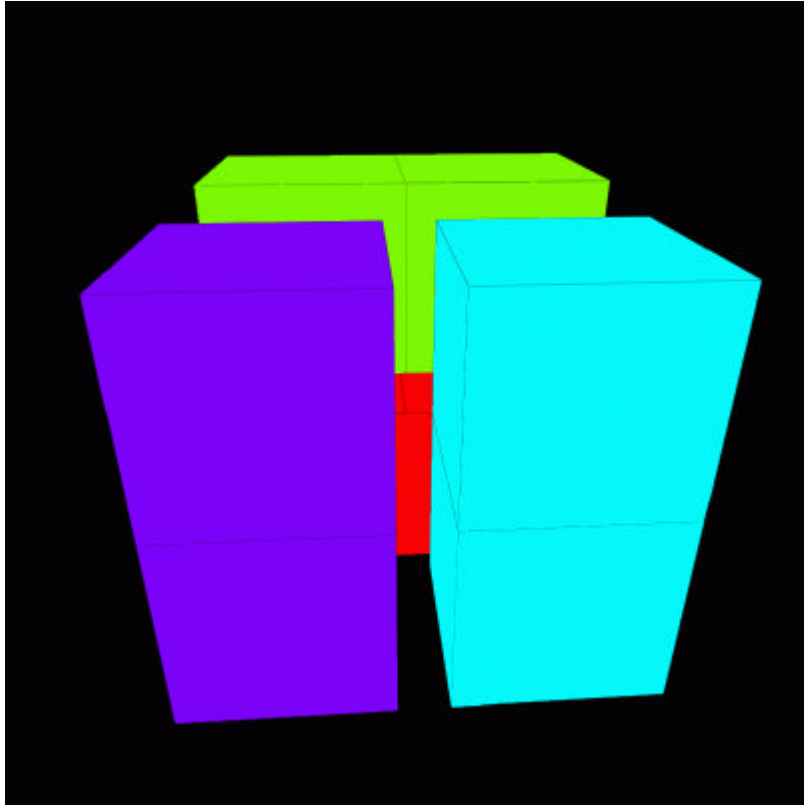


Figure 8: Balanced output mesh from the DRAMA repartitioner tool.

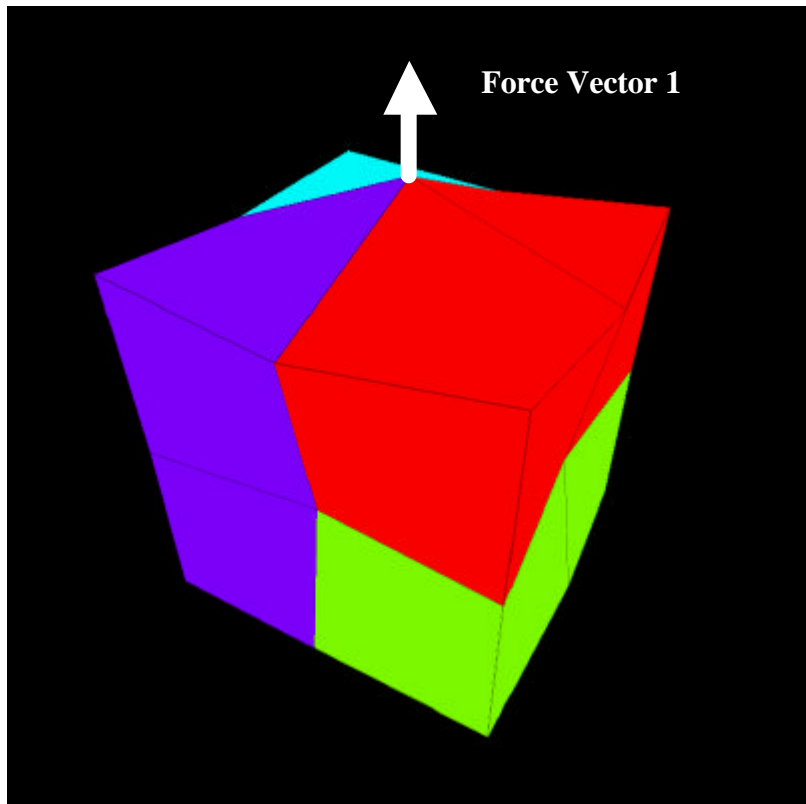


Figure 9: Deformed output mesh from the simulation with HeadFEM. Two external forces are applied symmetrically from above and below. The displacements were multiplied by a factor of 10^8 to emphasize the effect.

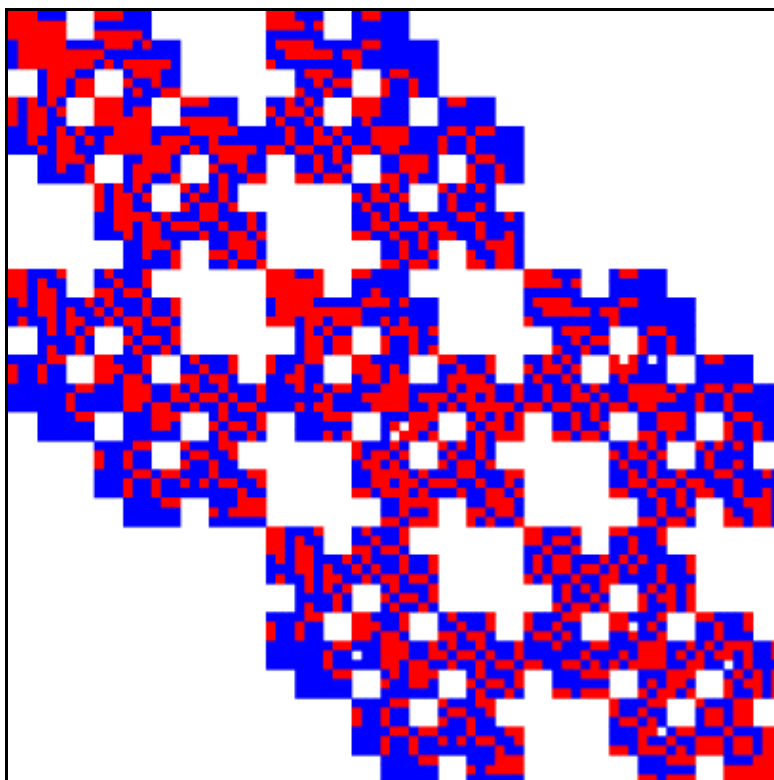


Figure 10: MatView [matview] visualisation of the global matrix corresponding to the original mesh produced by VGrid.

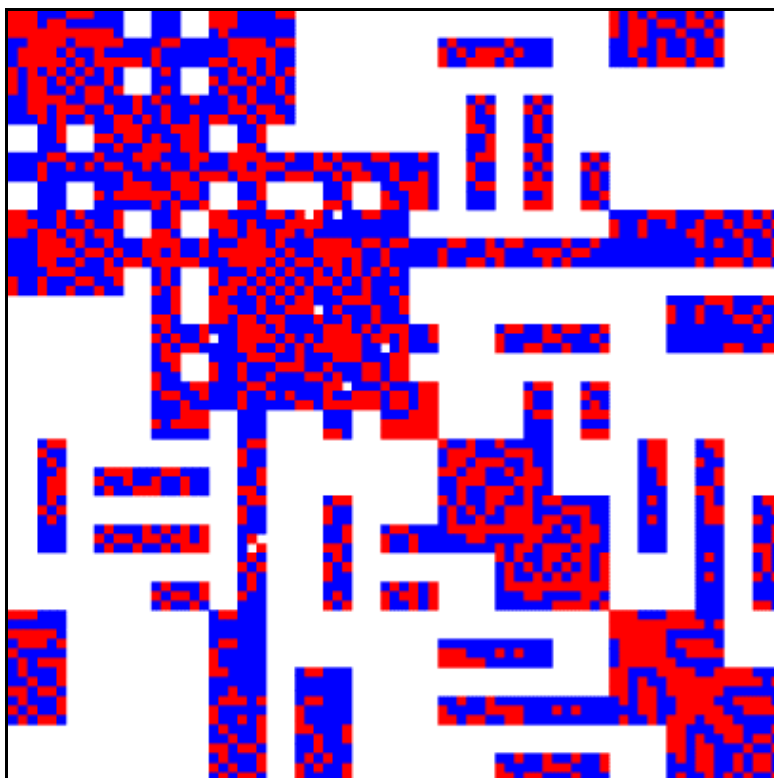


Figure 11: MatView visualisation of the global matrix corresponding to the balanced mesh produced by the re-partitioner tool (blue=negative values, red=positive entry).

7.3 How to access, install and use HeadFEM

The use of the HeadFEM software requires that the SimBio library *libsimbio.a* and the PILUTS solver library *libpiluts.a* have been installed on the system.

The installation of the HeadFEM version 2.0 package consists of the following steps:

1. Install the SimBio library *libsimbio.a*
2. Install the solver library *libpiluts.a*
3. Download the tar file *headfem2.tar.gz* from the SimBio server.
4. Unpack the release: `tar -xzf headfem2.tar.gz`
5. Build the system: `make`

To run the job on a parallel system (with MPI library installed) the following steps are necessary:

1. Copy the input mesh file *input.v* to the current working directory.
2. Start a parallel job: `mpirun -np 4 driver`.
3. Output in VISTA format: *output.v*

7.4 Future Planning

The FEI interface definition from Sandia National Laboratory [fei] is an emerging standard for the interface layer between FE-applications and linear solver libraries. It is planned to implement the FEI interface to support future extensions of HeadFEM and to be able to exploit public domain linear solver libraries with an FEI interface that are currently being developed [hypre, isis].

As the mesh generator VGrid creates brick, tetrahedral and hybrid meshes, the HeadFEM code has to be extended to enable the use of tetrahedral elements. The HeadFEM code will also be extended by non-linear FE features: It is planned

- to add methods for geometrically non-linear simulations (such as Newton-Raphson),
- to implement a non-linear material model (e.g. a viscoelastic tissue model).

If contact and friction phenomena become important we will consider

- to develop a contact/friction algorithm to take account of sliding interfaces such as brain and skull.

Furthermore the DRAMA partitioner tool will be exploited to find the optimal partitioning for the NEC PILUTS solvers used in HeadFEM. Besides the NEC solver routines the coupling of external solver libraries like Hypre, ISIS++ or Prometheus [prometheus] will be evaluated.

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