Applications of Automatic Mesh Generation and Adaptive Methods in Computational Medicine*

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Abstract

Important problems in Computational Medicine exist that can benefit from the implementation of adaptive mesh refinement techniques. Biological systems are so inherently complex that only efficient models running on state of the art hardware can begin to simulate reality. To tackle the complex geometries associated with medical applications we present a general purpose mesh generation scheme based upon the Delaunay tessellation algorithm and an iterative point generator. In addition, automatic, two- and three-dimensional adaptive mesh refinement methods are presented that are derived from local and global estimates of the finite element error. Mesh generation and adaptive refinement techniques are utilized to obtain accurate approximations of bioelectric fields within anatomically correct models of the heart and human thorax. Specifically, we explore the simulation of cardiac defibrillation and the general forward and inverse problems in electrocardiography (ECG). Comparisons between uniform and adaptive refinement techniques are made to highlight the computational efficiency and accuracy of adaptive methods in the solution of field problems in computational medicine.

Introduction

Computational Medicine is an emerging area of scientific computing which offers the investigator opportunities for discovery and application in both medicine and

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in numerical analysis. Computational Medicine encompasses a broad range of topics including bioelectric field simulation (modeling of electrical and magnetic fields from the brain and heart, and modeling of excitable tissues), biomechanical modeling (biomechanics, ergonomics, and hemodynamics), molecular biology, and imaging technology [1, 2, 3, 4, 5]. It is not the purpose of this paper to discuss the entire field of computational medicine, but to investigate accuracy issues in bioelectric simulations – issues that impact most other field problems in computational medicine.

Computational *electrophysiology* can be loosely defined as the simulation and modeling of macroscopic and microscopic bioelectric fields. The electrical activity in the human body is induced by the flow of charged ions across membranes of individual cells. The collective interaction of all the currents from groups of cells gives rise to electric potentials which are measured from, for example, the skull (EEG) or the torso surface (ECG). The registration of normal and abnormal bioelectrical signals has been used as a diagnostic tool for many years and extensive catalogs linking signals to pathologies have evolved. More recently, investigators have begun to develop mathematical descriptions of the origin of the electric signals they measure. The hope exists that these mathematical descriptions will provide medicine with new diagnostic tools which are based on physiological function and not empirical observation. In the field of electrocardiography, computational models of bioelectric phenomenon from sources in the heart have existed for over 25 years. The size and scope of the models have been limited by contemporary computational resources and by the relatively simple numerical algorithms utilized to approximate the continuous field equations. It has been shown that the electric signals in the body produced by the macroscopically viewed heart can be described as a solution to a quasi-static Poisson's equation [6]. While the theoretical solutions of such elliptic equations are not usually difficult (at least in the *direct* sense, when we know the nature of the sources — the complementary *inverse* problems are another story), computationally, there are many challenges to overcome in obtaining accurate approximations. Significant challenges include the construction of the geometrical model, the specification of the material properties, some of which are anisotropic, and the large scale nature of the computations.

One application of current interest in cardiac bioelectric field computation is the simulation of a defibrillation shock. Clinically, defibrillator electrodes are either implanted internally, or applied directly to the chest, in order to deliver sufficient electric energy to stop the irregular heart rhythms that signify a fibrillating heart. In the past, the placement of the electrodes for either type of defibrillator was chosen based on clinical trial and error. Only recently, has the sophistication of thorax and heart models permitted more realistic simulation of cardiac defibrillation. The aim of such models is to assist in determining the optimum electrode placement and strength of shock to terminate the fibrillation. The simulations involved in this case present similar computational challenges since, once again, the geometry of the torso is complex, the material properties (conductivities) are imperfectly known, and the resulting computations are extensive. Defibrillation gives rise to very large potential gradients near the edge of the electrodes. As the effectiveness of the simulations depends on accurately calculating the amount of current which passes from the electrodes to the heart, these gradients need to be computed accurately. Since the strength of the gradients falls off as $\frac{1}{r^2}$ from the source, adaptive refinement techniques are necessary for accurately computing the fields on and near the electrodes while still controlling the size of the resulting computation.

While the defibrillation problem represents the direct solution of Poisson's equation for electrical conduction (sources are known), another important application in cardiology is the electrocardiographic (ECG) inverse problem. An accurate solution to the inverse problem in electrocardiography would provide a noninvasive procedure for the evaluation of many cardiac abnormalities including myocardial ischemia [7, 8] and the localization of ventricular arrhythmias. The inverse ECG problem can be stated in most general terms as follows: given a subset of electrostatic potentials measured on the surface of the torso and the geometry and conductivity properties of the thorax, calculate the electric current sources within the heart and the resulting fields in the intervening conductive region (volume conductor). Mathematically this can be posed as an inverse source problem in terms of the primary current sources within the heart. Unlike the inverse problem of electrical impedance tomography, where the goal is to recover the magnitude and location of the various tissue conductivities, the conductivities are assumed known and the goal is to recover magnitude and location of the cardiac sources. The general inverse ECG problem does not, however, have a unique solution. In order to solve the general problem, one usually represents the heart's electrical activity by a collection of discrete source terms such as dipoles or other higher-order current generators. One then tries to recover magnitude, location and orientation of the simplified model sources (see [9] for recent review). Alternatively, if instead of discrete sources within the heart, one formulates the problem in terms of electrostatic potentials on a surface bounding the heart, the resulting problem does possess a unique solution[10]. In fact, this has been the approach used in most recent research, since, unlike discrete source models, it also offers to opportunity for direct validation through measurements of potentials on the heart surface. [11, 12, 13, 14, 15, 8]. Mathematically, instead of solving Poisson's equation, we solve a generalized Laplace's equation with Cauchy boundary conditions[1].

While this version of the inverse problem has a unique solution, the problem is still mathematically ill-posed in the Hadamard sense; i.e., the solution does not depend continuously on the data, such that small errors in the measurement of the voltages on the torso can yield unbounded errors in the solution. Hence the need for controlling discretization errors using adaptive methods. Interestingly, little research has been done to show the relationship between the discretization error and the solution error in an ill-conditioned system. We have found that controlling discretization errors by using adaptive methods provides a significant improvement in approximating ill-posed inverse problems.

As a result of the geometric complexities involved in bioelectric field simulations, we have also made efforts to tailor the automatic mesh generation capabilities applicable to problems in computational medicine. Standard techniques common in other engineering disciplines which involve piecewise parametric representations of the geometry do not work well for describing the irregular shapes of the various

[1]This is covered in more detail in the Mathematical Methods section

thorax inhomogeneities. Due to the large gradients that arise either from naturally occurring bioelectric sources such as the heart or from externally supplied fields such as those from defibrillation, adaptive methods are required to maintain a balance between solution accuracy and computational costs.

In this paper we elucidate upon our application of three-dimensional automatic mesh generation and adaptive refinement techniques applied to problems in computational medicine.

Mesh Generation

Bioelectric field simulations require the modeling of complex geometric domains such as those found in the human thorax (eg., heart, lungs, skeletal muscle, vasculartur e and the body surface). These different anatomical structures are extremely irregular and do not permit the efficient use of standard CAD/CAM descriptors commonly used to describe synthetic structures. Instead, the geometrical objects that comprise the geometrical model are described by sets of 2-D Magnetic Resonance Images (MRI) or Computed Tomography (CT) Images. The outlines of the different tissues must then be digitized (segmented) from the images.[2] The result is a set of contours (polylines or splines) connecting discrete points at the boundaries between organs and/or regions of different conductivity. The resulting point set is then used to construct a polygonal representation of the solution domain, i.e. a finite element mesh.

For the construction and simulation of anatomically correct models we utilized unstructured meshes of triangular or tetrahedral elements. Unstructured grids tend to capture the complex structures of human and animal anatomy more efficiently than structured grid. The meshes used for the research presented here ranged in size from thousands of elements for two-dimensional models to hundreds of thousands of elements for three-dimensional models.

The method we used to create meshes is based upon the Delaunay tessellation algorithm originally proposed by Watson [16] and later extended by Weatherhill [17]. The Delaunay criteria states that the circumsphere of any tetrahedron (triangle)[3] contains no other mesh points. The thrust of the Watson/Weatherhill algorithm is to efficiently insert a point into an existing grid (bounding simplex) in such a way that the Delaunay criterion is met. Certain tesselations are then deleted and new ones are subsequently created using the new point and a subset of the the old points. The general method is applicable to N-dimensions, although engineering applications usually require implementations in two or three dimensions.

A major component of efficient tessellation, and especially adaptive variants, is the use of appropriate data structures in the computer code. We utilized a data structure which contains all the information necessary to construct a tessellation satisfying the Delaunay constraint. This data structure is essentially a table containing the

[2]We note that the automatic segmentation of medical images is an ongoing research area. At this point in time, there does not exist a fully reliable automatic segmentation algorithm, thus we have developed semi-automatic algorithms which allow user intervention.

[3]In describing the algorithm, we use triangle or tetrahedron interchangeably.

four points (integers) of the tetrahedron, the four neighboring tetrahedra (integers), the origin of the sphere that circumscribes the tetrahedron (x,y,z), the radius of the circumscribing sphere (float), the origin of the inscribed sphere (x,y,z), and its associated radius (float). The inscribed sphere information is used during the point generation phase but is not required during the tessellation phase.

There are essentially six steps to the tessellation algorithm. The first step sets up the data structure describing an initial grid of tetrahedra. This grid is made up of eight convex hull points which form a bounding box around all of the points to be included in the mesh. The remaining steps determine how each new point is incorporated into the existing grid and how its addition effects the data structure. This is outlined in the following steps:

Delaunay Algorithm

Inputs:
n: number of points
DT: deleted tetrahedra
NT_DT: neighboring tetrahedra to deleted tetrahedra
T: newly created tetrahedra
N_T: neighboring tetrahedra to newly created tetrahedra

Define the convex hull and data structure
Begin
For Point$\leftarrow$ 1 to n Do
    Determine all tetrahedra to be deleted
        $\{DT_i\}$, i=1,dt
    For i$\leftarrow$ 1 to dt Do
        Determine neighboring tetrahedra $\{NT\_DT_j\}$, j=1,nt_dt
            to $\{DT_i\}$
    For j$\leftarrow$ 1 to nt_dt Do
        Connect Point to three points of $\{NT\_DT_j\}$
            to create $\{T_j\}$
    For j$\leftarrow$ 1 to nt_dt Do
        Find neighboring tetrahedra, $\{N\_T_k\}_j$, k = 1,4
            to $\{T_j\}$
    Expand and reorder the data structure with
        $\{T_j\}$ and $\{N\_T_k\}_j$
End

The efficiency of the above algorithm depends almost exclusively on the second step, which locates the tetrahedra that should be deleted. The searching begins at the end of the list and proceeds upwards until the first tetrahedron to be deleted is found. At this point, a tree search is conducted such that the deletion tetrahedron is the root of the tree and neighboring tetrahedra are leaves. The tree search stops when none of the leaves, i.e., neighboring tetrahedra, should be deleted. This step is the only one which performs a floating point computation, the calculation of the origin of the circumscribing sphere and the circumsphere radius. The remaining steps are independent of the number of points defining the mesh and are only local in nature. In addition, these steps are strictly logical with only integer comparisons to perform.

The mesh generation procedure consists of five steps as outlined in the following algorithm:

Mesh Generation Algorithm
Inputs: Boundary point representation (in contours)

Begin

- Triangulate Surfaces
- Construct Coarse Mesh - Delaunay Tessellation
- Determine Interior Tetrahedra
- Repeat:
  - Generate Interior Point
  - Tessellate Interior Point
- Until (point fails spacing and degree tests)
- Classify Regions

End

Starting with the boundary points extracted during the segmentation, one then proceeds to adequately represent the surface mesh (line segments in two-dimensions and triangles in three-dimensions). The next step is to construct a coarse mesh of tetrahedra from the boundary points and then to determine tetrahedra within the surface of interest. These interior tetrahedra are used in the fourth step, which iterates between the generation of a new point and subsequent tesselation until certain spacing criteria are satisfied.

The final step is to classify the tetrahedra by their material properties, e.g., which tetrahedra are considered to be in the heart, lungs, et cetera. Since the material properties of interest in bioelectric problems, electric conductivity, can be anisotropic, each tetrahedron must be assigned a tensor describing local conductivity. To classify a tetrahedron we had to localize the position of its centroid relative to the surfaces separating regions of different conductivity. To localize the element, we utilized a ray tracing approach [18] which projects a ray from the centroid of an element to a point at infinity and counts the instances the ray intersects with a triangulated surface. If the ray crosses through one triangulated surface an odd number of times, the point is considered to be interior to the surface; conversely, if it crosses the surface an even number of times, the tetrahedron is considered to be exterior to the surface.

Applications of Mesh Generation in Electrocardiology

In this next section we describe applications of automatic mesh generation to problems in cardiac electrophysiology.

Defibrillation

First we consider the problem of cardiac defibrillation. Of the million Americans who die each year of heart related causes, 470,000 are victims of sudden cardiac death caused presumably by ventricular fibrillation. Ventricular fibrillation is the final, potentially fatal stage in a cascade of cardiac arrhythmias, electrical conduction anomalies of the heart which often arise as a consequence of coronary heart disease and myocardial infarction. The most effective way to stop ventricular fibrillation once is has begun is to deliver a strong electrical shock to the heart, via the torso surface [19] (external) or the heart surface [20] (internal), i.e., to apply defibrillation [21].

Experimental studies using lab animals provide a controlled opportunity to study important parameters in defibrillation, e.g., electrode placement, shock strength, and shock duration, the results of which are often extrapolated to humans. Animal experiments also provide investigators with a means of assessing the accuracy of computational models, and basic assumptions about the mechanism underlying defibrillation. Recently, Deale and Lerman [22, 23] performed fundamental experimental studies, which concluded [22]

> *"...that for canine transthoracic defibrillation, 82% of the total delivered current is shunted between the electrodes by the thoracic cage, 14% is shunted by the lungs, and only 4% traverses the heart."*

Previous investigators [24, 25, 26] have predicted figures for the defibrillation current traversing the heart that are closer to 15%. Difference factors of 3–4 between models and conclusions based on experimental data suggest deficient models or misinterpretation of experimental data. The computer simulations were performed using canine anatomy with shock electrodes located geometrically similar to the experiment of Deale and Lerman [22]. They used a simple resistor model based on experimental measurements to calculate the data shown in the above figures. The difference between the simulations and experiments arise from using a 3-D model as opposed to a 1-D model.

One of the purposes of this research work was to estimate the accuracy of the experimental results for canine defibrillation and to assess different modeling assumptions. To replicate the experimental setup of Deale and Lerman [22], we constructed a computer model in which we paid special attention to the numerical accuracy of the simulations by implementing mesh refinement. Adaptive refinement was superior to uniform refinement in achieving reliable estimates of current densities on and near the electrodes. We obtained boundary points from MRI images and digitized photos of a dog torso anatomy. Using the method described above, we created both surface triangulations [27] and a tetrahedral volume mesh. The point spacing function, which controls spacing between points in the interior of the mesh, was initially set to match the spacing of the surface points.

Inverse ECG

As mentioned previously, the goal of the inverse problem in electrocardiography is to *image* the electric and potential fields due to bioelectric activity of the heart within the body using voltage measurements taken noninvasively on the body surface.

To study the direct and inverse problems in electrocardiography, we developed a series of two- and three-dimensional boundary element and finite element models based upon magnetic resonance images from a human subject [28, 29, 30]. Each of 116 MRI scans were segmented into contours defining torso, fat, muscle, lung, and heart regions. Additional node points were added to digitize each layer and were subsequently tessellated into tetrahedra using the Delaunay triangulation algorithm [28]. The resulting model of the human thorax contained approximately 675,000 volume elements, each with a corresponding conductivity tensor. Figure 1 illustrates the model construction process by showing a collage of the original MRI scan, a triangulated lung, and a portion of the tetrahedralization of the volume. An illustration of the two-dimensional model used for inverse simulation is shown in Figure 2 which represents the mesh for a two-dimensional finite element model, extracted from three-dimensional model of the human thorax shown in Figure 1.

Mathematical Methods

Mathematically, the problems of computational electrocardiology are governed by Poisson's equation for electrical conduction:

$$\nabla \cdot \sigma \nabla \Phi = -I_v \quad \text{in } \Omega \tag{1}$$

subject to the boundary conditions:

$$\Phi = \Phi_0 \text{ on } \Gamma_1 \text{ and } \sigma \nabla \Phi \cdot \mathbf{n} = 0 \text{ on } \Gamma_2 \tag{2}$$

where Φ and Φ_0 are electrostatic potentials, I_v are the primary cardiac current sources per unit volume, σ is the conductivity tensor, and Γ_1 and Γ_2 are surface boundaries which bound the solution domain, Ω. Once the electrostatic potentials are known, one can calculate the current density $\mathbf{J}$ according to:

$$\mathbf{J} = -\sigma \nabla \Phi. \tag{3}$$

The direct ECG problem is then characterized by solving (1) with Φ_0 equal to the voltages measured on the heart's surface, Γ_1 and the zero Neumann condition on the body surface, Γ_2. The general inverse ECG problem is stated as solving (1) for the primary cardiac currents, I_v according to the boundary conditions,

$$\Phi = \Phi_0 \text{ on } \Sigma \subset \Gamma_T \text{ and } \sigma \nabla \Phi \cdot \mathbf{n} = 0 \text{ on } \Gamma_T. \tag{4}$$

As noted previously, the solution to this problem in terms of cardiac source descriptions is not unique unless additional constraints are provided. A common approach is to solve a model problem in which the heart is broken up into N subdomains with the electrical activity of each subdomain represented by a variable dipole moment. One then seeks to determine the magnitude and direction of each of the dipoles as functions of time. Another approach to the inverse problem involves enclosing the heart with a bounding surface, and, instead of solving the Poisson equation in (1) for the primary cardiac currents, solving Laplace's equation for the potentials on the closed surface just outside the heart (according to the same boundary conditions as in (4)) [31]. The advantages of this formulation include that the solution to the resulting inverse problem is unique and that these solutions can be directly verified by measuring the potentials on the outer surface of the heart [32]. While the solution to this problem is unique, it is still ill-posed in the Hadamard sense that small errors in input data can cause large unbounded oscillatory errors in the solution data. One usually has to implement some kind of regularization scheme to attempt to restore the continuity of the solution back onto the data.

Finally, the defibrillation problem can be posed as solving Laplace's equation with boundary conditions similar to those in (2), replacing *a prior* knowledge of voltage on the heart boundary by that on the region of the torso under the defibrillation electrodes, that is, $\Phi = \Phi_0$ on $\Sigma \subset \Gamma_2$. Here, the sources are due to defibrillation pulses and the goal is to determine the resulting current density throughout the heart volume. Continuity conditions of the normal component of current density and potential hold at each of the conductivity interfaces.

The finite element method (FEM) was the preferred choice to approximate Laplace's equation since the material properties described by the conductivity, σ, have directional characteristics, i.e. are anisotropic. This anisotropic nature of the electrical conductivity inhibits the efficient use of the boundary element method. In addition, the unstructured meshes do not lend themselves to the use of finite differences or multigrid techniques for the solution method.

Briefly, the FEM is used to construct a potential ϕ^e in each element composed of a basis function. The approximate ϕ^e is then used to satisfy the governing equation in each element with some optimizing criteria. Tetrahedra were used as elements with linear basis functions as given by

$$\phi^e = \sum_{j=1}^{N} a_j u_j \tag{5}$$

The a_j's represent unknown coefficients to be solved for by some optimizing criteria for ϕ^e such that the governing equation is satisfied in some sense and u_j's represent the basis functions. A residual, R, exists due to the approximation of ϕ^e for the exact potential Φ, defined as

$$R = \nabla \cdot (\sigma \nabla \phi^e). \tag{6}$$

Applying the Galerkin method we have:

$$\int_{\Omega_e} \nabla \cdot (\sigma \nabla \phi^e) u_i d\Omega_e = 0.\ \mathrm{i} = 1,2,\ldots,\mathrm{N} \tag{7}$$

Green's theorem is applied to (7) giving rise to:

$$\int_{\Gamma_e} u_i (\sigma \nabla \phi^e) \cdot \mathbf{n} d\Gamma_e - \int_{\Omega_e} (\sigma \nabla \phi^e) \cdot \nabla u_i d\Omega_e = 0.\ \mathrm{i} = 1,2,\ldots,\mathrm{N} \tag{8}$$

The gradient of ϕ^e is given by

$$\nabla \phi^e = \sum_{j=1}^{N} a_j \nabla u_j. \tag{9}$$

(5) and (9) are substituted into (8) yielding,

$$\int_{\Omega_e} (\sum_{j=1}^{N} a_j \sigma \nabla u_j) \cdot \nabla u_i d\Omega_e = \int_{\Gamma_e} u_i (\sigma \nabla \phi^e) \cdot \mathbf{n} d\Gamma_e \ \mathrm{i} = 1,2,\ldots,\mathrm{N} \tag{10}$$

Rearranging (10) yields,

$$\sum_{j=1}^{N} a_j \int_{\Omega_e} (\sigma \nabla u_j) \cdot \nabla u_i d\Omega_e = \int_{\Gamma_e} u_i (\sigma \nabla \phi^e) \cdot \mathbf{n} d\Gamma_e \ \mathrm{i} = 1,2,\ldots,\mathrm{N} \tag{11}$$

thus yielding the familiar stiffness matrix and forcing vector,

$$K_{ij}^e = \int_{\Omega_e} (\sigma \nabla u_j) \cdot \nabla u_i d\Omega_e \ \mathrm{i} = 1,2,\ldots,\mathrm{N} \tag{12}$$

$$F_i^e = \int_{\Gamma_e} u_i (\sigma \nabla \phi^e) \cdot \mathbf{n} d\Gamma_e \ \mathrm{i} = 1,2,\ldots,\mathrm{N}. \tag{13}$$

Here, the stiffness matrix contains geometry and conductivity information while the forcing vector contains contributions from the Dirichlet boundary condition. For each element of the mesh, (12) and (13) are computed and are combined to form the global stiffness matrix and forcing vector. Summing the contributions from all the elements yields the linear system, $\mathbf{K\Phi} = \mathbf{f}$, in which we solve for the electrostatic potentials in the volume Ω. The linear system can, in principal, be solved by any number of standard methods. The very sparse nature, and often significant size of K, push the choice toward techniques that make use of spare matrix storage and iterative solutions.

For the direct ECG problem, this requires solving a linear system with a sparse, symmetric, positive definite matrix. The matrix ranges in size between approximately $N = 25,000 - 1,000,000$ depending on the level of mesh refinement. Due to the sparsity, we utilize a compressed-row storage method along with an iterative solver (SSORCG)[4] which recognizes the storage format and takes advantage of the symmetric structure of the matrix. Due to the quasi-static nature of the problem, we can distribute individual calculations for different time intervals over several workstations. For a single heartbeat, we perform approximately 500 system solves (for the voltages and current vectors), using the previous solution as the initial *guess* given to the solver (which, because of the continuity of time exhibited by the activation/recovery process in the heart, significantly reduces the number of iterations necessary for convergence).

For the defibrillation problems, the unknown voltages, Φ were solved using a preconditioned conjugate gradient iterative solver in SLAP (Sparse Linear Algebra Package) for matrices of size up to $N = 140,000$.

[4]Symmetric Successive Over Relaxation with a Conjugate Gradient preconditioner

Error Estimation

The essential feature of the FEM is that the approximate forms of the potential satisfies the governing equation in each element in some weighted sense. If we reduce the size of the elements, *h-refinement*, or increase the order of the basis function, *p-refinement*, the approximation improves [33]. While either approach can be applied globally, computational limits make it more efficient to apply refinement locally, to regions where it is deemed most beneficial. One way to monitor the overall effect of refinement is to compute the total energy, which must converge monotonically if refinement is progressing effectively. In the analysis of defibrillation, the large spatial gradients will occur on or near the electrodes. In anticipation of this, we can perform refinement within this region, potentially with either h- or p-type methods, or even a combination of the two.

We have implemented two different adaptive h-refinement techniques. One global method based on an estimate of the element energy error, derived from methods suggested by Lewis [34], and another method which utilizes the weak form of the approximation to estimate errors which are valid globally, but which can be applied locally. We briefly outline both of the methods below.

The error in the potential, e_Φ, is defined as the difference between the exact potential, Φ, and the calculated potential, $\hat{\Phi}$.

$$e_\Phi = \Phi - \hat{\Phi} \tag{14}$$

Similarly, the error in the gradient of the potential, q, is

$$e_q = q - \hat{q} \tag{15}$$

where $q = \nabla\Phi$ and $\hat{q} = \nabla\hat{\Phi}$. The error norm is defined as:

$$\|e_q\| = (\int_\Omega (\nabla\Phi - \nabla\hat{\Phi})^T \sigma (\nabla\Phi - \nabla\hat{\Phi}) d\Omega)^{\frac{1}{2}}. \tag{16}$$

Zienkiewicz [35, 36] has shown that

$$\int_\Omega (\nabla\Phi)^T \sigma (\nabla\hat{\Phi}) d\Omega = \int_\Omega (\nabla\hat{\Phi})^T \sigma (\nabla\Phi) d\Omega = \int_\Omega (\nabla\hat{\Phi})^T \sigma (\nabla\hat{\Phi}) d\Omega. \tag{17}$$

Using this result, (16) becomes

$$\|e_q\|^2 = \int_\Omega (\nabla\Phi)^T \sigma (\nabla\Phi) d\Omega - \int_\Omega (\nabla\hat{\Phi})^T \sigma (\nabla\hat{\Phi}) d\Omega \tag{18}$$

or equivalently,

$$\|e_q\|^2 = \|q\|^2 - \|\hat{q}\|^2 \tag{19}$$

Here, $\|q\|^2$ is a measure of the total energy in the domain. Using this, the percentage error, η, can be defined to be

$$\eta = \frac{\|e_q\|}{\|q\|} \cdot 100\% \tag{20}$$

This error measure gives a ratio of the energy difference and the total energy which is in effect a percentage error for each element.

The FEM we implemented used linear basis functions to describe the variation of the potential in each tetrahedral element. At every point in the mesh, the potential is uniquely specified. However, the gradient is not specified at every point in space but is defined to be constant over each element and discontinuous across element boundaries. Zienkiewicz showed that when the current densities arising from the gradients are globally smoothed, they provide a more accurate estimate of the energy than the energy using the constant current densities [35, 36]. Hence, (20) can be calculated using the energy due to the smoothed currents and the energy due to the constant currents. The smoothed current densities are now defined at the same nodal locations as the potentials and are continuous across element boundaries. The smoothing process used the Galerkin technique [34] and involved minimizing the difference between the two current densities,

$$\sigma(\nabla\tilde{\Phi} - \nabla\hat{\Phi}) \tag{21}$$

where $\nabla\tilde{\Phi}$ is the smoothed gradient representing the exact gradient and $\nabla\hat{\Phi}$ is the constant gradient from the FEM solution. This method produces a system of equations in the following form:

$$(\int_{\Omega_e} u_i u_j d\Omega_e)(\sigma\nabla\tilde{\Phi}_i) = (\int_{\Omega_e} \sigma\nabla\hat{\Phi}_i u_i d\Omega_e). \tag{22}$$

where u_i is a linear basis function defined at node i, $\nabla\tilde{\Phi}_i$ is the value of the smoothed gradient at that point, σ is the conductivity, and $\nabla\hat{\Phi}_i$ is the constant gradient resulting from the finite element solution. In equation (22), the current density, $\sigma\nabla\tilde{\Phi}_i$ is the unknown that is solved for at each node, i of the grid. Thus we calculate a new estimate, $\tilde{q}$, which can be used in place of the exact gradient, q. The current density now varies linearly in each tetrahedron and is continuous everywhere.

Once the energy error has been computed, the mesh refinement can begin. The error must be related to some parameter which guides the mesh refinement. We utilized a spacing function, h_e, which controls the size and number of elements [34]. This spacing function, h_e is defined to be the linear interpolation of the spacing values at the four nodes of the tetrahedron. A variable ξ is defined as the ratio of the element error to the average of the element errors:

$$\xi_e = \frac{||e_q||_e}{||\hat{e}_q||_e}. \tag{23}$$

If $\xi_e > 1$, then a new spacing function can be defined as

$$h^* = \frac{h}{\xi_e}. \tag{24}$$

Thus, the spacing values at each node of the element are reduced. This new spacing function will then increase the number of points in the regions of large errors. This whole process is repeated until the global error estimate falls below the specified level.

The algorithm does not depend on how the modification was made such that a different error estimate other than the one just described can be used by only modifying the spacing values in some fashion. This allows any number of error estimators to be used to guide the adaptive mesh refinement process.

In a similar manner, starting from the weak solution of (1) we can prove that $\Phi_h \in \Omega_h$, where Φ_h is the finite element solution and is the best approximation of the exact solution Φ in the sense that

$$\|\nabla\Phi - \nabla\Phi_h\| \leq \|\nabla\Phi - \nabla\tilde{\Phi}\| \quad \forall\, \tilde{\Phi} \in \Omega_h \tag{25}$$

where

$$\|\nabla\tilde{\Phi}\| = (\int_\Omega \nabla\tilde{\Phi}\cdot\nabla\tilde{\Phi})^{\frac{1}{2}}. \tag{26}$$

In particular, we can choose $\tilde{\Phi}$ to be the interpolant of Φ

$$\pi_h\Phi(N_i) = \Phi(N_i) \qquad i = 1,\ldots,M \qquad \pi_h\Phi \in \Omega_h. \tag{27}$$

With certain constraints on our elements, we can prove the following, well known relationships

$$\|\nabla\Phi - \nabla\pi_h\Phi\| \leq Ch \tag{28}$$

and

$$\|\Phi - \pi_h\Phi\| \leq Ch^2 \tag{29}$$

where C is a positive constant that depends on the size of the second partial derivative of Φ and the smallest angle formed by the sides of the elements in Ω_h. These estimates show that the error in both Φ and the gradient of Φ tend to zero as the discretization parameter, h, tends to zero. We can use these relationships to provide an adaptive algorithm for decreasing discretization error.

To make this a little more precise, we define the semi-norm:

$$|\tilde{\Phi}|_{H^r(\Omega)} = (\sum_{|\alpha|=r}\int_\Omega |D^\alpha\tilde{\Phi}|^2\,dx)^{\frac{1}{2}} \tag{30}$$

where

$$D^\alpha\tilde{\Phi} = \frac{\partial^{|\alpha|}\tilde{\Phi}}{\partial x_1^{\alpha_1}\partial x_2^{\alpha_2}} \qquad |\alpha| = \alpha_1 + \alpha_2 \tag{31}$$

are α-order partial derivatives and

$$H^K(\Omega) = \{\tilde{\Phi} \in L_2(\Omega):\ D^\alpha\tilde{\Phi} \in L_2(\Omega),\ |\alpha| \leq K\} \tag{32}$$

defines the Sobolev spaces. Given these definitions, we can then obtain the error estimates analogous to those in (28) and (29) for the finite element approximation [37, 38]:

$$|\Phi - \Phi_h|_{H^1(\Omega)} \leq |\Phi - \pi_h\Phi|_{H^1(\Omega)} \leq C[\sum_{K\in T_n}(h_k|\Phi|_{H^2(K)})^2]^{\frac{1}{2}} \tag{33}$$

or, in the $L_2(\Omega)$ norm,

$$\|\Phi - \Phi_h\|_{L_2(\Omega)} \leq \|\Phi - \pi_h\Phi\|_{L_2(\Omega)} \leq Ch^2|\Phi|_{H^2(\Omega)}. \tag{34}$$

For the potential gradients we have [39][5]:

$$\|\nabla\Phi - \nabla\Phi_h\|_{L_\infty(\Omega)} \le C\|\nabla\Phi - \nabla\pi_h\tilde{\Phi}\|_{L_\infty(\Omega)} \le C\max[h_K \max_{\alpha=2}\|D^\alpha\Phi\|_{L_\infty(\Omega)}]. \tag{35}$$

Given these previous error estimates for the finite element approximation, we can now use the estimates to decide where in our original finite element mesh the approximation is not accurate and create a recursive, adaptive algorithm to re-discretize in the appropriate areas. Suppose we want the accuracy of our finite element approximation to be within some given tolerance, δ, of the true solution, i.e.

$$|\Phi - \Phi_h|_{H^1(\Omega)} \ \le \ \delta. \tag{36}$$

Then, from the estimates above, we have, for example,

$$\sum_{K\in T_h}(h_k|\Phi|_{H^2(K)})^2 \ \approx \ \frac{\delta^2}{C^2}. \tag{37}$$

Thus, we redefine our mesh until,

$$\sum_{K\in T_h}(h_k|\Phi_h|_{H^2(K)})^2 \ \le \ \frac{\delta^2}{C^2}. \tag{38}$$

Here we can sum over all or part of the K elements in our tessellated geometry, T_h, and test to see if the error is less than our *normalized* tolerance. If the value of the error estimate exceeds the tolerance, then the element is 'flagged' for further refinement. One should note that the $H^2(\Omega)$ norm in (38) requires the second partial derivative of the finite element approximation. As stated previously, we have assumed a linear basis function for our fundamental element. Thus, we lack continuity of the second derivative and must approximate it using a centered difference (or other) formula based on first derivative information.

Of significant practical importance is choosing a reasonable tolerance, δ. Since the general location and bounds of the potential field are dictated by known physiological considerations, we can generate an initial mesh based upon simple field strength-distance arguments. One can estimate an upper bound of the potential (or electric) field by finding the field strength on a cylindrical (or circular) surface which encloses the actual geometry. This allows us to estimate the potential field and potential gradients which are used to produce the initial graded mesh. By this calculation, we are trying to assure that the errors far from the sources are minimal. We can then refine our finite element mesh by choosing the tolerance, δ, to be some fraction of the estimated error corresponding to the elements furthest from the sources. Thus we have used a minimax principle, minimizing the maximum error based upon initial (conservative) estimates of the potential field and potential gradients [40].

[5] We note that there a numerous possibilities for various norms and the ones given above should be seen as examples

Applications of Adaptive Methods in Electrocardiology

Defibrillation

We present two different model applications that use the adaptive techniques outlined earlier applied to defibrillation modeling. In defibrillation, it is important to know how the current is distributed in the thorax and what levels of current actually reach the heart. The flow of current is fundamentally affected by the inhomogeneities that are present in the thorax. Modeling defibrillation involves placing electrodes on a surface and applying *patches* of voltage in the form of Dirichlet boundary conditions. The first model application is the simulation of defibrillating electrodes placed on the surface of an isolated dog heart. The second simulation involves modeling external defibrillation on a dog thorax. In both cases, the energy norm described earlier was used to calculate the energy error which guided mesh refinement.

The isolated dog heart geometry was obtained from a group in New Zealand [41]. Two rectangular electrodes were placed on the surface of the isolated heart and a voltage difference was applied to simulate a typical defibrillation protocol. The conductivity of the heart was assumed to be homogeneous and isotropic throughout both the heart tissue and blood cavities. To demonstrate the effectiveness of mesh refinement, the total energy was examined during each iteration. The total energy for the adaptively refined mesh was compared to the total energy in a uniformly refined mesh. The adaptively refined mesh required fewer degrees of freedom than the uniformly refined mesh to achieve the same energy level.

The initial surface mesh of the isolated dog heart contained approximately 970 nodes and 6200 tetrahedra. After seven iterations of the refinement algorithm, the grid increased in size to 30,648 points and 195,823 tetrahedra. Shown below in Figures 3a–1d are (a) the initial surface mesh and (b-d), the refined meshes corresponding to the first, third, and fifth iterations of the refinement procedure. A plot of the total energy as a function of the number of degrees of freedom is illustrated in Figure 4.

Uniform refinement required twice as many degrees of freedom to achieve the same accuracy level as adaptive refinement. For example, 3,414 points were required in the uniformly refined mesh to achieve comparable accuracy as 1,700 points in the adaptively refined mesh.

In external defibrillation, much larger currents are injected into the torso to overcome the shunting effect of the inhomogeneities within the body. In particular, the skeletal muscle is a major obstacle to the flow of current into the heart region, at least in part because of its anisotropic nature [42]. To simulate this situation, we placed round electrodes on both sides of the torso surface of the dog thorax model [22, 23].

We constructed a base mesh with uniform spacing, then modified it using both uniform and adaptive refinement. To compare the two approaches, we monitored not the energies of uniform and adaptive mesh refinement, but other parameters that are more relevant to defibrillation, such as percentage of current shunted through the heart. While six different conductivity configurations were considered, to illustrate the utility of adaptive mesh refinement, only one case will be presented here. The skeletal muscle was assumed to be anisotropic using a cylindrical representation for

mesh	# of points	# of tetrahedra
small	26,068	165,592
medium	39,965	253,823
large	84,413	537,431

Table 1: Mesh statistics for the round electrode thorax model reflecting the number of tetrahedra and the number of points.

mesh	C_{IN}	C_B
small	33.094	14.929
medium	31.3504	14.1027
large	32.2083	13.6009

Table 2: Total current injected into system C_{IN} and the total current entering the body region, C_B using uniform refinement.

the fiber direction. The fibers were assumed to run in a circumferential direction with higher conductivities along the length of the fiber and lower conductivities normal to the fiber direction. The following conductivities in units of S/cm were used, $\sigma_{SK} = .0067\hat{h}_{theta} + .00043\hat{h}_r + .0067\hat{z}$, $\sigma_B = .00138$, $\sigma_L = .0005$, and $\sigma_H = .00232$ with subscripts SK, B, L, and H denoting skeletal muscle, body, lungs, and heart respectively [43]. We created three different uniformly refined meshes and from the smallest of these carried out adaptive refinement based on the error estimators described earlier. Table 1 gives the mesh statistics for the three uniformly refined meshes. Table 2 gives the total injected current and the current injected into the body region that is not shunted by the anisotropic skeletal muscle using uniform refinement. Table 3 contains similar results as Table 2 but is for adaptively refined meshes.

From the results of the external torso defibrillation example, we observed that C_{IN} and C_B showed no signs of convergence with the uniform refinement, while adaptive refinements improved with each iteration. Adaptive refinement clearly targets the large errors near electrode boundaries and yields grids which are both smaller, and hence more efficient, and more accurate. The computational effort in performing adaptive refinement based on energy error estimates yields a particularly attractive method for producing accurate and converging estimates of important defibrillation

# of points	C_{IN}	C_B
26,068	32.5056	14.9517
26,962	31.8607	14.8405
27,468	31.3137	14.7847
33,865	30.917	14.2227
39,868	31.6771	14.3627
48,979	30.931	14.4285
69,559	31.0604	14.33

Table 3: Input current shunted by the skeletal muscle region using adaptive remeshing

parameters close to sources.

Inverse ECG

For the initial studies on the effects of adaptive control of errors, we utilized a two-dimensional finite element model, extracted from our three-dimensional model of the human thorax. The two-dimensional model was constructed from a single transaxial magnetic resonance image located approximately 4 cm above the apex of the heart.

We simulated a simple bipolar source distribution on the surface of the heart model. Using the procedure described above, direct solutions were computed for different levels of mesh refinement and compared at the outer, torso boundary. Figure 2 shows the voltage at the outer boundary versus distance around the two-dimensional contour. The original mesh contained approximately 1500 elements while the final mesh, after five iterations of the adaptive algorithm, contained approximately 7000 elements. The maximum estimated error in the calculated potential was over 30% greater in the original mesh than in the final mesh and the maximum estimated error in the potential gradient was over 13% larger in the coarse mesh than in the refined mesh.

As noted above, h-adaption increases the number of degrees of freedom, and thus, the computational costs. Once again, one must balance accuracy against CPU time. However, since the relative error falls off rapidly with increasing degrees of freedom and then levels out after only a few iterations of the adaptive algorithm, it is not difficult to choose a reasonable balance.

For inverse ECG simulations we utilized heart voltages recorded during open chest surgery from a patient diagnosed with WPW syndrome (a potentially fatal arrhythmia) as the Dirichlet boundary condition for the direct problem. The tissue conductivities were assigned as fat = .045 S/m, fatpad = .045 S/m, lungs = .096 S/m, skeletal muscle (along the fiber) = .3 S/m, skeletal muscle (across the fiber) = .1 S/m, and an average thorax value = .24 S/m [43]. From forward solutions calculated using the adapted mesh we computed inverse solutions on the same mesh. The *L-curve* algorithm [44] was utilized to estimate the optimal *a priori* regularization parameter for Tikhonov regularization technique, which we used to compute the inverse solution matrix. Because the size of the two-dimensional finite element model was relatively small, the calculations stayed in the 256 MByte of dynamic memory on an IBM RISC-6000 model 580 (for the three-dimensional models a distributed iterative algorithm will be necessary). The inverse solutions were within 12.6% of those recorded originally, which compares favorably to previously reported values, which lay in the range of 20-40%, [45, 46, 47, 48], albeit for three-dimensional problems. An example of the current flow in the human thorax model is shown in Figure 5.

Conclusions

We have developed tools to automatically create and modify three-dimensional meshes for the complex geometries often associated with bioelectric field problems. Starting from surface contours derived from tomographic images, we can generate optimal (in the Delaunay sense), irregular surface (triangles) and volume (tetrahedra) descriptions, and attach to each element a tensor describing local tissue conductivity. In order to optimally balance modeling accuracy against computational cost, we have also devised, and tested, two different methods of adaptive mesh refinement, which are driven by error calculations specific to the finite element approach. In comparisons with experimental data, we have proven the utility of these methods in two relevant problems in cardiac electrophysiology. In one case, defibrillation in canine preparations was simulated in order to determine relative current density distributions within the heart and thorax. In another example, we estimate electric potentials on the heart surface from those on the body surface of a two-dimensional slice from a model of the human thorax. In both cases, adaptive mesh refinement produced large improvements in model accuracy, with only moderate increases in computational complexity.

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Figure Captions

Figure 1. A composite of the modeling process for the human thorax. An MRI scan is shown with a rendered image of the heart, a triangulated surface of the lung and a portion of the finite element mesh within the context of a cut away of the body surface.

Figure 2. A triangulated magnetic resonance image which forms the basis for finite element computations of the bioelectric fields within the thorax.

Figure 3a-d. A model of the isolated dog heart showing the initial surface mesh (a), and a cut-away view just below one of the electrodes (b)–(d) corresponding to the first, third and fifth iteration of the refinement process.

Figure 4. A plot of the total energy as a function of the number of points during adaptive refinement for the isolated dog heart. Energy is in Joules.

Figure 5. The electric current flow in the human thorax at one instance of time in the cardiac cycle.