Georg-Simon-Ohm-University of Applied Sciences Nuremberg

Report of the application project at the Faculty of AMP

Simulation of a medical therapy method with finite elements

Martin Michel

Keßlerplatz 12

DE-90489 Nuremberg

Advisor: Prof. Dr. rer. nat. Tim Kröger

Advisor: Prof. Dr. rer. nat. habil. Jörg Steinbach

Advisor: Prof. Dr. rer. nat. Thomas Lauterbach

Nuremberg, 01. January 1900

Contents

1. Introduction to radio frequency ablation

Lets talk about:

- Medical Treatment of Tumor

- Radio frequency ablation

- Why RFA Simulation is important

- Motivation / This project in General

2. Computer-aided simulation of radio frequency ablation

2.1. Discrete Numerical Simulation

- In real world physics models are often bounded by reality

- Geometrical boundary conditions are often vague

- In most cases there is no reasonable analytical approach to solve these problems

- Modern numerical approaches are very flexible in this regard

- Simulations done right can be easily modified and adapted to different models and boundaries

2.2. About Errors in simulations and numerical approaches

- see TUM dissertation

- There are different sources for errors following the simulation from the line from the real problem down to the discrete solution

- Idealization error: discrepancy between reality and the idealized reality and the idealized constitutive laws and boundary conditions -> Systems are often way more complex in reality, every patient is different

- Modeling errors: discrepancy between mathematical formulation and physical model -> e.g. using dimensionally reduced approaches, like linear dependencies or even constant parameters

- Discretization errors: discrepancy between the continous description and discrete discription of the model

- Solution errors: using iterative approximation methods and rounding errors

- It's basically a butterfly effect

- Optimizing one error source often conflicts with another one -> e.g. handling nonlinearity can cause fatal numerical errors (at least that's what Kroeger said ...)

2.3. The physics behind radio frequency ablation

- Generating electrical energy with a generator
- Generated heat is distributed on the tissue
- Temperature rises do to constant electrical energy input
- Interesting is: - Temperature distribution over time
- What else? TODO
- Electrical energy can be approximated by the potential of the electrodes on the probes

$$\varphi : TODO \tag{1}$$

$$ElectricalEnergy : TODO \tag{2}$$

- No energy is lost
- Electrical Energy becomes heat energy by Tissue resistance
- Heat Energy is distributed by heat equation

$$Heat equation : TODO \tag{3}$$

- Discretization of the equation in space and time domain
- Time can be modeled continuously or in discrete intervalls
- Discrete intervalls are is typically more practical in modeling but less efficient or exact
- Discrete intervalls can be refined if necessary

3. Mathematical aspects of discrete simulation

3.1. Theory of finite elements

3.1.1. Elliptical problems

- Elliptical problems in general
- build up system of PDE's to describe problem
- Using the cylindric domain, different domains

3.1.2. Parabolic problems

- Parabolic / time-dependent problems
- Ignoring time dependency first and calculate the resulting elliptical problem - Build system of equations for elliptical problem
- Describe the parabolic PDE as an ODE with matrices from elliptical PDE
- Solving the system of ODE equations over discrete time intervalls
- Runge-Kutta
- For this simulation, backward euler / implicit euler formula does the job

3.1.3. FEM in Electrostatics

- General info
- special domain
- boundary conditions

3.1.4. FEM in Temperature Fields / perhaps Fluid Dynamics

- General info
- boundary condition (heat source or sink)
- In this simulation, heat source is from electrical energy

3.2. Numerical solution of system of ODE's

3.3. Axial symmetrie

- Using axial symmetrie to simplify computations
- reducing one dimension 3D -> 2D
- problems are aquivalent
- significant savings calculations time and complexity
- approach: fourier decomposition in angular direction to reduce dependency on the angular φ
- using static models, only dependency on space
- maybe Torus elements
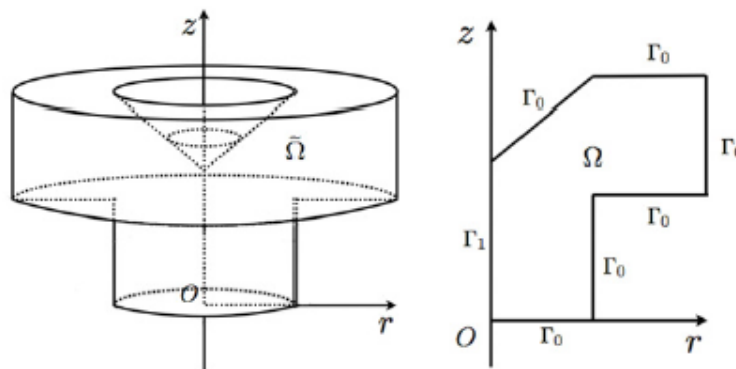
A three-dimensional axisymmetric domain $\bar{\Omega}$ (left); the corresponding two-dimensional half section Ω (right).

Figure 1: Schematic projection on 2D half section

4. Discretization of PDEs

4.1. Computational Domain

- Using one needle, whole geometry domain is axis symmetric around one needle
- Problem can be reduced to 2D problem using ring elements and cylindric coordinates
- Eliminate dependency on angular ϕ from the calculations
- For visualisation, symmetric results can be reconstructed to 3D
- Whole calculation will be in cylindric coordinates

4.2. FEM in cylindric Coordinates

- Rewrite the equations to cylindric coordinates
- Calculations are made on a cross-section with angular phi = 0
- Define boundaries -> new artificial boundary around the rotation axis to be taken into consideration
- Explain how the new boundary can be treated

Laplace in cartesian coordinates:

$$\nabla^2 := \Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{4}$$

Laplace in cylindric coordinates:

$$\Delta := \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \tag{5}$$

TODO : Write something

Laplace in polar coordinates:

$$\Delta := \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \tag{6}$$

4.3. PDE for Electric potential

4.3.1. Weak formulation of the problem

4 areas can be distinguished from a mathematical point of view
- Inner domain
- Fixed Potential of electrodes
- Outer boundaries with no fixed potential -> Robin
- Rotation axis, artificial boundary -> Neumann

Constant material parameters:

4.3.2. Inner Domain

- The electric potential of the inner domain is described as :

$$-\nabla \cdot (\sigma(x,y,z,t)\nabla\varphi(x,y,z,t)) = 0 \tag{7}$$

- Elliptical boundary problem
- Assuming constant material parameters: $\nabla\sigma = 0$
- Solution is independent from σ so we can cut it out - Equation becomes Laplaces' equation, phi becomes time independent

$$-\Delta\varphi(x,y,z) = 0 \tag{8}$$

- Using a cylindric domain, we can use cylinder coordinates (see ref Laplace in cylinder)

$$-\Delta\varphi(r,\phi,z) = -\frac{1}{r}\frac{\partial\varphi}{\partial r} - \frac{\partial^2\varphi}{\partial r^2} - \frac{1}{r^2}\frac{\partial^2\varphi}{\partial\phi^2} - \frac{\partial^2\varphi}{\partial z^2} = 0 \tag{9}$$

- Since the domain has axis symmetry, the solution for φ is independent from the angular ϕ
- So equation simplifies to

$$-\Delta\varphi(r,z) = -\frac{1}{r}\frac{\partial\varphi}{\partial r} - \frac{\partial^2\varphi}{\partial r^2} - \frac{\partial^2\varphi}{\partial z^2} = 0 \tag{10}$$

4.3.3. Electrodes

- Potential difference on the electrodes is fixed by definition
- For calculations, potential will be defined as ± 1

$$\varphi = \pm 1 \tag{11}$$

4.3.4. Outer boundary

- one approach is a simplification with natural boundary conditions

$$n \cdot \nabla \varphi = 0 \tag{12}$$

- In cylindrical coordinates

$$TODO \tag{13}$$

- In actual RFA treatment, there is a mass to nullify the potential in the outer region
- For the lower boundary, this behaviour can be easily modeled with dirichlet conditions

$$\varphi = 0 \tag{14}$$

4.3.5. Rotation axis

- this is an artificial boundary
- To keep the axis symmetry, here must apply natural neumann bundary conditions
- Othe conditions would break the symmetrie
-

$$n \cdot \nabla \varphi = 0 \tag{15}$$

- Use input from article

4.4. Calculation of electrical energy

- φ can be calculated on every discrete point
- Calculate power for every point
- Tissue Resistance
- Effective power
- Calculate electric energy from electric power

4.5. PDE for temperature Distribution

4.5.1. Weak formulation

From physics above, the temperature distribution is modeled by the heat equation:

$$\partial_t(\rho c T) - \nabla \cdot (\lambda \nabla T) = Q \tag{16}$$

The heat equation is a well known parabolic partial differential equation.

We are assuming ρ and c are constant

ρ = density

c = specific heat capacity

λ = thermal conductivity, which is depending on T

T = T(r,z,t) = temperature

Q = Q(r,z,t) = heat energy

Cylindrical coordinates: see 'Transient Heat Transfer in a Partially Cooled Cylindrical Rod' from Lawrence Agbezuge

$$\rho c \frac{\partial T}{\partial t} - \frac{d\lambda}{dT}\left[\left(\frac{\partial T}{\partial r}\right)^2 + \left(\frac{\partial T}{\partial z}\right)^2\right] - \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) = Q \tag{17}$$

For the first run, we assume *lambda* is also constant too, which greatly reduces the complexity of the problem to the form

$$\rho c \frac{\partial T}{\partial t} - \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) = Q \tag{18}$$

TODO: explain Q her

$$Q_{total} = Q_{rf} + Q_{perf} \tag{19}$$

- Q_{rf} is described above
- Q_{perf} is blood perfusion

- TODO: Maybe explain this in the physics above???

5. Applied FEM technologies

5.1. Weak solutions

5.1.1. Electric potential

Electric potential / Laplace's equation in cylindrical domain:

$$a_w(u,v) := \int_\Omega (\partial_r u \partial_r v + \partial_z u \partial_z v) r \, dr \, dz = \int_\Omega f v r \, dr \, dz \tag{20}$$

- $u \in H_r^1(\Omega) \cap \{v|_{\Gamma_0} = 0\}$
- $v \in H_r^1(\Omega) \cap \{v|_{\Gamma_0} = 0\}$

Approximate with linear regression functions
Linear regression functions for reference triangles:

$$\phi_1(\xi, \eta) = 1 - \xi - \eta \tag{21}$$

$$\phi_2(\xi, \eta) = \xi \tag{22}$$

$$\phi_2(\xi, \eta) = \eta \tag{23}$$

Specific PDE for electric potential, inner domain:

$$a_w(u,v) := \int_\Omega (\partial_r u \partial_r v + \partial_z u \partial_z v) r \, dr \, dz = 0 \tag{24}$$

5.1.2. Temperature Distribution

This is basically the problem above but as a hyperbolic problem
Using semidiscrete solution and iterate solution over time
We are applying method of the discontinuous galerkein fem

For reference see Jung, Langer : Methode der finiten Elemente für Ingenieure, chapter 7.1

Weak formulation for the problem:

We are looking for $u(r,z,t) \in V_{g1}$ with $\dot{u} \in L_2(\Omega)$ for almost every $t \in (0,T)$, so

$$(\dot{u},v)_0 + a(t;u,v) = \langle F(t),v \rangle \; for \; all \; v \in V_0 \tag{25}$$

and for amost every $t \in (0,T)$ is the "Anfangsbedingung -> suche englische Formulierung"

$$(u(r,z,0),v)_0 = (u_0,v)_0 \; for \; all \; v \in V_0 \tag{26}$$

The formal model above is given by

$$
\begin{aligned}
(\dot{u},v)_0 &= \int_\Omega \dot{u}(r,z,t)v(r,z)drdz = \int_\Omega \frac{\partial u(r,z,t)}{\partial t}v(r,z)drdz, \\
a(t;u,v) &= \int_\Omega \left[\lambda_1(r,z,t)\frac{\partial u}{\partial r}\frac{\partial v}{\partial r} + \lambda_2(r,z,t)\frac{\partial u}{\partial z}\frac{\partial v}{\partial z} \right] \cdot r \cdot drdz + \int_{\Gamma_3} \alpha(r,z,t)u(r,z,t)v(r,z)ds, \\
\langle F(t),v \rangle &= \int_\Omega f(r,z,t)v(r,z)drdz + \int_{\Gamma_2} g_2(r,z,t)v(r,z)ds + \int_{\Gamma_3} \alpha(r,z,t)u_A(r,z,t)v(r,z)ds, \\
V_{g_1} &= TODO, \\
V_0 &= TODO
\end{aligned}
$$

Adapted for the temperature distribution, assuming λ and all material parameters are constant:

$$a_w(t;u,v) := \int_\Omega \rho c(\partial_t u \cdot v)drdz + \int_\Omega \lambda(\partial_r u \partial_r v + \partial_z u \partial_z v)rdrdz = \int_\Omega fvrdrdz \tag{27}$$

5.2. Discretization / Triangulation

- Grid generation and refinement
- 2D domain
- initial coarse grid trinagulation can be done by hand
- coarse grid can be refined by algorithm

- refinement of triangle into 4 new pieces
- insert picture here

5.3. Assembling system of equation

- assemble elementwise
- use symmetrie of elements if koefficients are constant or allow it
- Add boundary conditions afterwards
- grouping of similar calculations allow more vectorized operations

5.4. Solving the system of equations

5.5. Error estimations

5.5.1. Element Error on 2D geometry

- H1-Norm
- L2-Norm

- The analytical solution of the problem is unknown, but we can estimate it by calculating different element sizes on different fine grids

Idea: Define geometric some geometric coordinates on triangle and look for best matching or choose some points on different geometrical entities

Refine triangles around that point and see whether the error is smaller on the finer grid

5.5.2. Time step error on discrete intervalls

See Skript Numerik 2 Kroeger, after some take make a smaller or larger time step and compare the difference of results, use the smaller steps for calculation

6. Other numerical aspects

6.1. Numerical integration

- quadrature on discrete points

6.2. Numerical gradient on discrete points

- "Testfunction nähern Ersatzlösung an "
- gradient is constant on every triangle
- however, gradient is needed on discrete points

6.3. Surface integral

- sum of integral of every single triangle

6.4. Grid refinement

- refine triangle uniformly into 4 new ones

7. Applied simulation

7.1. Generating TestData / Get reference data

- Material parameters see Stein TODO
- Using specification data from electrical generator

7.2. Solving the PDEs

7.3. Combine everything to continous time dependent simulation

7.4. Interpretation of result numbers

- Interprete numbers
- Compare with data from experiment or other simulations
- TODO compare with other simulations

8. Programming technologies

8.1. Performance Optimization

8.2. MatLab vs C++

- Could have done the whole simulation using only MATLAB
- MATLAB is a scripting language that calls Fortran Subroutines, which are highly efficient in calculating problems of linear algebra
- However, MATLAB has to call these subroutines in an efficient way to take these performance advantages
- It is extremely easy to write bad and inperformant code in MATLAB, if it is used in the wrong way
- Efficient implementation required hardcoding routines and is very stiff
- To me it was important to write flexible code, that can be easily adapted and extended to try out different modification
- This is way easier when using loops and subroutines instead of hard coded implementations, also the code because way more easier to read and fix
- So I was going for a combined implementation of MatLab and C++
- When using flexible code design, C++ allows performance advantages in using loops etc over MATLAB
- However, MATLAB allows easy function hadnling, what makes the algorithms more accessible for the reader
- In the end I combined the advantages of both languages

- MatLab serves as frame for the pre- and postprocessing, like grid generation and graphical output of the numerical results.
- Also the scripts serve as a mathematical documentation of the whole simulation for the reader
- Computation intense subroutines are done in C++

8.3. Graphical output

9. Summary and Outlook

9.1. Project Summary

- One could argue that writing a simulation from scratch is a waste of time
- There are many highly useful numerical software solutions for numerical simulation and numerical problems
- Usually there is no need to write an own detailed implementation
- Creating own scripts and implementations helps to understand numerical problems and error sources
- This approach helps enormously to increase the ability to use these software products effectively and to generate better simulations and is mandatory to improve
- There can also be no software developer without understanding how a computer works numbers

9.1.1. strengths and flaws

- why is it good, why is it bad - good: numerical results do match the general expectation
- bad: model is to simplified to represent real world conditions

9.1.2. future modifications

- Material parameters are dependent on Temperature and potential ->
- Using variable instead of fixed material parameters
- Take the evaporation of water into account
- Different types of perfusion

- Defining more realistic and complex boundary conditions
- Perhaps a second needle in a 3D simulation

9.2. State of the current Research

- Research in the simulation of medical therapy methods
-

9.3. Other FEM projects and software

- FENICS
- COMSOL
- ANSYS

References

[1] Tim Kröger et. al. *Numerical Simulation of Radio Frequency Ablation with State Dependent Material Parameters in Three Space Dimensions*. Springer, 2006.

[2] Hiroki Watanabe et. al. *Temperature Dependence of Thermal Conductivity of Liver Based on Various Experiments and a Numerical Simulation for RF Ablation*. IEEE EMBS 2010 : 32nd Annual International Conference of the IEEE Engineering in Medicine and Biology Society, 2010.

[3] Thomas Stein. *Untersuchungen zur Dosimetrie der hochfrequenzstrominduzierten interstitiellen Thermotherapie in bipolarer Technik*. Institut für Med./Techn. Physik und Lasermedizin der Freien Universität Berlin, 1999.

[4] Klaus Knothe u. Heribert Wessels. *Finite Elemente, Eine Einführung für Ingenieure, 5. Auflage*. Springer Vieweg, 2017.

[5] Michael Jung u. Ulrich Langer. *Methode der finiten Elemente für Ingenieure, Eine Einführung in die numerischen Grundlagen und Computersimulation, 2. Auflage*. Springer Vieweg, 2013.

[6] Aklilu T. G. Giorges. *Finite Element and Finite Difference Methods for Elliptic and Parabolic Differential Equations*. InTech, 2016.

[7] John Loustau. *Numerical Differential Equations, Theory and Technique, ODE Methods, Finite Differences, Finite Elements and Collocation*. World Scientific, 2016.

[8] Arndt Bode et. al. *Partielle Differentialgleichungen, Numerik und Anwendungen, Konferenzen Band 18*. Forschungszentrum Jülich GmbH, 1996.

[9] Claus-Dieter Munz. *Numerische Behandlung gewöhnlicher und partieller Differenzialgleichungen, Ein anwendungsorientiertes Lehrbuch für Ingenieure, 4. Auflage*. Springer Vieweg, 2019.

[10] Hengguang Li. *Finite element analysis for the axisymmetric Laplace operator on polygonal domains, Journal of Computational and Applied Mathematics*. Elsevier, 2011.

[11] *Transient Heat Transfer in a Partially Cooled Cylindrical Rod, Transactions of the ASME Vol. 131*. ASME Digital Collection, 2009.

[12] Christian G. Sorger. *Generierung von Netzen für Finite Elemente hoher Ordnung in zwei und drei Raumdimensionen*. Technische Universität München, Lehrstuhl für Computation in Engineering, 2012.

[13] Wolf Dieter Pietruszka. *MATLAB und Simulink in der Ingenieurpraxis, Modellbildung, Berechnung und Simulation, 4. Auflage*. Springer Vieweg, 2014.

[14]   Jichun Li. *Computational Partial Differential Equations Using MATLAB*. CRC Press, 2009.

[15]   P.I. Kattan. *MATLAB Guide to Finite Elements, An Interactive Approach*. Springer, 2003.

[16]   Norbert Heiderich. *Technische Probleme lösen mit C/C++, Von der Analysis bis zur Dokumentation, 4. Auflage*. Hanser, 2020.

[17]   Michael McLaughlin. *C++ Succinctly*. Syncfusion Inc., 2012.

[18]   Stefan Kuhlins. *Die C++ Standardbibliothek, Einführung und Nachschlagewerk, 4. Auflage*. Springer, 2005.

[19]   Physicists like to think that all you have to do is say 'These are the conditions now what happens next?'. *Richard Feynman*. The Character of Physical Law, 1965.

[20]   Not only is the Universe stranger than we think it is stranger than we can think. *Werner Heisenberg*. Across the Frontiers, 1972.

A. Source code Visual C++

Listing 1: For loop to print numbers from 1 to 10

```
1  // Print numbers from 1 to 10
2  #include <stdio.h>
3  int main() {
4    int i;
5    for (i = 1; i < 11; ++i)
6    {
7      printf("%d ", i);
8    }
9    return 0;
10 }
```

B. Source code MatLab

TODO