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Report of the application project at the Faculty of AMP

Simulation of a medical therapy method with finite elements

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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

- TODO

- Study approach to study finite elements and behaviour of convergence
- FEM simulation for RFA in 2D space domain with discrete time solutions
- The modeled problem is a 3D problem
- By modeling one needle there, is a axis symmetrie in the domain
- 3D axis symmetric cylindrical domain can be described with 2D torus elements

2. Computer-aided simulation of radio frequency ablation

2.1. Discrete Numerical Simulation

- Physical relationships can be described by physical laws which are described by mathematical relationships
- Usually highly complex systems that are described by ODEs, PDEs and statistics
- Phxsic can be approximated by simplified models
- In real world physics these models are usually bounded by reality
- In most physic fields excluding quantum mechanics and modern theoretical physics, "grobe" models are determinated, definite mathematical solutions can be found
- Since the physics is determinated, simulations can be done instead of experiment and measurement
- In practise, geometrical dimensions of points of interest are often usually vague
- In many cases there is no reasonable analytical approach to solve these problems, especially in the field of engineering

- Modern numerical approaches are very flexible in this regard
- "Statt glatter analytischer lösung gibt es ein beliebig genaue Näherung"
- Simulations done right can be easily modified and adapted to different models and boundaries
- These models are usually discribed by PDEs
- TODO: most frequently used methods

- Finite difference method
- Finite element method
- Find more
- In this approach we will model radio frequency ablations with simple finite element techniques

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

- Needles stuck in tissue have electrodes with generate a potential
- Generating electrical energy by power of an extern generator
- Energy does not get lost
- Heats the tissue, temperature rises do to continuing energy input
- Generated heat is distributed on the tissue,

- Thus additionaly there is a cooling effect by the perfusion of blood
- Heated tissue can kill harmful cells
- The whole process is regulated from outside

- Interesting for our simuation is:
- Temperature distribution over time
- What else? TODO

- For the simulation, we will use a RFA model as described following kroeger
- For simplicity, material parameters are seen constant
- In real world, material parameters are highly dependant on body conditions, temperature and vary heavily with different patients
- For some "Untersuchungen hierzu" , see Stein

- Electrical energy depends on the electrical power
- Power is defined by potential of the domain

$$-\nabla \cdot (\sigma(x,y,z,t)\nabla\varphi(x,y,z,t)) = 0 \tag{1}$$

Power applied by the probe:

$$p(x,y,z,t) = \sigma(x,y,z,t) \cdot |\Delta\varphi(x,y,z,t)|^2 \tag{2}$$

Due to tissue resistance, the effective power of the generater is obtained by a scaling. Thus can be modeled as follwing

$$Q_{rf} = p(x,y,z,t) \cdot \frac{p_{eff}(t)}{p_{total}(t)} \tag{3}$$

$$p_{total}(t) = \int_\Omega p(x,y,z,t)dx \tag{4}$$

$$p_{eff}(t) = \frac{4 \cdot p_{setup} \cdot R_{tis}(t) \cdot R_I}{(R_{tis}(t) + R_I)^2} \tag{5}$$

$$R_{tis}(t) = \frac{U^2}{p_{total}(t)} \tag{6}$$

- TODO : explain parameters

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

$$\partial_t(\rho c T) - \nabla \cdot (\lambda \nabla T) = Q \tag{7}$$

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

- Additionaly to temperature destribution, there is the cooling effect of perfusion

$$Q_{total} = Q_{rf} + Q_{perf} \tag{8}$$

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

$$Q_{perf}(x,y,z,t) = ??v?? \cdot \rho_{blood} c_{vlood} \cdot (T_{body} - T(x,y,z,t)) \tag{9}$$

- Discretization of the equation in space and time domain
- Time dependecy 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

- As described above, the whole simulation will be done on a 2D half section representing the 3D axis symmetric geometry

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

- Ritz-Galerkin-Verfahren, for Details see ref book TODO
- This documentation will be focused on the 3D -> 2D aspect

- Using the cylindric domain, different domains, will be described later

3.1.2. Assembling system of equations

- Systems of equations by finite number of elements calculated with shape function
- solution is approximation of real solution

$$Matrix \tag{10}$$

3.1.3. Boundary conditions

- Dirichlet with trick, define value to be solution of variable
- TODO

- Neumann boundary with curve integral

$$f = f_{vol} + f_{surf} \tag{11}$$

$$b = \int_{\Gamma_2} g \cdot \phi_i dS \tag{12}$$

- Note : In 2D dimension the surface integral is around the boundary line
- For natural boundary conditions $g(x) = 0$, the surface integral added is zero, which is a trivial solution

3.1.4. Parabolic problems

- Parabolic / time-dependent problems
- Usually involve an elliptic problem with additional time dependent factor

- Ignoring time dependency at 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

3.1.5. FEM in Electrostatics

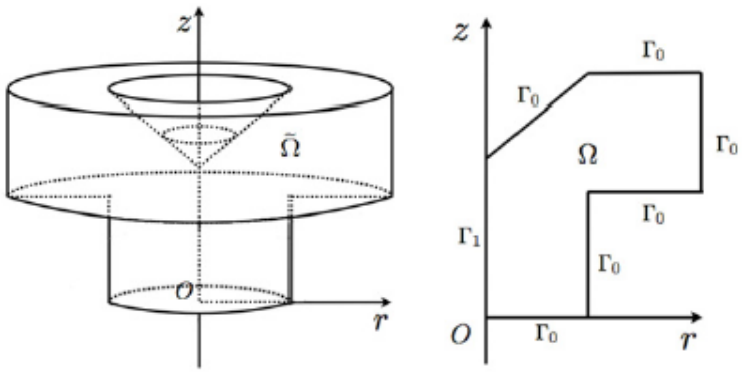
- General info
- special domain
- boundary conditions

3.1.6. 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. 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 $\tilde{\Omega}$ (left); the corresponding two-dimensional half section Ω (right).

Figure 1: Schematic projection on 2D half section

- TODO: write this more formal - Lax-Milgram-Lemma and Poincaré inequality on 3D-Domain determine a unique solution
- $u \in H_r^1(\Omega) \cap \{v|_{\Gamma_0}\}$ - Trace-operator
- rotation axis becomes an artificial boundary on 2D half section

- A more formal description can be found in :
- Use input from article TODO

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:

$$\nabla^2 := \Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{13}$$

Laplace in cylindric coordinates:

$$\Delta := \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \tag{14}$$

TODO : Write something

Laplace in polar coordinates:

$$\Delta := \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \tag{15}$$

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 :

$$-\nabla \cdot (\sigma(x,y,z,t)\nabla\varphi(x,y,z,t)) = 0 \tag{16}$$

- 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

$$-\Delta\varphi(x,y,z) = 0 \tag{17}$$

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

$$-\Delta\varphi(r,\phi,z) = -\frac{1}{r}\frac{\partial\varphi}{\partial r} - \frac{\partial^2\varphi}{\partial r^2} - \frac{1}{r^2}\frac{\partial^2\varphi}{\partial\phi^2} - \frac{\partial^2\varphi}{\partial z^2} = 0 \tag{18}$$

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

$$-\Delta\varphi(r,z) = -\frac{1}{r}\frac{\partial\varphi}{\partial r} - \frac{\partial^2\varphi}{\partial r^2} - \frac{\partial^2\varphi}{\partial z^2} = 0 \tag{19}$$

4.3.3. Electrodes

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

$$\varphi = \pm 1 \tag{20}$$

4.3.4. Outer boundary

- one approach is a simplification with natural boundary conditions

$$n \cdot \nabla\varphi = 0 \tag{21}$$

- In cylindrical coordinates

$$TODO \tag{22}$$

- 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

$$\varphi = 0 \tag{23}$$

4.3.5. Rotation axis

- this is an artificial boundary, as discribed above
- To keep the axis symmetry, here must apply natural neumann bundary conditions
- Other conditions would break the trace operator
-

$$n \cdot \nabla\varphi = 0 \tag{24}$$

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:

$$\partial_t(\rho c T) - \nabla \cdot (\lambda \nabla T) = Q \tag{25}$$

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

$$\rho c \frac{\partial T}{\partial t} - \frac{d\lambda}{dT}\left[\left(\frac{\partial T}{\partial r}\right)^2 + \left(\frac{\partial T}{\partial z}\right)^2\right] - \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) = Q \tag{26}$$

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

$$\rho c \frac{\partial T}{\partial t} - \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) = Q \tag{27}$$

TODO: explain Q her

$$Q_{total} = Q_{rf} + Q_{perf} \tag{28}$$

- Q_{rf} is descripted 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:

$$a_w(u,v) := \int_\Omega (\partial_r u \partial_r v + \partial_z u \partial_z v) r dr dz = \int_\Omega f v r dr dz \tag{29}$$

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

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

$$\phi_1(\xi, \eta) = 1 - \xi - \eta \tag{30}$$
$$\phi_2(\xi, \eta) = \xi \tag{31}$$
$$\phi_2(\xi, \eta) = \eta \tag{32}$$

Specific PDE for electric potential, inner domain:

$$a_w(u, v) := \int_\Omega (\partial_r u \partial_r v + \partial_z u \partial_z v) r dr dz = 0 \tag{33}$$

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

$$(\dot{u}, v)_0 + a(t; u, v) = \langle F(t), v \rangle \; for\; all\; v \in V_0 \tag{34}$$

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

$$(u(r,z,0), v)_0 = (u_0, v)_0 \; for\; all\; v \in V_0 \tag{35}$$

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:

$$
a_w(t;u,v) := \int_\Omega \rho c(\partial_t u\cdot v)drdz + \int_\Omega \lambda(\partial_r u\partial_r v + \partial_z u\partial_z v)rdrdz = \int_\Omega fvrdrdz \tag{36}
$$

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. ODE for parabolic problems

5.5. Solving the system of equations

- direct solver would be preferred in general
- if numbers of element grows, this computations takes up lots of memory
- up from a certain point, high amount memory can't be efficiently handled with RAM anymore
- using additional memory is extremely costly in terms of calculation speed
- since matrix is sparse, iterative solver can be very fast
- iterative solver is preferred if elements grow in numbers
- TODO : when should you use iterative solver

5.6. Error estimations

5.6.1. 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 sized 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

5.6.2. 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 "
- in our case, gradient is constant on every triangle
- actually discrete gradient on vertices is interesting
- vertices as average value of surrounding triangles

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 TODO

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 accessable 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

- Data can be easily recreated
- Solution is axis symmetric, so values apply for every angle ϕ
- This gets 3D data in cylindrical coordinates
- Can be reevaluated into cartesian coordinates to be plotted
- Discrete points are linear interpolated

9. Summary and Outlook

9.1. Project Summary

- One could argue that writing a numerical 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
- However, 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
- Implementing the algorithms on own trains understanding of numerical problems
- Should be programmed by everyone working with finite elements at least once

9.1.1. strengths and flaws

- good: numerical results do match the general expectation
- "zuverlässige" convergency
- numerical solution matches "qualitativ" the expectations
- Implementation can be easily adopted to more complex approaches

- bad: model is way to simplified to represent real world conditions of RFA
- Even further modifications would not change the results heavily

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
- Basic algorithm can be adopted to 3D problems

9.2. State of the current Research

- Research in the simulation of medical therapy methods
- TODO

9.3. Other FEM projects and software

- There is a lot of good commercial FEM software out there
- Matlab PDE toolbox, libraries with efficient implementation of almost every aspect on solving PDEs
- COMSOL Multiphysics, a High-Power simulation program with model builder and GUI

- ANSYS, like COMSOL but a little weaker but more widely used

- Also, good open source software
- FENICS
- FREEFEM

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A. Source code Visual C++

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

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

B. Source code MatLab

TODO