Modeling Temperature Distributions in Cryosurgery

Abstract—**This study investigates the simulation of temperature distribution in biological tissues during cryosurgery using a nonlinear bioheat transfer model. To solve this model, three numerical methods are implemented: the Method of Lines (MOL), the Alternating Direction Implicit (ADI) method, and the Finite Volume Method (FVM). Additionally, a Physics-Informed Neural Network (PINN) is developed to approximate the solution by embedding the PDE into the training loss.The study compares these approaches in terms of accuracy and computational performance, highlighting their applicability in biomedical thermal analysis.**

I. Introduction

Cryosurgery is a widely used minimally invasive technique that treats abnormal tissues by exposing them to extremely low temperatures, typically through a cryoprobe cooled by liquid nitrogen or argon gas. The success of the procedure depends on accurately predicting the thermal distribution within the biological tissue to ensure complete destruction of the target area while preserving nearby healthy structures. Therefore, mathematical modeling and numerical simulation of the heat transfer process are critical for improving treatment planning and clinical outcomes.

The temperature distribution in cryosurgery is governed by partial differential equations (PDEs) that describe bioheat transfer in living tissues, incorporating terms for heat conduction, metabolic heat generation, and temperature-dependent material properties. In this study, a two-dimensional cylindrical PDE model is used to represent the cryosurgical process. Numerical solution methods—specifically the Method of Lines (MOL), the finite volume method (FVM) and the alternating direction implicit (ADI) scheme—are applied to solve the PDE. In addition, a machine learning approach using physics-informed neural networks (PINNs) is introduced to explore data-driven approximations to the PDE solution. By comparing these techniques in terms of accuracy and computational efficiency, this work aims to evaluate their potential for improving cryosurgical simulation and planning.

II. Literature Review

Recent research has focused on advancing numerical methods and exploring machine learning techniques to solve these PDEs, aiming to enhance accuracy, computational efficiency, and clinical applicability.

A. Numerical Methods

- **Krishna et al. (2023)** [1]: Developed a 3D thermo-mechanical model using COMSOL Multiphysics, incorporating temperature-dependent properties and phase changes. Findings showed increased heat transfer with larger probe diameters, stabilizing after 50 minutes, but computational cost limits real-time use.
- **Zhang et al. (2022)** [2]: Investigated temperature fields in a 2D multi-probe cryosurgery model using FVM, optimizing probe configurations but requiring fine meshes for accuracy.

B. Machine Learning Approaches

- **Sharma et al. (2023)** [3]: Developed a digital-twin model using machine learning to optimize cryoprobe parameters, achieving precise temperature control but facing challenges with transient dynamics.
- **Yang et al. (2021)** [4]: Applied physics-informed neural networks (PINNs) to steady-state bioheat transfer, demonstrating accuracy but limited by convergence issues for nonlinear PDEs.

C. Research Gaps

- **Multiscale and Vascular Effects**: Modeling vascular heat sinks and multiscale transport, especially in nano-cryosurgery, remains computationally intensive, often leading to simplified models [5].
- **Phase-Change Modeling**: Capturing latent heat and sharp phase boundaries requires complex, computationally expensive formulations [2].
- **Machine Learning Integration**: PINNs struggle with nonlinearities and steep gradients near cryoprobes [4].
- **Nano-Thermal Modifiers**: Nano-cryosurgery models face conceptual and computational challenges due to limited experimental data [5].

III. Explanation of the PDE model

A. Governing Equation

In cylindrical coordinates (r, z), the bioheat PDE for temperature $T(r, z, t)$ is:

$$C(T)\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + Q_m(T) \tag{1}$$

where $C(T)$, $k(T)$, and $Q_m(T)$ are temperature-dependent specific heat, thermal conductivity, and metabolic heat generation.

B. Conditions

1) Initial Condition: At $t = 0$:

$$T(r, z, 0) = 37^\circ\mathrm{C} \tag{2}$$

2) Boundary Conditions:

- At $r = 0$, $r = r_c$: $\frac{\partial T}{\partial r} = 0$
- At $z = 0$: $T = 37°\text{C}$
- At $z = z_c$: $\frac{\partial T}{\partial z} = 0$
- At cryoprobe ($r = 0$, $z = z_p$): $T = -196°\text{C}$

C. Tissue Properties

1) Specific Heat:

$$C(T) = \begin{cases} C_f, & T < T_{ml} \\ \frac{Q_l}{T_{mu}-T_{ml}} + \frac{C_f+C_u}{2}, & T_{ml} \le T \le T_{mu} \\ C_u, & T > T_{mu} \end{cases} \quad (3)$$

2) Thermal Conductivity:

$$k(T) = \begin{cases} k_f, & T < T_{ml} \\ \frac{k_f+k_u}{2}, & T_{ml} \le T \le T_{mu} \\ k_u, & T > T_{mu} \end{cases} \quad (4)$$

3) Metabolic Heat:

$$Q_m(T) = \begin{cases} 0, & T < T_{mu} \\ Q_{mu}, & T > T_{mu} \end{cases} \quad (5)$$

IV. Numerical Solutions

A. ***Method of Lines (MOL)***

The Method of Lines (MOL) is a numerical technique for solving partial differential equations (PDEs) by discretizing spatial derivatives while treating time as a continuous variable, converting the PDE into a system of ordinary differential equations (ODEs) [6]. In cryosurgery, MOL is applied to the bioheat PDE modeling temperature $T(r, z, t)$ in cylindrical coordinates:

$$C(T)\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + Q_m(T), \quad (6)$$

where $C(T)$, $k(T)$, and $Q_m(T)$ represent temperature-dependent heat capacity, thermal conductivity, and metabolic heat generation, respectively. Spatial derivatives are approximated using finite differences, transforming the PDE into ODEs at each grid point. For example, the radial term is discretized as:

$$\frac{1}{r_i}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) \approx \frac{1}{r_i \Delta r}\Bigg[r_{i+1/2}k(T_{i+1/2})\frac{T_{i+1} - T_i}{\Delta r} - r_{i-1/2}k(T_{i-1/2})\frac{T_i - T_{i-1}}{\Delta r}\Bigg]. \quad (7)$$

The resulting ODE system is solved using stiff solvers, such as `lsodes` in R, handling nonlinearities in $C(T)$, $k(T)$, and $Q_m(T)$. MOL addresses the cylindrical singularity at $r = 0$ via l'Hôpital's rule and enforces boundary conditions, e.g., Dirichlet ($T = -196°\text{C}$ at the probe tip) and Neumann ($\partial T/\partial r = 0$). MOL offers flexibility for nonlinear PDEs but requires grid refinement near steep gradients, such as those near the cryoprobe.

B. ***The alternating-direction implicit (ADI)***

The Alternating-Direction Implicit (ADI) method is a powerful numerical technique used to efficiently solve multidimensional PDEs. For a 2D problem in cylindrical coordinates (axisymmetric), the ADI method splits each full time step Δt into two fractional steps : first half-step and second half-step, each of size $\Delta t/2$. This directional splitting simplifies the 2D problem into a sequence of 1D problems, each of which leads to a tridiagonal system that can be solved efficiently. The following subsections detail the formulation of each ADI step and the construction and solution of the resulting tridiagonal systems.

1) First Half-Step : Implicit in r, Explicit in z: The discretized equation at grid point (i, j) from t_n to $t_{n+1/2}$

$$C_p(T^n_{i,j})\frac{T^{n+1/2}_{i,j} - T^n_{i,j}}{\Delta t/2} = Lr + Lz \quad (8)$$

Where :

$$L_r = \frac{k(T_{i,j})}{r_i \Delta r^2}\Big[r_{i+1/2}(T^{n+1/2}_{i+1,j} - T^{n+1/2}_{i,j}) - r_{i-1/2}(T^{n+1/2}_{i,j} - T^{n+1/2}_{i-1,j})\Big] \quad (9)$$

$$L_z = \frac{1}{\Delta z^2}\Big[k(T^n_{i,j+1})(T^n_{i,j+1} - T^n_{i,j}) - k(T^n_{i,j-1})(T^n_{i,j} - T^n_{i,j-1})\Big] + Q_m(T^n_{i,j}) \quad (10)$$

2) Second Half-Step: Implicit in z, Explicit in r: The discretized equation from $t_{n+1/2}$ to t_{n+1}:

$$C_p(T^{n+1/2}_{i,j})\frac{T^{n+1}_{i,j} - T^{n+1/2}_{i,j}}{\Delta t/2} = Lr + Lz \quad (11)$$

Where :

$$L_r = \frac{k(T^{n+1/2}_{i,j})}{r_i \Delta r^2}\Big[r_{i+1/2}(T^{n+1/2}_{i+1,j} - T^{n+1/2}_{i,j}) - r_{i-1/2}(T^{n+1/2}_{i,j} - T^{n+1/2}_{i-1,j})\Big] \quad (12)$$

$$L_z = \frac{1}{\Delta z^2}\Big[k(T_{i,j})(T^{n+1}_{i,j+1} - T^{n+1}_{i,j}) - k(T_{i,j})(T^{n+1}_{i,j} - T^{n+1}_{i,j-1})\Big] + Q_m(T^{n+1/2}_{i,j}) \quad (13)$$

3) Solution of the Tridiagonal System: Each implicit step in the ADI method leads to a tridiagonal system of the form:

$$a_m T_{m-1} + b_m T_m + c_m T_{m+1} = d_m, \quad (14)$$

where a_m, b_m, and c_m are coefficients that depend on thermal conductivity $k(T)$, grid spacing, and specific heat $C_p(T)$, while d_m contains contributions from the explicitly treated direction and the source term Q_m. The index m generically represents the spatial coordinate being solved implicitly (either r or z), depending on the current ADI half-step. This system is efficiently solved using a custom `tridiag()` function based on the Thomas algorithm.

C. General Overview: Solving PDEs Using the Finite Volume Method (FVM)

The **Finite Volume Method (FVM)** is a widely used numerical technique for solving partial differential equations (PDEs), particularly those that represent conservation laws such as heat conduction. The method transforms PDEs into algebraic equations by applying the conservation principle to small control volumes within the computational domain.

Steps in the Finite Volume Method

1) **Define the Computational Domain:**
Radial length rc = 5, discretized into nr = 6 nodes,Axial length zc = 10, discretized into nz = 11 nodes,Time interval: tf = 120 seconds, output at 5 time points

2) **Generate Mesh Grids:**
Uniform grid spacing in r: dr = rc / (nr - 1), Uniform grid spacing in z: dz = zc / (nz - 1), 2D mesh formed using sequences: r and z

3) **Compute Face Fluxes** For each internal control volume, compute conductive heat fluxes across faces:
   - **Radial direction (r):** Use the harmonic mean to evaluate k at interfaces.

   $$F_r = k_{r,\text{interface}} \cdot \frac{\Delta T}{\Delta r}$$

   Multiply by the cylindrical surface area:

   $$A_r = 2\pi r \cdot \Delta z$$

   - **Axial direction (z):** Similar flux evaluation is done using axial interfaces.

   $$A_z = \pi \left(r^2_{i+\frac{1}{2}} - r^2_{i-\frac{1}{2}} \right)$$

4) **Discretize the Governing Equation**
The unsteady heat equation is discretized in integral form over each control volume:

$$C_p(T) \cdot \frac{dT}{dt} = \frac{1}{V} \left(q_r + q_z + Q_m \cdot V \right)$$

Where:
   - V is the volume of the control cell,
   - q_r, q_z are the net radial and axial heat fluxes,
   - Q_m is the internal heat generation term.

5) **Time Integration**
For each time step, the temperature in each control volume is updated using:

$$T^{n+1} = T^n + \Delta t \cdot \frac{q_r + q_z + Q_m \cdot V}{C_p(T) \cdot V}$$

Temperatures are updated iteratively over the entire domain.

D. Physics-Informed Neural Networks

PINN ARCHITECTURE

- A neural network with 5 hidden layers, each containing 64 neurons and using the `tanh` activation function, was used to approximate the temperature field $T(r, z, t)$.
- The input variables (t, r, z) were normalized to the range $[-1, 1]$ to improve training stability.

PHYSICS-INFORMED LOSS

The loss function combined multiple components to enforce the physics and constraints of the problem:

- **PDE Residual:** Enforced the bioheat transfer equation, incorporating piecewise definitions of specific heat $C(T)$, thermal conductivity $k(T)$, and metabolic heat generation $Q_m(T)$.
- **Boundary Conditions:**
  - Neumann: $\frac{\partial T}{\partial r} = 0$ at $r = 0$ and $r = r_c$, and $\frac{\partial T}{\partial z} = 0$ at $z = z_c$.
  - Dirichlet: $T = T_s$ at $z = 0$.
- **Initial Condition:** $T(r, z, 0) = T_o$.
- **Point Constraint:** $T(0, z_p, t) = T_p$ to enforce the cryoprobe temperature at the probe tip.

TRAINING

- The network was trained using the Adam optimizer with a learning rate of 10^{-3} for 40k epochs.
- L-BFGS optimizer (LR=10^{-3}, 1k epochs).
- Loss weights were set to emphasize the point constraint ($w_{\text{point}} = 50$) and the initial/boundary conditions ($w_{\text{ic}} = w_{\text{bc}} = 10$).
- Collocation points were resampled every epoch.

V. RESULTS

Due to the extensive number of simulations and the high-resolution plots generated for different numerical methods and machine learning approaches, this section presents only a table that compares the methods to each other.

For a complete collection of all plots and comparative results, including:

- Temperature profiles over time for each numerical method
- Machine learning prediction outputs versus ground truth,

please refer to the dedicated GitHub repository:

project GitHub repository.

The repository includes organized folders with method-wise results, code snippets, and instructions for reproducing the figures.

A. Comparison

We compared the errors using the Mean Absolute Error (MAE) metric and analyzed the time complexity across the entire computational grid ($nr = 6 \times nz = 11$).

Method	Execution Time (s)	MAE	Max Error
MOL	0.1599	–	–
ADI	3.25	0.36347	16.8947
FVM	0.07	0.3339	13.539
ML	0.22	0.51088	15.3535

TABLE I: Performance comparison of numerical and machine learning methods for solving the cryosurgery heat equation. The Method of Lines (MOL) is used as a reference solution for error calculations.

VI. Improvements and Future Work

The present work successfully implements multiple numerical schemes—namely the Method of Lines (MOL), Alternating Direction Implicit (ADI), Finite Volume Method (FVM), and Machine Learning (ML)—to simulate temperature distributions in cryosurgery. Each method was executed within a consistent computational environment, allowing for direct comparative analysis of both computational performance and accuracy.

As shown in Table I, the FVM achieved the fastest execution time (0.07 seconds) while maintaining a relatively low mean absolute error (MAE = 0.3339), indicating strong potential for real-time simulation. However, despite its speed, slight compromises in accuracy were observed compared to MOL. Future improvements for FVM could include mesh refinement near cryoprobe boundaries and adaptive control volume sizing to further boost accuracy without compromising speed.

The ADI method exhibited the highest computational cost (3.25 seconds) among all solvers. While it maintained acceptable accuracy (MAE = 0.36347), its performance may not be suitable for real-time applications in its current form. This highlights an opportunity to explore parallelized or GPU-accelerated ADI implementations, which could drastically reduce runtime while preserving the method's numerical stability advantages.

Machine Learning (ML) achieved a reasonable runtime (0.22 seconds) but exhibited the highest MAE (0.51088) and a max error comparable to numerical methods. This reflects the limitations of training purely on synthetic datasets. Enhancing the ML model using transfer learning from experimental or clinical thermographic data could improve generalizability and accuracy. Additionally, incorporating physics-informed neural networks (PINNs) or hybrid ML–PDE models may bridge the gap between data-driven speed and physics-based accuracy.

From a modeling perspective, the current simulation assumes a symmetric cylindrical domain with uniform discretization. Clinical realism can be significantly improved by introducing patient-specific anatomical geometries, extracted from imaging modalities such as MRI or CT, and solving them using finite element methods (FEM) on structured or unstructured meshes. This would enable localized resolution enhancement near critical regions, such as cryoprobe tips or highly perfused tissues.

The boundary conditions used in all methods are simplified (e.g., Dirichlet boundaries for symmetry and probe contact). Incorporating more realistic boundary effects, such as variable surface heat flux, convective losses, or contact resistance, could improve fidelity. Similarly, dynamic modeling of material properties—like phase-change-aware thermal conductivity or perfusion-driven heat capacity—would enhance the biophysical accuracy of the simulation.

References

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