Parameters analysis of a porous medium model for treatment with hyperthermia using OpenMP

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Abstract. Cancer is the second cause of death in the world so treatments have been developed trying to work around this world health problem. Hyperthermia is not a new technique, but its use in cancer treatment is still at early stage of development. This treatment is based on overheat the target area to a threshold temperature that causes cancerous cell necrosis and apoptosis. To simulate this phenomenon using magnetic nanoparticles in an under skin cancer treatment, a three-dimensional porous medium model was adopted. This study presents a sensibility analysis of the model parameters such as the porosity and blood velocity. To ensure a second-order solution approach, a 7-points centered finite difference method was used for space discretization while a predictor-corrector method was used to time evolution. Due to the massive computations required to find the solution of a three-dimensional model, this paper also presents a first attempt to improve performance using OpenMP, a parallel programming API.

1. Introduction
According to the World Health Organization (WHO), cancer is the second cause of death in the world. There are several kinds of treatments trying to mitigate this world health problem, like radiotherapy, chemotherapy or even surgical extraction. An attempt to minimize trauma due to invasive treatments is the use of local hyperthermia, which is a minimally non-invasive therapy based on overheat the target area up to a threshold temperature that causes necrosis and apoptosis of the cancerous tissue. One important point is how to heat the tumor: according to [1], magnetic nanoparticles are a good choice. Due to the biocompatibility with the human body, iron oxides magnetite ($Fe_3O_4$) and maghemite ($\gamma - Fe_2O_3$) are the most used nanoparticles.

In this work, hyperthermia is modeled as follows. The bioheat transfer is modeled as a porous medium[2], but using the external heat as shown in [3]. The heat generation due to the nanoparticles is modeled as suggested by [1]. Then a sensibility analysis of the blood velocity and porosity is carried out. Finally, this paper presents a parallelization strategy applied to the numerical method in order to speedup the simulation time since its solution in the three-dimensional domain demands a huge computational time. The parallelization was implemented using OpenMP, a parallel programming API.

2. Bioheat Transfer Model
The transient bioheat model adopted in this work is based on the theory of porous media in biological tissues adapted from [2]. This model, in a well-posed problem, can be written as:
\[
\left\{\begin{array}{l}
[\rho c_p (1 - \varepsilon) + \rho_b c_{pb} \varepsilon] \frac{\partial T}{\partial t} = \nabla \cdot \kappa \nabla T + \beta \frac{\rho_b (u_0)_{AVG} \varepsilon c_{pb}}{\delta} (T_b - T) + \\
(1 - \varepsilon) (Q_m + Q_r), \\
\alpha T + \gamma \nabla T \cdot \vec{n} = f, \\
\end{array}\right. \\
\begin{array}{l}
T (\cdot, 0) = T_0, \\
\end{array}
\] \\
\text{in } \Omega \times I, \\
\text{on } \Gamma \times I.
\]

where \(\kappa = (1 - \varepsilon) k_t + \varepsilon k_b\); \(\rho, c_p\) and \(k_t\) are density, specific heat and thermal conductivity of the tissue, respectively; \(\rho_b, c_{pb}, k_b\) and \((u_0)_{AVG}\) are density, specific heat, thermal conductivity and velocity of the blood, respectively; \(\varepsilon, \delta\) and \(\beta\) are porosity of the medium, average distance between the transverse blood vessels and a correction factor, respectively; \(T_b\) is the blood temperature; \(Q_m\) is the metabolic heat source; \(Q_r\) external spatial heating.

3. Numerical Scheme and Parallel Strategy

The finite difference method in both time and space is employed to solve Eq. (1). Briefly, the domain \(\Omega \cup \Gamma \subset \mathbb{R}^3\) is discretized into a set of equally spaced points defined by \(S = \{x_i, y_j, z_k\} : i = 0, \ldots, I_x; j = 0, \ldots, I_y; k = 0, \ldots, I_z\) with \(I_x, I_y\) and \(I_z\) being the number of intervals of length \(\Delta x, \Delta y\) and \(\Delta z\), respectively in each direction. To ensure a second order convergence, the 7-points centered finite difference scheme [4] was applied for the spatial discretization. To march in time, the time domain \(I\) was partitioned into \(I_T\) equal time intervals of length \(\Delta t\), and an explicit alpha-family of time integration method [5] was adopted into Eq. (1) as shown by Alg. 1. According to [5], the use of \(r_f = 2\) and \(\alpha = 0.5\) in this scheme ensures a second order convergence when applied to linear equations.

**Algorithm 1: Parallel Predictor-Multicorrector Algorithm**

```plaintext
1 begin
2 # pragma omp parallel
3 foreach n in I_t do
4 # pragma omp for
5 foreach T in Omega U Gamma do
6 if (r = 0) then
7 T^n+1,i,j,k = T^n,i,j,k + (1 - \alpha) \Delta t \frac{\partial T^n,i,j,k}{\partial t}
8 end if
9 \frac{\partial T^{n+1,i,j,k}}{\partial t} = \left[ \frac{1}{\rho (1 - \varepsilon) + \rho_b c_{pb} \varepsilon} \right]_{i,j,k} \Phi(T_{i-1,j,k}, T_{i+1,j,k}, T_{i,j-1,k}, T_{i,j+1,k}, T_{i,j,k}, T^{n+1,i,j,k}) +
10 \frac{\beta \rho_b (u_0)_{AVG} \varepsilon c_{pb}}{\delta} \left( T_b - T_{i,j,k} \right) + \left( Q_m + Q_r \right) (1 - \varepsilon)_{i,j,k}
11 T^{n+1,i,j,k} = T^{n+1,i,j,k} + \alpha \Delta t \frac{\partial T^{n+1,i,j,k}}{\partial t}
12 end foreach
13 end for
14 end foreach
15 end
```

In Alg. 1, \(T^n_{i,j,k} \approx T(x_i, y_j, z_k, t_n)\), and \(\Phi(T^{n+1}_{i,j,k}, T^{n+1}_{i+1,j,k}, T^{n+1}_{i,j-1}, T^{n+1}_{i,j+1}, T^{n+1}_{i,j,k}, T^{n+1}_{i,j,k} = q^{n+1}_{x,i,j,k} + q^{n+1}_{y,i,j,k} + q^{n+1}_{z,i,j,k}\), where \(q^{n+1}_{x,i,j,k} = \frac{1}{\Delta x^2} \left[ k_{i+1/2,j,k} \left( T^{n+1}_{i+1,j,k} - T^{n+1}_{i,j,k} \right) - k_{i-1/2,j,k} \left( T^{n+1}_{i,j,k} - T^{n+1}_{i-1,j,k} \right) \right]\) (all the other fluxes are approximated in a similar manner). Due to the fact that \(\kappa\) is a piecewise continuous function, the harmonic mean \(\bar{k}_{i+1/2,j} \approx \frac{2k_{i,j} k_{i+1,j}}{k_{i,j} + k_{i+1,j}}\) was adopted to ensure the flux continuity.
4. Simulation Results
The aforementioned mathematical model was used to simulate the hyperthermia in a cubic domain with lengths equal to 0.1 m in each direction, discretized using $\Delta x = \Delta y = \Delta z = \Delta = 0.001$ m and over 3000 s of simulation time with $\Delta t = 1$ s, in addition to a tumor formed by two intercepted spheres seated at (0.5, 0.5, 0.5) m and (0.4, 0.4, 0.4) m with radius of 0.015 m and 0.01 m, respectively. All the parameters used to perform the simulation are shown in Tab. 1 and are in accordance with the literature [6, 7]. In addition, the heat generated by the nanoparticles is mathematically modeled as a function $Q_r(\vec{x}) = \sum_{i=1}^{n} A_i e^{-r(\vec{x}^2)/r_0^2}$ with one ($n = 1$) injection point seated at (0.05,0.05,0.05) m; and considering $A = 1.3 \times 10^6$ W/m$^3$ and $r_0 = 3.1 \times 10^{-3}$ m.

$$c\quad (J/Kg^\circ C)\quad 4000.0\quad 4000.0$$
$$c_b\quad (J/Kg^\circ C)\quad 4000.0\quad 4000.0$$
$$k_t\quad (W/m^\circ C)\quad 0.51\quad 0.56$$
$$k_b\quad (W/m^\circ C)\quad 0.64\quad 0.64$$
$$\rho\quad (Kg/m^3)\quad 1000.0\quad 1000.0$$
$$\rho_b\quad (Kg/m^3)\quad 1000.0\quad 1000.0$$

To evaluate the sensibility analysis, two parameters were chosen: blood velocity and porosity. For the porosity analysis, the velocity was fixed in 1.6 mm/s with the porosity values ranging from 0.001 to 0.1 in increments of 0.02 at the tumor tissue, whereas for the blood velocity analysis the porosity was fixed in 0.06 with the blood velocity values ranging from 1.5 mm/s to 4.5 mm/s in increments of 0.6 mm/s, according to the experimental data shown in [6], at the tumor tissue. These parameters were chosen mainly because both are not constant at the body. As shown at [6] the blood velocity depends on the cancer stage, and the porosity can vary as well, it depends on, for instance, the shape of the cell and the interstitial fluid [8].

First of all, it is important to observe that these temperature curves represent an hyperthermia treatment since they are qualitatively in accordance with experimental data in [1]. Furthermore, according to Fig. 1(a) it is possible to observe that increasing the value of the porosity parameter in 100 times affects the steady state temperature in an hyperthermia treatment about 4°C; moreover, Fig. 1(b) shows that increasing the value of the blood velocity in 3 times results in a difference of 1.4°C, i.e. this model is more sensitive to the velocity of blood than to the medium porosity. Finally, it is worthwhile to note that the hyperthermia treatment starts having effects at 43°C, and in some cases it is necessary to use more injection points [1].

All the simulations were performed in a SMP Linux (3.9.2-200) computer with two Intel Xeon CPUs E5620 with 2.40GHz of clock frequency, the Hyper-Threading option turned off and 12 GB of RAM. Each CPU has four cores, so a total of 8 cores were available. The speedup was computed using the average of three executions. The standard deviation for these executions was below 2.73%. According to Fig. 2, the best speedup result, 7.12, was obtained using the dynamic scheduling with chunk size equals to 1. The speedup results are quite encouraging since the serial version was executed in 11.5 min and the best parallel version executed in 1.62 min using 8 cores.

5. Conclusions
This work presented a parameter analysis of the blood velocity and the medium porosity using a bioheat model in porous media. It has been observed that the mathematical model is more sensitive to blood velocity parameter when compared to porosity. Furthermore, a finite difference
strategy was employed to solve the equations and a parallel implementation was used to speedup the simulation up to 7.1 times in a 8 core processor. As future work, we plan to handle with more complex porous media bioheat models, e.g. two phases, and try a parallelization strategy using GPUs as shown in [9].

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Figure 1. Influence of porosity (a) and blood velocity (b) at the point (0.048, 0.048, 0.048) m inside the tumor.

Figure 2. Speedup analysis