

# Parallel algorithms for adaptive time-stepping in radiofrequency liver ablation simulation: implementation on an IBM Blue Gene/P computer

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**Abstract**—This work concerns the mathematical modeling and computer simulations of the heat transfer process. The core is solving the time-dependent partial differential equation of parabolic type. Instead of a uniform discretization of the considered time interval, an adaptive time-stepping procedure is applied in an effort to decrease the simulation time. The procedure is based on the local comparison of the Crank Nicholson and backward Euler approximations. Computer simulation on geometry obtained from a magnetic resonance imaging (MRI) scan of the patient is performed. Results of some preliminary numerical experiments performed on a selected test problems are presented and discussed

## I. INTRODUCTION

THE minimally invasive treatment called radio-frequency ablation (RFA) guided by imaging techniques, the doctor inserts a thin needle through the skin and into the tumor, (see Fig. 1, [11]). High-frequency electrical energy delivered through this needle heats and destroys the tumor. The circuit is closed with a ground pad applied to the patient's skin.

The right procedure parameters are very important for the successful killing of all of the tumor cells with minimal damage on the non-tumor cells.



Fig. 1. CT Scan, Showing Radio-Frequency Ablation of a Liver Lesion

Computer simulation on geometry obtained from a magnetic resonance imaging (MRI) scan of the patient is performed.

In this work, an adaptive time stepping algorithm is applied to the simulation in order to reduce the computational time.

The rest of the paper is organized as follows. The mathematical and numerical models are shortly presented in Section 2. The adaptive time-stepping algorithm is described in Section 3.

Section 4 is devoted to the computer simulations and analysis of the results obtained on an IBM Blue Gene/P supercomputer. Finally, some concluding remarks can be found in Section 5.

## II. THE MATHEMATICAL AND NUMERICAL MODELS

The bio-heat time-dependent partial differential equation [4], [5] is the governing equation describing the RFA process. It can be presented as follows:

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + J \cdot E - \alpha h_B (T - T_B), \quad (1)$$

where the thermal energy arising from the current flow is described by  $J \cdot E$  in (1) and  $\alpha h_B (T - T_B)$  accounts for the heat loss due to blood perfusion in the capillaries. The heat produced from metabolic functions of the liver is neglected. The initial and boundary conditions which are used in this approach are as follows:

$$T = 37^\circ\text{C} \quad \text{when } t = 0 \text{ at } \Omega, \quad (2a)$$

$$T = 37^\circ\text{C} \quad \text{when } t \geq 0 \text{ at } \partial\Omega, \quad (2b)$$

$$-k \frac{\partial T}{\partial n} = \alpha (T - T_B) \quad \text{when } t \geq 0 \text{ at } \Gamma_R \quad (2c)$$

The notations which are used in (1) and (2) are given below:

- $\Omega$  – the entire domain of the model;
- $\partial\Omega$  – the boundary of the domain;
- $\Gamma_r$  – the boundary of the blood vessel;
- $\rho$  – density [ $\text{kg}/\text{m}^3$ ];
- $c$  – specific heat [ $\text{J}/\text{kg K}$ ];
- $k$  – thermal conductivity [ $\text{W}/\text{m K}$ ];
- $J$  – current density [ $\text{A}/\text{m}$ ];
- $E$  – electric field intensity [ $\text{V}/\text{m}$ ];
- $t$  – time [ $\text{s}$ ];
- $T$  – temperature [ $\text{K}$ ];
- $T_B$  – blood temperature ( $37^\circ\text{C}$ );
- $w_B$  – blood perfusion coefficient [ $\text{s}^{-1}$ ];
- $h_B = \rho_B c_B w_B$  – convective heat transfer coefficient accounting for the blood perfusion in the model;
- $\alpha$  – tissue state coefficient;
- $n$  – the outward-pointing normal vector of the boundary.

The cumulative damage integral  $\Psi(t)$  is used as a measure of ablated region [1], [9]:

$$\Psi(t) = \ln \left( \frac{c(0)}{c(t)} \right) = A \int e^{-\frac{\Delta E}{RT(t)}} dt, \quad (3)$$

where  $c(t)$  is the concentration of living cells,  $R$  is the universal gas constant,  $A$  is the “frequency” factor for the kinetic expression [ $s^{-1}$ ], and  $\Delta E$  is the activation energy for the irreversible damage reaction [ $J \text{ mol}^{-1}$ ]. The values used  $A = 7.39 \times 10^{39} s^{-1}$  and  $\Delta E = 2.577 \times 10^5 J \text{ mol}^{-1}$  are taken from [1]. Tissue damage  $\Psi(t) = 4.6$  corresponds to 99% probability of cell death. The value of  $\Psi(t) = 1$ , corresponding to 63% probability of cell death is significant, because at this point the tissue coagulation first occurs and blood perfusion stops.

The tissue state coefficient  $\alpha$  is expressed as

$$\alpha(t) = \begin{cases} e^{-\Psi(t)} & \text{if } \Psi(t) < 1, \\ 0 & \text{if } \Psi(t) \geq 1. \end{cases}$$

In the presented algorithm the bio-heat problem (1) is solved in two steps (see [9] for more details):

- 1) Finding the heat source  $J \cdot E$  using that: (a)  $E = -\nabla V$  ( $V$  is the electric potential in the computational domain  $\Omega$ ), and (b)  $J = \sigma E$ , where  $\sigma$  is the electric conductivity [ $S/m$ ];
- 2) Finding the temperature  $T$  by solving the heat transfer equation (1) using the heat source  $J \cdot E$  obtained in the first step.

For the numerical solution of (1) the finite element method in space is used ([7]). *Linear conforming tetrahedral elements* are used in this study. They are directly defined on the elements of the used unstructured mesh (see Fig. 2). An *algebraic multigrid* (AMG) preconditioner is used [3]. The time derivative is discretized via finite differences and the both the *backward Euler* and the *Crank-Nicolson* schemes are used ([8]).

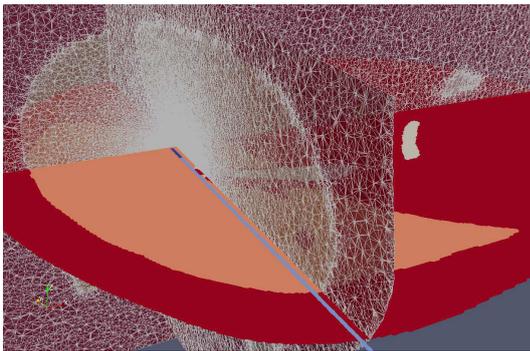


Fig. 2. Inserted RF Probe and the Finite Element Mesh

Let the matrices  $K$  and  $M$  be the stiffness and mass matrices from the finite element discretization of (1):

$$K = \left[ \int_{\Omega} k \nabla \Phi_i \cdot \nabla \Phi_j d\mathbf{x} \right]_{i,j=1}^N,$$

$$M = \left[ \int_{\Omega} \rho c \Phi_i \Phi_j d\mathbf{x} \right]_{i,j=1}^N.$$

Let us also denote with  $\Omega_B$  the subdomain of  $\Omega$  where we account for the blood perfusion (the liver tissue) and with  $M_B$  the matrix

$$M_B = \left[ \int_{\Omega} \delta_B h_B \Phi_i \Phi_j d\mathbf{x} \right]_{i,j=1}^N,$$

where

$$\delta_B(x) = \begin{cases} \alpha & \text{for } x \in \Omega_B, \\ 0 & \text{for } x \in \Omega \setminus \Omega_B. \end{cases}$$

The influence of the Robin boundary conditions given in (2c) and the electric field intensity is presented by:

$$M_R = \left[ \int_{\Gamma_R} \alpha \Phi_i \Phi_j d\mathbf{x} \right]_{i,j=1}^N, \quad (4)$$

and

$$F = \left[ \int_{\Omega} J E \Phi_i \Phi_j d\mathbf{x} \right]_{i,j=1}^N, \quad (5)$$

Then, the spatially discretized parabolic equation (1) can be written in matrix form as:

$$M \frac{\partial T}{\partial t} + (K + M_B + M_R) T = F + M_B T_B + M_R T_B. \quad (6)$$

### III. ADAPTIVE TIME-STEPPING ALGORITHM

To ensure accuracy and not waste computational effort, it is important to adapt the time steps to the behavior of the solution.

The time discretization for both backward Euler method and the Crank-Nicolson one can be written in the form

$$\begin{aligned} & (M + \tau^n \theta (K + M_B + M_R)) T^{n+1} \\ & = (M - \tau^n (1 - \theta) (K + M_B + M_R)) T^n \\ & + (\tau^n \theta + \tau^n (1 - \theta)) (F + M_B T_B + M_R T_B), \end{aligned} \quad (7)$$

where the current ( $n$ -th) time-step is denoted with  $\tau^n$ , the unknown solution at the next time step – with  $T^{n+1}$ , and the solution at the current time step – with  $T^n$ . If we set the parameter  $\theta = 1$ , (7) gives a system for the backward Euler discretization. When  $\theta = 0.5$  (7) becomes Crank-Nicolson one. The solution of the linear system (7) with  $\theta = 1$  and  $\theta = 0.5$  gives us  $T_{BE}$  and  $T_{CN}$  respectively.

A suitable adaptive time-stepping procedure is based on a local comparison of the backward Euler ( $T_{BE}$ ) and Crank-Nicolson ( $T_{CN}$ ) approximations for the current timestep, and is controlled by the ratio

$$\eta = \frac{\|T_{CN} - T_{BE}\|}{\|T_{BE}\|}. \quad (8)$$

This approach has a down side, that solving two linear systems is required to obtain  $T_{BE}$  and  $T_{CN}$ . This is, from the computational point of view, expensive. Nevertheless overall decrease in computational time is expected.

The algorithm below, describing our adaptive time-stepping procedure, is based on the one for adaptive time stepping for processes in spent nuclear fuel repositories [2]. It has several parameters:

- 1)  $\tau^1$  – initial timestep;
- 2)  $N_{\text{Adapt}}$  – a parameter showing how often the adaptive time stepping strategy is applied, e.g.  $N_{\text{Adapt}} = 1$  shows that the adaptive time stepping is used on each step while  $N_{\text{Adapt}} = 3$  – that the adaptive time stepping is performed at every third time step,  $N_{\text{Adapt}} = 0$  indicates that all time steps are non-adaptive.
- 3)  $\lambda_{\text{NonAdapt}}$  – a parameter showing whether and by how much the time step is multiplied, in non-adaptive time steps, e.g.  $\lambda_{\text{NonAdapt}} = 1$  means that the time step is not changed, while  $\lambda_{\text{NonAdapt}} = 1.2$  means that the time step on the current level is multiplied by 1.2 for the next time level.
- 4)  $\varepsilon_{\text{min}}$  and  $\varepsilon_{\text{max}}$  are minimal and maximal thresholds for the error estimate  $\eta$ .

*Algorithm 1 (Adaptive Time-Stepping Procedure):*

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1. for  $k = 1, 2, \dots$  until the end of time do
2.   if CurrentStepIsAdaptive( $N_{\text{Adapt}}, k$ )
3.     then
4.       do
5.         compute  $T_{\text{BE}}, T_{\text{CN}}$  with  $\tau^k$ 
6.         compute  $\eta$ 
7.         if  $\eta < \varepsilon_{\text{min}}$  then  $\tau^{k+1} = 2\tau^k$ 
8.         if  $\eta > \varepsilon_{\text{max}}$  then  $\tau^k = 0.5\tau^k$ 
9.         while  $\eta > \varepsilon_{\text{max}}$  // if too big error
10.          // stay on the same timestep
11.           $T^{k+1} = T_{\text{BE}}$ 
12.        else
13.          compute  $T_{\text{BE}}$  with  $\tau^k$ 
14.           $T^{k+1} = T_{\text{BE}}$ 
15.           $\tau^{k+1} = \tau^k \lambda_{\text{NonAdapt}}$ 
16.        end if
17.      end if
18.    end for

```

The last timestep is always truncated to the time of simulation.

Inner PCG iteration with the BoomerAMG [3] preconditioner, part of the software package HYPRE [10], is used for the solution of (7). The preconditioner is reconstructed if the number of inner iterations goes above 12. The reconstruction takes place before the solution of the next timestep.

#### IV. COMPUTER SIMULATIONS AND ANALYSIS OF THE OUTPUT RESULTS

The IBM Blue Gene/P computer, located at the Bulgarian Supercomputing Center, is used for the simulations and numerical experiments with the new adaptive time stepping algorithm. This machine consists of two racks, 2048 Power PC 450 based compute nodes, 8192 processor cores and a total of 4 TB random access memory. Each processor core has a double-precision, dual pipe floating-point core accelerator. Sixteen I/O nodes are connected via fiber optics to a 10 Gbps Ethernet switch.

The material properties which are used in the simulations are taken from [4]. The applied electrical power is 15 W, and the simulation is done for 7 minutes.

We run several test to choose a suitable set of values for the threshold parameters  $\varepsilon_{\text{min}}$  and  $\varepsilon_{\text{max}}$ . As a quantitative criterion of quality of the solution we used two volumes – the volume  $Vol_1$ , which is the volume of the tissue, where the cumulative damage integral  $\Psi$  is greater than 1, and  $Vol_{4,6}$  – the volume of the tissue, where  $\Psi > 4.6$ . The results of the nonadaptive algorithm with step  $\tau = 1$  s were compared with the ones from adaptive runs. As a result of these tests we found that an acceptable variation in the two important volumes less than 3 % occurs when the threshold interval is  $[2.5 \times 10^{-4}, 1.25 \times 10^{-3}]$  and this interval is used in the further computer simulations.

Based on these preliminary tests, a number of runs were done both using 128 and 1024 processors. Uniformly refined mesh was used for the runs on 1024 processors. Some of the output results obtained during the simulations are presented in Table I and Table II. An excellent scalability is observed – we solve eight times bigger problems on eight times more processors for almost the same time. One can see in both tables that the best results with regards to CPU time and number of the inner iterations are obtained when the adaptive strategy is applied at each second time step and meanwhile, at the intermediate time steps  $\tau$  is multiplied by 1.2. In this case, comparing the total CPU times of the algorithm without the adaptive time-stepping and using this strategy, it is seen that the time of the new algorithm is almost three times shorter.

#### V. CONCLUSIONS

The first experimental results show that the new algorithm is scalable. The tests allowed us to find some suitable parameters and showed the practical usefulness of the developed solver for such kind of computer simulations. One can observe that the computing time is decreased more than three times, the number of outer iterations is decreased from 420 to 71, and the number of inner iteration decreases from 2233 to 535. This preliminary results are a good motivation for further improving the algorithm and doing more simulations.

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TABLE I  
NUMBER OF ITERATIONS AND THE CPU TIME IN THE ADAPTIVE TIME-STEPPING ALGORITHM IN THE CASE OF 128 PROCESSORS.

$N_{\text{Adapt}}$	$\lambda_{\text{NonAdapt}}$	No. of inner iterations	No. of outer iterations	CPU time [s]	$Vol_1$ $\text{cm}^3$	$Vol_{4.6}$ $\text{cm}^3$
0	1.0	2233	420	7608	22.14	15.60
1	1.0	917	102	3968	22.72	15.93
2	1.0	731	104	3137	22.63	15.87
	1.2	535	71	2321	22.87	16.00
3	1.3	587	77	2624	22.87	16.02
	1.0	700	113	3053	22.58	15.83
	1.2	539	76	2329	22.88	16.03
	1.3	592	77	2559	22.81	15.97

TABLE II  
NUMBER OF ITERATIONS AND THE CPU TIME IN THE ADAPTIVE TIME-STEPPING ALGORITHM IN THE CASE OF 1024 PROCESSORS.

$N_{\text{Adapt}}$	$\lambda_{\text{NonAdapt}}$	No. of inner iterations	No. of outer iterations	CPU time [s]	$Vol_1$ [ $\text{cm}^3$ ]	$Vol_{4.6}$ [ $\text{cm}^3$ ]
0	1.0	604	420	7259	22.21	15.65
1	1.0	777	101	4234	22.70	15.92
2	1.0	594	101	3488	22.70	15.92
	1.2	478	71	2619	23.01	16.10
3	1.3	539	77	2982	22.94	16.07
	1.0	549	104	3121	22.70	15.93
	1.2	455	76	2530	22.85	16.01
	1.3	514	75	2740	22.94	16.06

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