AUTOMATIC MESH REFINEMENT FOR 3D NUMERICAL SIMULATION OF THERMAL DIFFUSION IN SILICON

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Abstract

Within the frame of the european PROMPT-II project (esprit project 24038), the fields of interest at IEMN-ISEN are related to the 3D simulation of thermal annealing process steps. In particular, the implementation of a 5-species diffusion model is under developement what emphasises the requirement for a "clever" control of the space and time discretization. This paper presents such an automatic refinement tool based on the computation of an error estimator.

1. Introduction

In DIFOX-3D, the 3D module for the simulation of thermal annealing steps, developed at ISEN, the diffusion equations are solved with the finite element method on a tetrahedronal mesh with linear shape functions. In order to guarantee the accuracy of the numerical simulations and to avoid prohibitive calculation times, we are implementing an adaptive process to control dynamically the discretization of time and space and which consists in : 1) the mesh generation, 2) the solution of the non-linear equation, 3) the calculation of the refinement criterion, 4) the mesh/time refinement. During the refinement step, the elements having unacceptable errors are refined by the use of an efficient local mesh generator ([1]).
Our time-dependent problem is discretizated simultaneous in time and space ([2-3]). Thus, we use an analytical approach to optimize the discretization in time and space. The adaptive method we have chosen is based on sharp a posteriori error estimates. We have first to derive

the formula for the error. We show that this formula can not be given explicitly since the problem is not linear. This means that we have to re-write it differently what leads to a modified formula corresponding to a linearized continuous problem (the dual problem). The next step is to over-estimate this global error formula. Here, we use the properties of the finite element method as well as those of analytical mathematics.

2. Computation of the error estimator

The diffusion equation in R^3 with Neumann and Dirichlet boundaries conditions is:

$$\nabla(D(u)\nabla u) = \frac{du}{dt} \qquad \text{in } \Omega \text{xI} \qquad (1)$$

Considering a sequence of discrete time steps, $I_n = [t_n, t_{n+1}[$ the corresponding time intervals of length k_n, and T_n a triangulation into triangles K of diameter h_K associated with each I_n.

Furthermore, let $W_n = \{\ v \in H_0^{\ 1}(\Omega)\colon v|_K \text{ is linear } \forall K \in T_n\}$ (2)

Let ([3]) $V_n = \{v \in H^1(\Omega x I_n)\colon v(x,t) = w_0(x) + t w_1(x),\ w_i \in W, (x,t) \in \Omega x I_n\}$ (3)

and we define $V = \prod_{n=0}^{N-1} V_n$ where $t_N = T$ is a given final time. Below we shall seek an approximate solution U in the finite-dimensional space V, consisting of piecewise linear functions in x and t, continuous in space and discontinuous in time at the discrete time levels n.

Equation (1) can be rewritten in its weak form as follows, in using the Galerkin scheme, called discontinuous Galerkin method (DG-method):

Find $U \in V$ $\quad B(U;U,v) = (u_0, v_0^{\ +}) \qquad \forall v \in V,$ (4)

We note that the exact solution u of equation (1) satisfies (4).

We shall now derive an error representation formula by substraction: let $e=u-U$

$$\text{E}(u,U;e,v) = 0 \qquad \forall v \in V, \qquad (5)$$

We obtain an equation of the error. We shall now associate the linearized dual problem:

$$E(u,\ U; w,z) = (w_N, e_N) \qquad (6)$$

By integration by part of this equation, we obtain z as solution of the dual problem.

We choose w=e in this for deriving a representation error formula. Finally

$$(e_N, e_N) = \sum_{n=0}^{N-1} \int_{I_n} \{(U_t, Z - z) + (D(U)\nabla U, \nabla(Z - z)) - \langle Fl(U) | Z - z \rangle\} dt + \qquad (7)$$
$$\sum_{n=0}^{N-1} ([U]_n, Z_n^{\ +} - z_n^{\ +})$$

We obtain, under certains assumption, that:

$$\|e_N\| \le C_N \max_{n \le N-1} \varepsilon_n(U,h_n,k_n) + \varepsilon_N \tag{8}$$

Suppose we want to achieve error control within a given tolerance TOL with a given norm. Discarding for simplicity ε_N and setting $C = max_N C_N$, we obtain the following error control:

$$\varepsilon_n\,(U,h_n,k_n) \le TOL/C \qquad n=0,1,2,... \tag{9}$$

So, our adaptive version may now be formulated as choosing sucessively h_n and k_n such that the corresponding finite element solution satisfies (9).

As a practical implementation of this method, we consider the following adaptive algorithm for choosing W_n : for each $n=1,2,...$, with $T_n^{\,0}$ a given initial space mesh and k_{n0} an initial timestep, determine meshes T_n^j with N_j elements of size $h_{nj}(x)$, and timestep k_{nj} and corresponding approximate solutions U^j defined on I_{nj}, such that for $j=0,1,...$

$$k^2_{n,\,j+1} min\left(\gamma max_{t \in I_{nj}}\left(\left\|\frac{(D(U^j) - J_n D(U^j))}{k_{n,\,j}}\right\|\right), (\gamma + \beta_1 + 1)\left\|\frac{[U^j]_n}{k^2_{n,\,j}}\right\|, \quad \forall\, K \in T_n^j \right. \tag{10}$$

$$\left.\gamma max_{t \in I_{nj}}\left\|\frac{Fl(U^j)}{k_{n,\,j}}\right\|\right) = \frac{TOL}{2}$$

$$\beta_2 max_{t \in I_{nj}}\left\|h^2_{n,(j+1)}\delta(U^j)\right\| + \beta_1 max_{t \in I_{nj}}\left\|h^2_{n,\,j+1} Fl(U^j)\right\| + \tag{11}$$

$$(\gamma + \beta_1 + 1)\left\|h^2_{n,\,j+1}\frac{[U^j]_n}{k_{n,\,j}}\right\| = \frac{TOL}{2\sqrt{N_j}}$$

3. Refinement process

We have decided to work with percentage. We compute then the percentage of the spatial error estimate on one element by (10), and the mesh is then refine if this percentage exceeds a prescribed value. For the temporal error estimate (11), we have different errors on each element, and we compute also a percentage to decide if we need to refine the timestep. For the refinement, we can choose k_n as large as possible by equidistribution. It leads to consider the algorithm in Fig. 1.

A question remains which has not been solved for time being. The insertion of a new vertice in an element can be performed either in the volume, on the faces or on the edge of the tetrahedron.

The error estimator is tested on the simple case of a diffusion step of Boron at 900°C during 60 minutes (Fig. 2). We have first considered the case of a linear diffusion (we have to modify the error estimator to adapt it to a linear problem). Numerical simulations have shown that for the linear problem, the temporal refinement does not decrease the global error (Table 1).

Elements number	Spatial error estimator	Percentage spatial
96	0.155	100 %
324	8.20e-02	53 %
768	4.97e-02	32 %
1500	3.32e-02	21 %
2592	2.37e-02	15 %
4116	1.77e-02	11 %
6144	1.38e-02	9 %
12000	8.97e-03	6 %

Table 1: Evolution of the error according to the mesh space

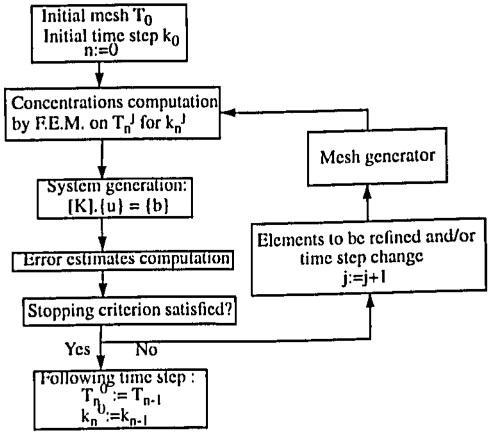

Fig. 1 : refinement algorithm

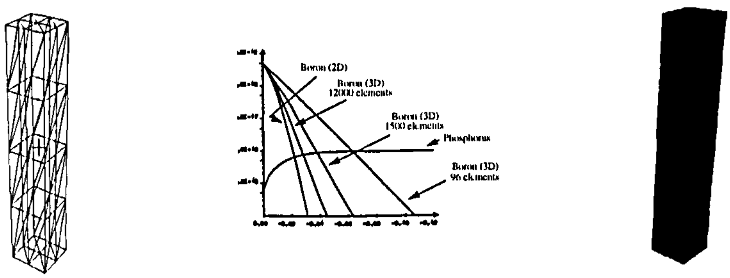

Fig. 2 : a) initial mesh, b) comparison of curves and c) Most refined mesh for the simulation of diffusion of boron at 900°C during 60 minutes.

5. References

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