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Adaptive Multigrid Strategies for Simulation of Diffusion Processes[1]

S. Mijalković, D. Pantić, Z. Prijić, N. Stojadinović
Faculty of Electronic Engineering, University of Niš,
Beogradska 14, 18000 Niš, Yugoslavia

Abstract

Robust and efficient grid refinement strategies for an adaptive multigrid simulation of diffusion processes from implanted impurity profiles have been presented. The refinement criteria are based on global and local discretization errors estimated by extrapolation techniques. The local discretization error for the initial grid refinement and the global discretization error for the grid refinement during diffusion simulation are compatible and controlled by the same, problem independent, relative error parameter.

1 Introduction

An adaptive grid generation method, which properly resolve discrete solutions and operators in different parts of the simulation domain, is a highly desirable feature for efficient and robust process simulation programs. However, the formulation of adaptive grid structures and strategies for the simulation of diffusion processes, where remeshing approach have to simultaneously accommodate space and time dimensions, introduces some critical design challenges:

- Since adaptive grid structures are subjected to frequent changes during simulation in order to follow the evolution of the discrete solution, the remeshing strategies have to allow for an easy and efficient addition (or deletion) of refined grid areas.
- The grid structures have to be as regular as possible in order to minimize the prolongation of interpolation errors introduced during the data transfer from the old to new generated grid structures.
- Effective self–adaptive strategies should be based on an easily controllable discrete approximation accuracy estimator.
- The adaptive grid structures for the initial solution and the solution evolution have to be generated by using compatible error estimators and the same tolerance level.
- The adaptive grid strategy should be capable of running efficiently on parallel machines.

In the present single–grid adaptive methods for the discrete approximation of diffusion process problems [1,2], i.e. the methods which use a single adaptive grid structure, the adaptivity is generally achieved by introducing a nonregularity into the grid structure. However, it is well known that the grid nonuniformity reduces the accuracy of discrete approximation, significantly increases the information contents necessary for

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the grid structure modifications and reduces the parallelization abilities. This shortcomings typically result in lengthy global refinement processes which drastically reduce the simulation efficiency.

In this paper we present an alternative adaptive grid approach based on the multi–level local grid structures which successfully meets the desirable requirements for an efficient adaptive grid strategy and eliminates the most critical shortcomings of the single–grid adaptive approaches.

2 A multi–level refinement process

The principal idea of the multigrid adaptivity is to accomplish the grid refinement (or coarsening) in terms of extending (or contracting) noncoextensive, properly aligned uniform local grids on different discretization levels. The principal formulation of multigrid adaptivity is rather general and independent of the particular discretization approach. However, let us confine, for convenience, to the regular adaptive multi–level structure which is suitable for the two–dimensional finite–difference discretization.

The basic discrete structure for the formulation of an adaptive multigrid system is an uniform lattice:

$$L(h) = \{\mathbf{p}|\ \mathbf{p} = (\alpha h, \beta h);\ \alpha, \beta \in Z\}\ . \tag{1}$$

with meshsize h. In the multigrid context significant role play only uniform lattices with discrete meshsizes $h_l = h_1/2^{l-1}$ $(l \in Z)$ where l denotes discretization level $(l \geq 1)$ and h_1 is the coarsest meshsize. Consequently, $L_l \equiv L(h_l)$ represent an uniform lattice on l–th discretization level. Using the term of the uniform lattice an uniform grid on the l–th discretization level is

$$G_l = L_l \cap D_l\ . \tag{2}$$

$D_l \subset \mathbf{R}^2$ is a two dimensional continuous domain where discrete approximation at least require the presence of l–th discretization level. The whole adaptive multi–level structure is a set of uniform grids

$$G = \{G_1, G_2, \ldots, G_M\} \tag{3}$$

where on the first k discretization levels $(k \geq 2)$ the uniform grids are global covering the whole simulation domain D while the other grids are local covering only $D_l \subset D_{l-1}$ and serve to produce different levels of refinement. M denotes the maximum discretization level defined with $\text{area}(D_{M+1}) = 0$.

The general multi–level refinement process is based on the successive generation of new finer local discretization levels provided that some error estimator and tolerance level are known on the currently highest discretization level. Suppose that the coarse grid G_l is given and that the error estimator and tolerance level indicate that elementary discretization cell Ω_p surrounding grid point $\mathbf{p} = (x_p, y_p)$ has to be refined. Instead of introducing a new partition of Ω_p, the elementary refinement structure

$$E_{l+1}(\mathbf{p}) = \{\mathbf{q}|\ \mathbf{q} = (x_p + \nu_x \cdot h_{l+1}, y_p + \nu_y \cdot h_{l+1});\ |\nu_x| \leq k,\ |\nu_y| \leq k\}\ . \tag{4}$$

has to be introduced on the $(l+1)$st discretization level. In (4) k is the width of the elementary refinement structure. The width k has to be selected so to adjusts the overlap between the subregion Ω_r covered by elementary refinement structure and $D_l \setminus \Omega_p$. In multi–level adaptive techniques [3] this overlap is necessary to assure that coarse grid solution can be reliably used for the formulation of Dirichlet boundary condition at the internal boundaries of the local uniform grids. However, the size of the overlap area must not introduce unnecessary grid refinement. In that sense, elementary refinement structure with width $k = 2$ seems to be an optimal choice.

The generation of a new discretization level is completed with unification of all elementary refinement structures introduced over all coarse grid discretization cells which have been found to require a better grid resolution. With the given error estimator and tolerance level on the currently finest discretization level l, the next discretization level is generated as it is described in Algorithm 1.

Algorithm 1 (Local Grid Refinement)

Here G_l, ε and Tol are given local uniform grid on the currently finest discretization level l, the discrete error estimator and the tolerance level, both defined on G_l. This algorithm produces a local uniform grid G_{l+1} which refines the grid G_l.

1. Set $G_{l+1} = \emptyset$
2. Repeat Steps 3 for all $\mathbf{p} \in G_l$
3. If($\varepsilon_l[\mathbf{p}] > \mathrm{Tol}[\mathbf{p}]$)
   Set $G_{l+1} := G_{l+1} \cup E_{l+1}[\mathbf{p}]$
   [End of If structure]
   [End of Step 2 loop]
4. Exit

It should be noted that the multi–level refinement process is tightly coupled with adaptive multigrid algorithm [4] which actually supplies the refinement process with the discrete solutions at different discretization levels in order to be used for the formulation of the required error estimators and tolerance levels.

In order to handle the adaptive time integration a nonuniform grid in time dimension should be introduced. The simplest approach is to use the same time–step size for all discretization levels in space. Naturally, the space adaptive multi–level structure should be regenerated at each discrete moment of time. It is important to note that the interpolation of the previous discrete solution defined on $G(t_{n-1})$ into $G(t_n)$ takes place only at the new generated parts of the corresponding local grids, since due to the strictly regular nature of the adaptive multi–level structure the grid points of the remaining local grid parts do not change their positions.

3 Refinement criteria

The adaptive simulation of diffusion processes requires two different grid refinement processes in space dimensions: one for the adaptive discrete approximation of impurity profiles for initially implanted impurity profiles which are introduced at the beginning of processing or superposed to the existing impurity profiles at the certain stage of processing and other for the adaptive discrete approximation of the intermediate impurity profiles during the diffusion process simulation.

3.1 Grid refinement during diffusion process simulation

In the case of space–grid refinement during the diffusion process simulation the error estimator

$$\varepsilon_l = |(C)_l - C_l| \tag{5}$$

is the ultimate goal of all adaptive approaches for the simulation of the diffusion processes. In (5) $(C)_l$ is the continuous solution of the diffusion problem presented on the l–th discretization level while C_l is the corresponding discrete solution. Since for the

impurity distribution typically holds $C > C_{\min}$ where $C_{\min}$ is the minimum concentration of interest for simulation the tolerance level naturally has the form

$$\mathrm{Tol} = \mathrm{Rel} \cdot C_l + C_{\min} \tag{6}$$

where Rel is the problem independent relative error parameter.

It is important to note that due to inability of the single–grid adaptive approaches [1,2] to efficiently and accurately estimate global discretization error (5), those are restricted to the application of some approximation of the local discretization error with fixed problem dependent tolerance levels.

On the other hand, an adaptive multigrid algorithm [4] naturally generates discrete solutions of discrete diffusion problem on different local discretization levels which is suitable for the direct estimation of the global discretization error using Richardson extrapolation described in Algorithm 2.

Algorithm 2 (Estimate Global Discretization Error)

Here G_{l-1}, G_l, C_{l-1} and C_l are local uniform grids on the two successive discretization levels and corresponding discrete solutions of impurity diffusion problem. p is the order of the discrete approximation. This algorithm produces the approximation of the global discretization error ε_l.

1. Repeat Step 2 and 3 for all $\mathbf{p} \in G_{l-1} \cap G_l$
2. Set $(\varepsilon_l)_{l-1} := (2^p - 1)^{-1} \cdot ((C_l)_{l-1} - C_{l-1})$
3. Set $\varepsilon_l := (\varepsilon_l)_{l-1}$
4. [End of Step 1 loop]
5. Repeat Step 6 for $\mathbf{p} \in G_l \setminus G_{l-1}$
6. Set $\varepsilon_l := I((\varepsilon_l)_{l-1})$
7. [End of Step 5 loop]
8. Exit

It is important to note that the global discretization error of the l-th discretization level is estimated on the subgrid which belongs to the coarser discretization error $l-1$. Therefore, it is necessary to interpolate ε_l from $(l-1)$th to l-th discretization level by using the operator I.

3.2 Initial grid refinement

In order to formulate a refinement criterion for the initial grid, which should approximate implanted profiles with the same tolerance level (6), the following error estimator has been introduced:

$$\varepsilon_l = \left(\left(\int_{\Delta D} C dD \right)_l - \int_{\Delta D} (C)_l \right) / \Delta D \, . \tag{7}$$

where $(C)_l$ is the continuous implanted impurity profile presented at the l-th discretization level. This error estimator actually approximates the error in the local dose contents inside the elementary grid cell ΔD and represent the local discretization error of the discrete operator:

$$W_l((C)_l) = \int_{\Delta D}^{l} (C)_l \, / \, \Delta D \, . \tag{8}$$

Adaptive multigrid discretization implies the existence of the compatible discrete operators (8) on different discretization levels which is suitable for the application of the local discretization error extrapolation technique which is described in Algorithm 3.

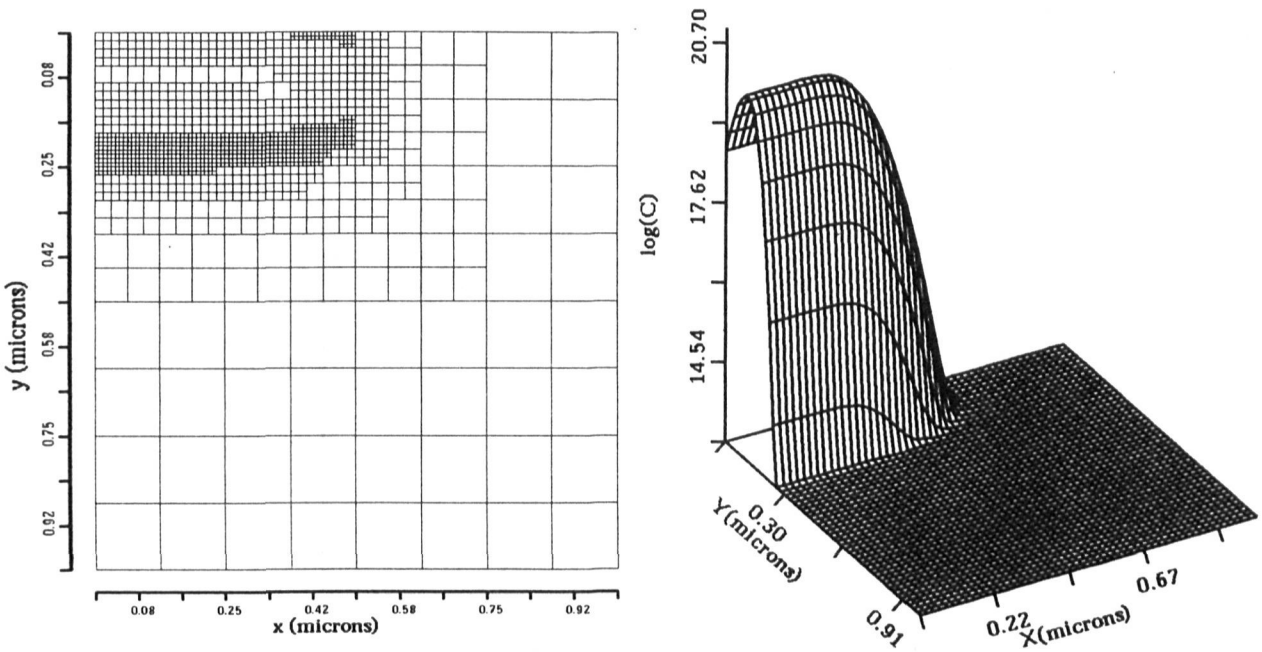
Algorithm 3 (Estimate Local Discretization Error)

Here G_{l-1}, G_l, $(C)_{l-1}$ and $(C)_l$ are local uniform grids on the two successive discretization levels and corresponding discrete presentation of implanted impurity profiles. p is the order of the discrete approximation. This algorithm produces the approximation of the local discretization error ε_l.

1. Repeat Step 2 and 3 for all $\mathbf{p} \in G_{l-1} \cap G_l$
2. Set $(\varepsilon_l)_{l-1} := (2^p - 1)^{-1} \cdot (W_{l-1}((C)_{l-1}) - ((W_l(C)_l)_{l-1})$
3. Set $\varepsilon_l := (\varepsilon_l)_{l-1}$
4. [End of Step 1 loop]
5. Repeat Step 6 for $\mathbf{p} \in G_l \setminus G_{l-1}$
6. Set $\varepsilon_l := I((\varepsilon_l)_{l-1})$
7. [End of Step 5 loop]
8. Exit

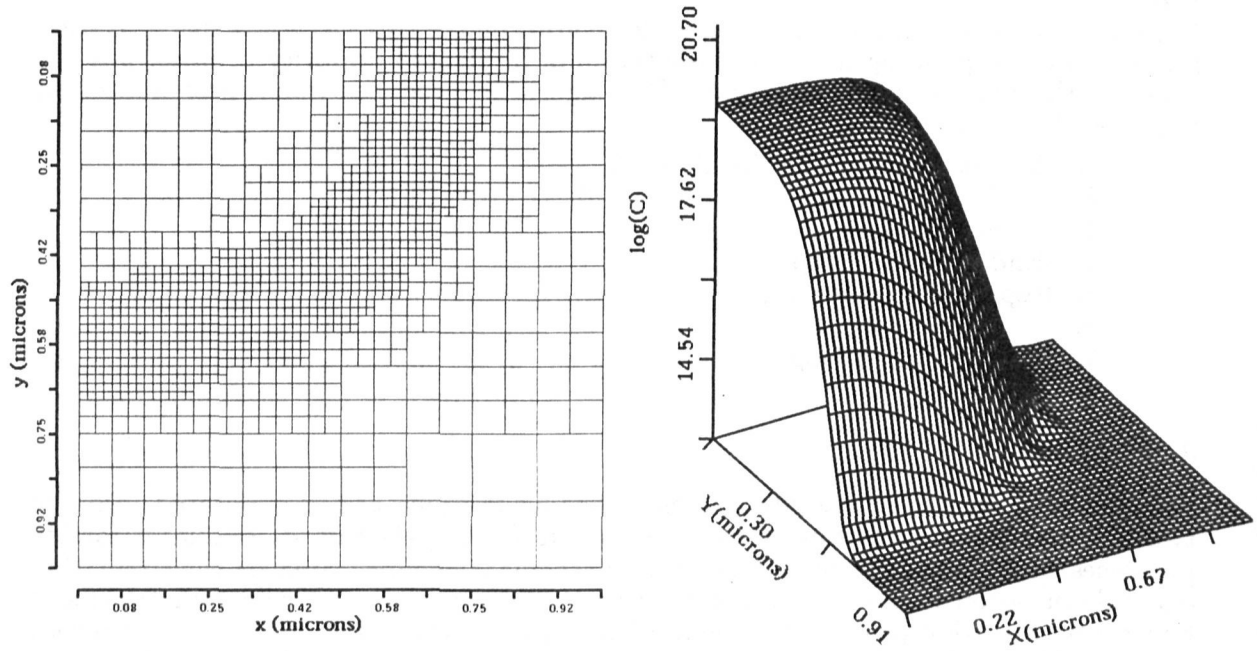
4 Example

All multigrid strategies described in the previous sections are incorporated into the two dimensional process simulation program **MUSIC** (**MU**ltigrid **S**imulator for **IC** processes) [5]. The adaptive grid generation scheme is demonstrated by the simulation example of boron implantation and diffusion. The adaptive multigrid structures and boron concentration profile after the implantation process ($30keV$, $10^{15}cm^{-2}$) are shown in Fig.1. The final multigrid structures and boron concentration profile after 30 minutes diffusion at $1000°C$ are shown in Fig.2. The one dimensional boron profile and grid evolution during the diffusion process is shown in Fig.3.



a) b)

Figure 1: The adaptive multigrid structures (a) and boron concentration profile after ion implantation (b).



a) b)

Figure 2: The final multigrid structures (a) and boron concentration profile after diffusion (b).

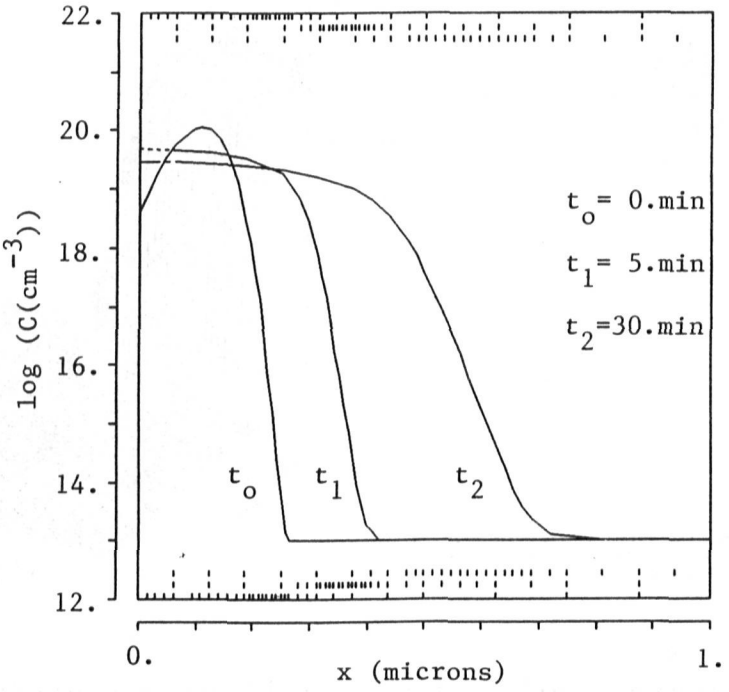


Figure 3: One dimensional profile and grid evolution during diffusion process.

5 Conclusion

The multi–level local grid concept offers a unique and qualitatively different adaptive environment than any single–grid adaptive approach because it gives the required nonuniform resolution of the discrete approximation by using only uniform local grids which makes the implementation and handling of global adaptive structures easy and inexpensive.

In this paper we have presented efficient and robust adaptive strategies which take advantage of the discrete solutions and operators on different discretization levels. Moreover, the refinement criteria for the initial grid generation and grid modifications during diffusion simulation are based on the local and global discretization error with the same tolerance level controlled by the problem independent parameter.

6 References

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