ANISOTROPIC MESH REFINEMENT FOR THREE-DIMENSIONAL DIFFUSION SIMULATION

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ABSTRACT

We present a computational method for locally adapted conformal anisotropic tetrahedral mesh refinement. The element size is determined by an anisotropy function which is governed by an error estimation driven ruler according to an adjustable maximum error. Anisotropy in refinement is taken into account to reduce the amount of elements compared to strict isotropic refinement. The spatial resolution in three-dimensional unstructured tetrahedral meshes for diffusion simulation can be dynamically increased.

INTRODUCTION

In the numerical solution of practical problems of physics engineering such as semiconductor process and device simulation, one often encounters the difficulty that the overall accuracy of the numerical approximation is deteriorated by local exaltations. An obvious remedy is to refine the discretization in the critical regions [1]. The question than is how to identify these regions and how to obtain a good balance between the refined and unrefined regions such that the overall accuracy is optimal. These considerations clearly show the need for error estimators which can be extracted a posteriori from the computed numerical solution and the given data of the problem. The error should be local and should yield reliable upper and lower bounds. The global upper

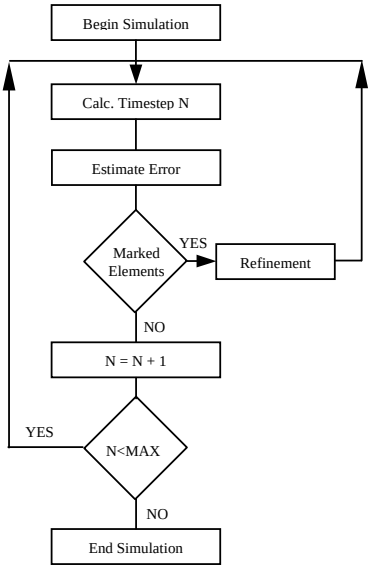

Fig.1. Simulation procedure

bounds are sufficient to obtain a numerical solution with an accuracy below a prescribed tolerance. Local lower bounds are necessary to ensure that the grid is correctly refined according to an adjustable error using a (nearly) minimal number of grid-points. As shown in **Fig. 1**, during the calculation of a time step a combination of error estimation and refinement mechanism is necessary to deliver higher accuracy, if needed, by increasing the spatial resolution.

ANISOTROPIC REFINEMENT

Using strict isotropic meshes for three-dimensional process simulation is not practicable [2]. The necessity to keep the computational time low, and the limitation of memory requires anisotropic adapted meshes. In [3], e.g., the element shapes are controlled by a tensor-based metric space for representing mesh anisotropy over the domain. Anisotropy is defined by three orthogonal principal directions and an aspect ratio in each direction. The three principal directions are represented by three unit vectors $\vec{\xi},\vec{\eta}$ and, $\vec{\zeta}$ and in these directions the amounts of stretching of a mesh element are represented by three scalar values λ_x,λ_y and λ_z respectively. Using $\left(\vec{\xi},\vec{\eta},\vec{\zeta}\right)$ and $\left(\lambda_x,\lambda_y,\lambda_z\right)$ two matrices **R** and **S** can be defined:

$$\mathbf{R} \equiv \begin{pmatrix} \xi_x & \eta_x & \zeta_x \\ \xi_y & \eta_y & \zeta_y \\ \xi_z & \eta_z & \zeta_z \end{pmatrix} \text{ and } \mathbf{S} \equiv \begin{pmatrix} \lambda_\xi & 0 & 0 \\ 0 & \lambda_\eta & 0 \\ 0 & 0 & \lambda_\zeta \end{pmatrix}. \qquad (1)$$

By combining matrices **R** and **S**, a 3×3 positive definite matrix **M** is obtained

$$\mathbf{M} \equiv \mathbf{RSR}^{\mathbf{T}} \qquad (2)$$

that describes the three-dimensional anisotropy.

The basic refinement step in our algorithm is tetrahedral bisection which is well investigated by, e.g. Arnold [4]. When bisecting a tetrahedron, a particular edge - called the *refinement edge* - is selected and split into two edges by a new vertex. As new tetrahedra are constructed by refinement, their refinement edges must be selected carefully to take anisotropy into account without producing degenerately shaped elements. In order to identify which edge should be cut, the length of the edges is calculated in a metric space [5].

A set S with a global distance function (the metric g) which for every two points x, y in S gives the distance between them as a nonnegative real number $g(x, y)$ is called the metric space [6]. The distance function must also satisfy

$$\begin{aligned} &g(x,y) = 0 \Leftrightarrow x = y \\ &g(x,y) = g(y,x) \\ &g(x,y) + g(y,z) \geq g(x,z) \end{aligned} \qquad (3)$$

In our implementation this metric varies over the domain, and hence the length of an edge depends on its position. In case the *anisotropic length* is greater than an adjustable value, the edge is cut in the middle. Calculating the length of an edge in a metric space can be seen as calculating a line integral. In general an arc length ℓ_C is defined as the length along a curve C: $\ell_C = \int_C ds$. **M** as defined in (2) represents a metric when viewed as positive definite tensor $M = M(x, y, z)$ over the entire domain. Roughly spoken, the metric tensor m_{ij} defines how to compute the distance between any two points in a given space. Its components can be viewed as multiplication factors which must be placed in front of the differential displacements dx_i in a generalized Pythagorean theorem

$$ds^2 = g_{11}dx_1^2 + g_{12}dx_1 dx_2 + g_{22}dx_2^2 + \cdots . \qquad (4)$$

The length of a line segment PQ in a metric space is calculated by [7]

$$\ell_{PQ} = \int_0^1 \sqrt{PQ^T \cdot M\left(P + tPQ\right) \cdot PQ}\, dt \qquad (5)$$

where $M(P + tPQ)$ is the metric at point $P + tPQ, t \in [0,1]$.

In case the anisotropic length of an edge exceeds an adjustable limit, this edge is cut in the middle. This process is performed for all edges over the tetrahedral domain resulting in a mesh, which follows the anisotropy tensor field given by (2).

The crux of the matter is to find a suitable anisotropic tensor function which describes the stretching direction and the stretching factors for a specific diffusion problem. Another problem is to find an error estimation which detects those regions where a higher spatial resolution is need. An answer to these questions can be found when looking at the characteristics of the diffusion problem.

DIFFUSION AND DISCRETIZATION

Diffusion can be viewed as the transport of matter caused by a gradient of the chemical potential. This mechanism is responsible for the redistribution of dopant atoms in a semiconductor during a high-temperature processing step. The underlying ideas can be categorized into two major approaches, namely, the continuum theory of Fick's diffusion equation and the atomistic theory [6]. We are using the continuum theory approach which describes the diffusion phenomenon by:

$$\vec{J} = -D \cdot grad(C) \qquad (6)$$

$\vec{J}$ denotes the diffusion flux, D is the *diffusion coefficient* or *diffusivity*, and C is the concentration of the dopant atoms. In general, the diffusion models used in semiconductor process simulation are strongly nonlinear, because the diffusion coefficients depend, e.g., on the impurity concentration and the point defects distribution [7]. These dependencies result in coupled equation systems for impurities and point defects. Additionally, chemical reactions and convection problems have to be considered in the models. However, for better understanding of our refinement techniques, the following explanation is based on the linear parabolic diffusion problem, given by (6).

There are mainly two discretization schemes for PDEs in complicated domains namely the: *finite element* (FE) method and the *finite volume* (FV) (finite box) method. In our diffusion simulator we use the Galerkin approach of the finite element method with linear shape functions and lumping mass with backward Euler time discretization [8]. In two dimensions finite elements and finite boxes give exactly the same discretization, if in the case of finite element the mass matrix is lumped. Therefore, the usage of a customary Delaunay mesh guarantees that the solution does not contain any non-physical negative concentrations [9]. In three dimensions, the situation changes drastically, since the good properties of finite elements on a Delaunay mesh are lost [7]. In many practical cases, one cannot rely on a good quality of the finite element mesh. Then, additional strategies are pursued: e.g., mesh refinement combined with time step reduction. According to standard finite element theory, the discretized solution (using the backward Euler-method) will converge to the exact solution if meshing granularity and time step size tend to zero.

ANISOTROPY FUNCTION AND ERROR ESTIMATION

By applying a finite element discretization the gradient of the dopant concentration is constant over an element and varies from one element to another. According to the diffusion law given by (6) it is obvious that strong variations of the gradient from one element to an adjacent one yield an approximation error when compared to the proper continuos gradient field. This gradient approximation error causes a diffusion flux error which gives rise to a violation of the law of mass conservation.

According to the discussion of a posteriori gradient recovery error estimation by Ainsworth [10], the basic idea is to estimate the error per cell by watching the jump of the solution along the faces of each cell. In our implementation the error estimation is performed by calculating the gradient field of the solution in every element over the domain, where only a small variation in adjacent vectors is allowed. As shown in **Fig. 1**, if the variation of the gradient vectors are to high, the element is marked for the refinement procedure.

The question about the right anisotropy tensor function is more difficult. One of the best choice is to use the HESSIAN matrix of the given dopant profile. The HESSIAN matrix therefore must be given analytically which requires a twice continuously differentiable initial profile, which is inconvenient. The advantage of using the HESSIAN matrix is that it excellently reflects the curvature of the dopant profile and guarantees a good approximation in regions with high derivatives. Another possibility is to use the piecewise constant gradient field for the stretching directions and the estimated error for the stretching factors. This method is more general and shows good practical behavior.

In the next section we show an example of the gradient field approach where the gradient field denotes the stretching directions and the error estimation denotes the stretching factor.

EXAMPLE

The left part of **Fig. 2** shows the initial coarse mesh which carries the dopant concentration. The right part shows the corresponding gradient field and iso-surfaces. The gradient vectors are calculated over every tetrahedron. The orientation of the gradient is turned towards higher concentration values perpendicular to the iso-surfaces of the dopant concentration. The gradient varies much stronger along the short edges of the structure. In this example the piecewise constant gradient field is used for the stretching directions and the

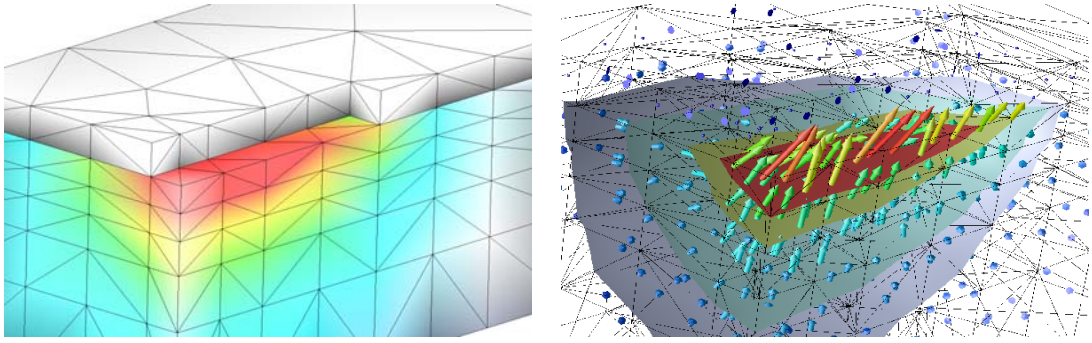

Fig. 2. Dopant concentration. Initial mesh (left). Gradient field and iso-surfaces (right).

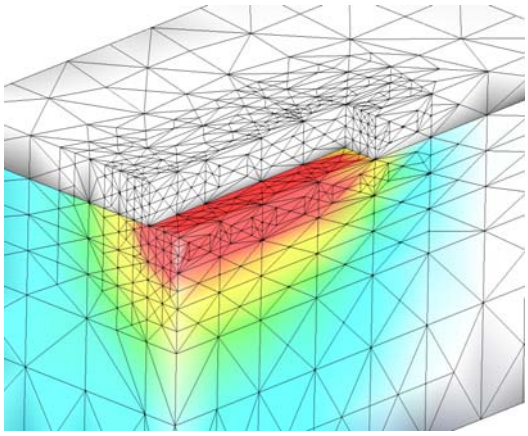

Fig. 3. Refined anisotropic mesh

estimated error for the scaling factors. The results of this refinement strategy can be seen in **Fig. 3**. After refinement the edge length along the long side of the cuboid does not change much, but on the short side a much higher density arises and the resolution is increased. To find a good balance between refined and unrefined regions it is mandatory to take element shapes into considerations and to refine elements belonging to the upper mesh mask structure as a consequence.

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