Comparison between a Posteriori Error Indicators for Adaptive Mesh Generation in Semiconductor Device Simulation

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Nowadays, device simulators are essential tools for designing VLSI devices and much effort is being made to improve their user-interfaces. For example, unified systems have been developed which allow consecutive process and device simulations, and multi-window based simulation environments have been constructed which assist users to operate simulators.

Optimizing discretization mesh, however, is still left to users and this reduces the practicality of device simulators. The adaptive meshing technique resolves this problem by refining the mesh automatically according to the discretization error. Adaptive mesh generation consists of 1) solving semiconductor device equations, 2) evaluating an discretization error indicator, and 3) refining the mesh elements with the large indicator value. These steps are repeated while some element retains the large indicator value. It is crucial to select appropriate indicators for ensuring the precision in calculated device characteristics on the adapted mesh. Although several indicators were already proposed [1–4], more reliable and simpler indicator is desirable especially for the current continuity equation. In this paper, simple error indicators are incorporated into the typical adaptive mesh device simulator HFIELDS [3] and their practicality is examined.

In HFIELDS, the discretization mesh is adaptively generated by using the curvature β of electrostatic potential ψ (or quasi Fermi potentials ϕ_n, ϕ_p) as an error indicator. The indicator β is estimated simply by $\psi''(1+(\psi')^2)^{-1/2}(dx)^2/2$. To limit $\beta(\psi)$ is almost equivalent to limiting the spatial change of $\nabla\psi$, and this reduces the discretization error in the Poisson equation effectively. In the case of the current continuity equation, to limit $\beta(\phi)$ is not effective since current density is proportional to $\nabla\phi$ times carrier density and carrier density varies by several orders of magnitude. Therefore, another indicator should be introduced that either takes account of the carrier density or directly estimates the error in current density.

In the case of MOSFETs simulation, lateral current density varies abruptly near the Si surface along the vertical direction, and this spatial variation in current density can be used as an error indicator. When the discretization mesh is based on box grid, such an indicator is useful as

$$\gamma_r = \frac{|J_1 - J_2|}{\max(|J_1|, |J_2|)} \tag{1}$$

where J_1 and J_2 are current densities along two parallel edges of a box. Essentially, the indicator γ_r examines the uniformity of current density normal to the control volume boundary. Although γ_r can be evaluated easily, it is well defined only for the box based mesh.

As an error indicator for the current continuity equation which is applicable to general triangular mesh, the theoretical error estimator proposed in [5] can be applied. This estimator is based on L_2 norm of flux density error vector $(\boldsymbol{F}-\boldsymbol{F}^*)$, where $\boldsymbol{F}$ denotes calculated flux density (electric field or current density) and $\boldsymbol{F}^*$ denotes the true one. The error estimator for each mesh element E_i is given by

$$\eta_i = \left(\int_{E_i} |\boldsymbol{F}-\boldsymbol{F}^*|^2 \, dV\right)^{\frac{1}{2}}. \tag{2}$$

η is applicable to the error estimation for both the Poisson and the current continuity equations.

In order to estimate η, flux density must be defined at every point in the element. Regarding $\boldsymbol{F}$, uniform flux density in each triangular element can be defined which satisfies

$$(F_1 - \boldsymbol{F}\cdot\boldsymbol{n}_1)\, d_1 = (F_2 - \boldsymbol{F}\cdot\boldsymbol{n}_2)\, d_2 = (F_3 - \boldsymbol{F}\cdot\boldsymbol{n}_3)\, d_3 \tag{3}$$

where F_i denotes flux density along i-th edge e_i of the element, $\boldsymbol{n}_i$ denotes unit direction vector of e_i[2], and d_i denotes length of e_i's control volume boundary limited inside of the element. $\boldsymbol{F}$ defined by (3) gives the same current flow outgoing each control volume as that approximated by the control volume method. Since $\boldsymbol{F}^*$ is unknown, $\boldsymbol{F}^*$ is estimated as follows. First, flux density at each mesh point $\boldsymbol{F}_v$ is estimated by taking a weighted average of flux density values along neighboring edges. Then, $\boldsymbol{F}^*$ is approximated by piecewise linear function formed by $\boldsymbol{F}_v$ within each element.

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[1] This work was carried out while the author was at the D.E.I.S., Università di Bologna.

[2] The edge direction is assumed to be cyclic, i.e. $e_1 = (v_1, v_2), e_2 = (v_2, v_3), e_3 = (v_3, v_1)$ where v_i denotes the vertex point.

Practicality of the error indicator γ_r and η is compared through their application to MOSFET simulation (Fig.1). HFIELDS is used for solving semiconductor device equations and adaptive mesh generation starting from the coarse mesh shown in Fig.2. Since HFIELDS uses triangular mesh based on finite box grid, γ_r can be applied.

Fig.3, 4 and 5 show generated meshes optimized by only $\beta(\psi)$, by $\beta(\psi)$ and γ_r, and by η, respectively. The mesh optimized only by $\beta(\psi)$ is too coarse around the channel inversion layer to obtain a precise drain current. By using γ_r together with $\beta(\psi)$, or by using η, a fine mesh is generated around channel region. Although obtained meshes are slightly different around *pn* junctions, this does not affect the drain current. Fig.6 shows the variation of drain current during the optimization procedure. The mesh optimized by $\beta(\psi)$ and γ_r (B) has approximately 100 more points than that optimized by η (C), though the same drain current is obtained. The reason is because γ_r uses a relative error and thus mesh points are also generated around the region where relatively small current flows. Another disadvantage is that γ_r may not generate a fine mesh when the carrier generation-recombination is significant and the current direction is almost uniform.

The error estimator η is applicable regardless of mesh element shape and it is superior to the other two indicator sets examined here with respect to the optimization ability. Since this indicator is deduced by theoretical investigation, it is expected that this indicator is suitable regardless of device structures and bias conditions.

References

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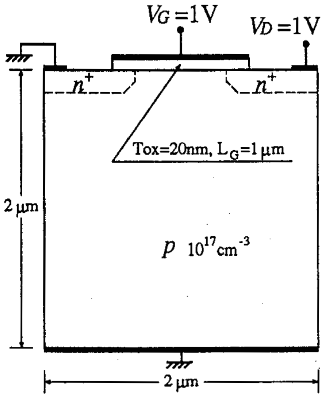

Figure 1: Simulated MOS structure.

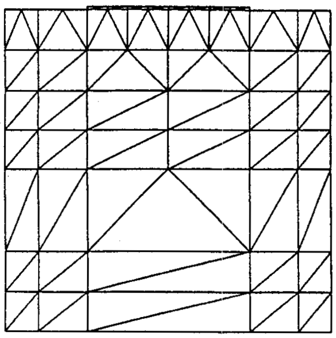

Figure 2: Initial discretization mesh.

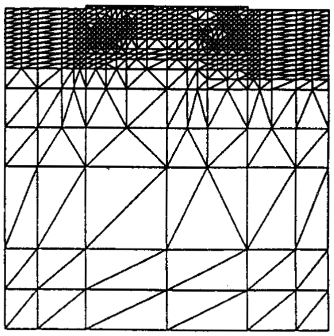

Figure 3: Optimized mesh according to the indicator $\beta(\psi)$.

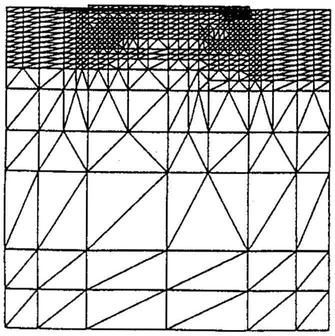

Figure 4: Optimized mesh according to $\beta(\psi)$ and γ_r.

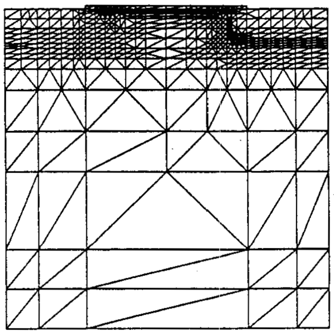

Figure 5: Optimized mesh according to η.

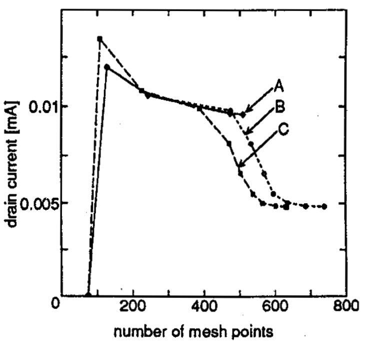

Figure 6: Drain current as a function of the number of mesh points.Used error indicators are A:$\beta(\psi)$, B:$\beta(\psi)$ and γ_r, C:η.