3D Mesh Generation with Wavelet-Driven Adaptivity

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***Abstract*— In this paper we show the effectiveness on 3-dimensional domains of a Wavelet-based Adaptive Method (WAM), which is able to drive a progressive adaptation of computational meshes suited for semiconductor device simulation in order to capture sensible regions. An improved two-step wavelet analysis is performed on some relevant physical variables, allowing for a highly selective refinement of domain regions with stringent resolution requirements for simulation accuracy; moreover, a mesh quality control algorithm ensures a smooth grading of element sizes and eliminates bad configurations affecting convergence. Complex real structures can thus be handled with negligible computational overhead and with no skilled control from the user. Simulation results related to a 3D p-n diode and to different nMOSFET driver geometries demonstrate the capability of the proposed automatic tool to ensure good convergence and accuracy properties with considerable advantages over reference manually-constructed meshes of much larger size.**

***Keywords*— wavelet, device simulation, adaptive meshing.**

I. Introduction

The accuracy of semiconductor device simulations strongly depends on the characteristics of the computational grids used for the solution of partial differential equations governing the device behavior. Mesh generation is thus a delicate task, which normally requires deep physical insight and a difficult trade off between the resolution level necessary to achieve the desired precision and the computational cost determined by the corresponding grid size. Moreover, the task becomes more and more challenging as the dimensionality of the problem and the complexity of the domain increase: great expertise and long time are then required for the user to construct an appropriate mesh for each specific simulation. In this framework, automatic mesh adaptation algorithms would represent a very useful tool able to relieve the user from such a critical and time-consuming task.

In order to optimize the number of unknowns which arise from the discretization of device equations, many adaptive strategies were proposed in literature: most refinement methods are driven by the use of the local truncation error (in both Poisson and current continuity equations [1]), or by other *a-posteriori* error indicators that either utilize solutions of local Dirichlet problems, or measure jumps of relevant quantities [2]. While providing a means to control the simulation accuracy, these approaches generally introduce a significant computational overhead, which can easily become unbearable when complex simulation domains are involved, as is often the case in three-dimensional simulations.

Recently, a new refinement procedure has been proposed [3], which is able to construct anisotropic two-dimensional grids, whose density remarks the internal structure of physical relevances, by means of fast algorithms [4] available for the Wavelet Transform (WT). The method exploits the powerful localization properties which arise from the optimality of WT for the characterization of Besov spaces. Such spaces are suited to capture the layer behavior of the solution of the PDEs which model the electronic devices.

In the following sections we present an extension of this algorithm, implemented to deal with complex 3D geometries. Since 3D simulations are notoriously extremely challenging due to the large grid size usually required to accurately describe the device domain, the proposed software does not arise from a straightforward generalization of the 2D case, but includes significant modifications aiming at a considerable selectivity improvement of the refinement strategy, which avoids redundant nodes insertion. Another major issue is mesh quality: while the presence of obtuse angles can affect convergence and accuracy of standard finite-volume simulators, in literature no algorithms are known which can in general guarantee a Delaunay tetrahedralization of 3D domains without any obtuse angles [5]. In contrast, the dyadic structure of our grids allows for a simple correction procedure [6] which eliminates all obtuse angles in element faces parallel to coordinate axes, with clear benefic effects on simulations.

A p-n diode with 3D-shaped junction and complex nMOS driver geometries have been chosen as test structures to demonstrate the capabilities of our tool to deal with anisotropy and large simulation domains, ensuring both mesh quality and good convergence and accuracy properties.

II. The WAM approach

The wavelet representation of functions originates a set of projection coefficients (*details*), structured over different resolution levels (or *scales*): low level coefficients describe the smooth features of the data, spanning over broad intervals, while the high level ones are associated with strongly localized high frequency singularities [3][4]. The multiresolution nature of the WT thus allows for zooming procedures which progressively reduce the uncertainty of singularities location: in fact rapid variations in the solution shapes, such as sharp changes in low order derivatives or even jumps, generate high wavelet coefficients distributed on the space-scale plane as shown in the example of Fig. 1.

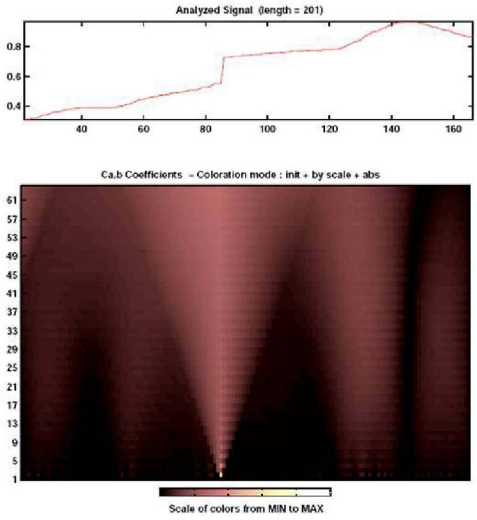

Fig. 1. WT of a discontinuous signal (top figure). The pixel intensity represents the modulus of wavelet coefficients for a certain position (abscissa value) at a given scale (ordinate). Strong gradients and singularities could be localized following local maxima across the space-scale plane with a zooming procedure.

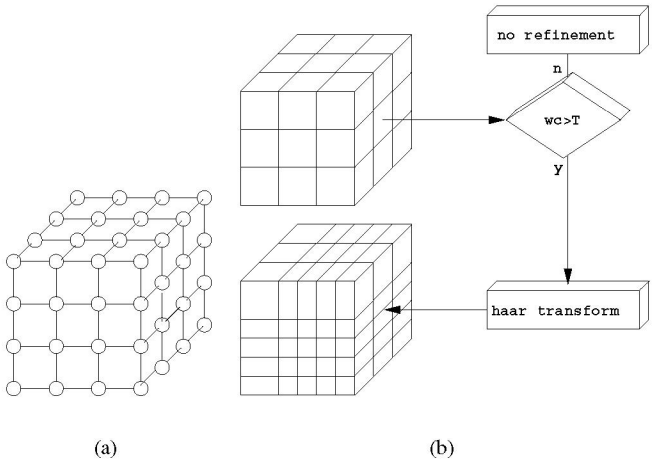

Fig. 2. (a) 3D wavelet support. (b) Details of the Wavelet refinement. The wavelet coefficient (wc) is calculated convolving 4^3 samples of the computational grid. A further step based on the Haar Transform is added to the algorithm presented in [3] to keep the number of inserted vertices as low as possible.

An important application of this kind of analysis is the adaptive approximation of functions by means of a simple threshold procedure that keeps the largest wavelet coefficients only: this task is equivalent to constructing an adaptive approximation grid, whose resolution is locally increased where the signal is irregular. Our approach exploits this technique: a partial solution is calculated on a coarse grid, which is then iteratively and automatically refined only in the regions where the wavelet coefficients calculated on the preliminary results are greater than a given threshold. The refinement algorithm inserts the new nodes in dyadic positions: this allows to construct admissible stencils for coefficient computation on higher levels and consequently the procedure can be iterated to improve the resolution in sensible regions with a zooming analysis across scales. In the following cases, we consider the transformation on the electrostatic potential φ and on carrier concentrations n, p, but different strategies based on other physical quantities are possible as well.

III. 3D SELECTIVITY AND GRID QUALITY IMPROVEMENT

The analysis which drives the adaptive refinement consists in the calculation of detail coefficients by convolving the considered function samples on a number of grid points depending on the particular wavelet chosen. In our case, the choice of the db2 wavelet [7] implies the use of four equidistant samples in each direction for the computation of a single coefficient: 3D details are then obtained by convolving 4^3 grid samples (the stencil or "support" of the wavelet computation, see Fig. 2(a)). Three directional coefficients can be calculated on each support by using a high-pass filter in one direction and low-pass filters in the others. Each coefficient provides a global information on the regularity properties of the analyzed function over an area whose extension depends on the support size corresponding to the current resolution level. However, a certain amount of redundancy is intrinsically introduced by this kind of approach since the whole support is refined even in case of a sharp singularity localized in a small portion of it. While in 2D this is not a relevant issue, in the 3D case the insertion of unnecessary nodes can easily make the mesh size grow too large: for this reason the original refinement strategy has been improved in order to achieve a greater selectivity.

In the modified approach, if a sensible region is detected by means of the db2 analysis, a further transformation step based on the Haar wavelet [8] is performed to drive the anisotropic grid construction. Since the Haar support only includes two samples in each direction, a 3D db2 stencil can be split into 3^3 Haar supports: the new analysis step thus provides additional informations on the localization of singularities, allowing to refine the larger db2 support only partially according to specific criteria on Haar coefficient ratios. By means of the multidirectional analysis, different portions of the original support can also be refined in different directions, thus providing a better resolution of the anisotropic characteristics of the solution. Fig. 2(b) schematically illustrates the described procedure, which considerably improves the refinement selectivity, producing up to a 20% reduction in the number of new nodes insertion.

To provide the possibility of integrating the adaptive method in the framework of conventional device simulators, some requirements have to be fulfilled: in particular, the finite volumes method implemented in standard simulator engines works better if vertices connectivity is defined by a Delaunay mesh without obtuse angles. In two dimensions, due to the semiregular nature of the wavelet-based grid, the number of grid patterns generating obtuse triangles is small, and for each

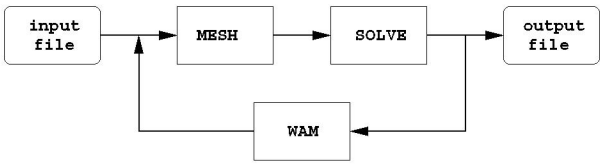

Fig. 3. Block diagram of the validation tool.

one we were able to define a stable correction strategy [6] based on either edge swapping or the insertion of Steiner points. The problem in 3D is much more challenging; however, since our approach is still dyadic, an extension of the correction algorithm has been implemented, which considerably improves the quality of the mesh by eliminating all obtuse element faces parallel to coordinate planes. The procedure has proved to be stable and the number of added nodes is small; on the other hand the introduction of such a step produces great benefits to the solution accuracy in most cases and it is often essential even for simulation convergence.

IV. The validation tool

The wavelet-based refinement module (WAM) has been inserted into the validation tool depicted in Fig. 3, providing the convenient interfacing with a mesh generator block (MESH) and a standard device simulator engine (SOLVE).

MESH analyzes an input file describing the device to be simulated, and, according to geometry and materials, generates some data structures containing both mesh definition and grid points classification suitable for a device solver based on the Scharfetter-Gummel box method, so the validation tool naturally fits into the framework of conventional TCAD softwares. The MESH module is implemented by TETGEN [9], a C++ open source tool that supports Delaunay tetrahedralizations and the insertion of additional points into the mesh. The latter feature provides an efficient interfacing mechanism for the refiner block. The simulation phase results are then used by the refinement module, that represents the WAM extension to 3D problems described above. Once the wavelet-based refinement algorithm has been performed, the correction procedure checks the new grid in order to eliminate the wrong configurations. Then the meshing module is invoked again to build a boundary Delaunay mesh from the resulting set of points. This cycle goes on until a stopping criterion is satisfied.

Our approach can be performed during a quasistationary simulation with a fully adaptive strategy, i.e. adapting the mesh at each bias step. This capability is essentially due to a gradual adaptation strategy which preserves the computational grid from strong variations in nodes location between two consecutive bias steps, thus preventing convergence issues and numerical artifacts in the IV characteristics. As far as the recomputation of the solution on the adapted grid is concerned, extensive numerical tests suggest that with the proposed refinement strategy nonlinear node block Jacobi iteration or homotopy techniques can be completely avoided, even when one has to deal with complex and numerically challenging

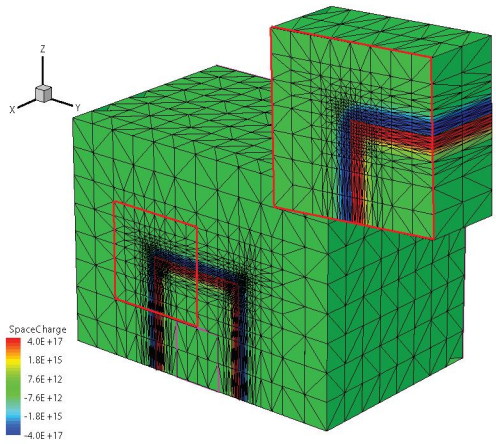

Fig. 4. 3D anisotropic refinement of a p-n diode.

problems such as breakdown simulations, preserving accuracy and reducing CPU time.

V. Simulation results

The automatic refinement strategy has been applied to simulate a set of 3D test structures including a diode and various nMOS drivers with different geometries.

The p-n junction provides a simple but effective test case to highlight the anisotropic capabilities of our tool. Fig. 4 shows how the refinement correctly follows the junction shape, increasing the resolution only in the required directions, with smooth transitions in the profile corners. The improved strategy also ensures good selectivity properties, so that the great majority of mesh points are concentrated in domain regions where the relevant physical phenomena take place.

In Fig. 5 the meshes for two different-shaped n-channel MOSFET drivers are shown; the device structures were selected to test the refiner behavior when dealing with complex geometries and large domains. The figure illustrates some interesting features; in particular, it is important to notice: (1) how the adaptive strategy accurately meshes the regions which have stringent requirements, (2) the absence of obtuse triangles, (3) the smooth grading of mesh elements.

The accuracy of the contact current calculated with our meshes was estimated in comparison with a reference simulation performed with meshes of much larger size. The effectiveness of the WAM approach is influenced by the choice of the threshold which discriminates the relevant wavelet coefficients: an analysis of such an influence for the 3D p-n diode is depicted on Fig. 6, showing how a good choice provides the same degree of accuracy with a great saving in the number of grid points. Moreover the same trend appears at all the successive levels of the wavelet analysis, thus allowing to perform the threshold selection at the first level, when the mesh size is still very small.

Finally, Fig. 7 demonstrates how the obtuse triangle correction procedure is essential to ensure simulation accuracy: the masking of such procedure produces a poor match with reference results in forward bias and definitely compromises

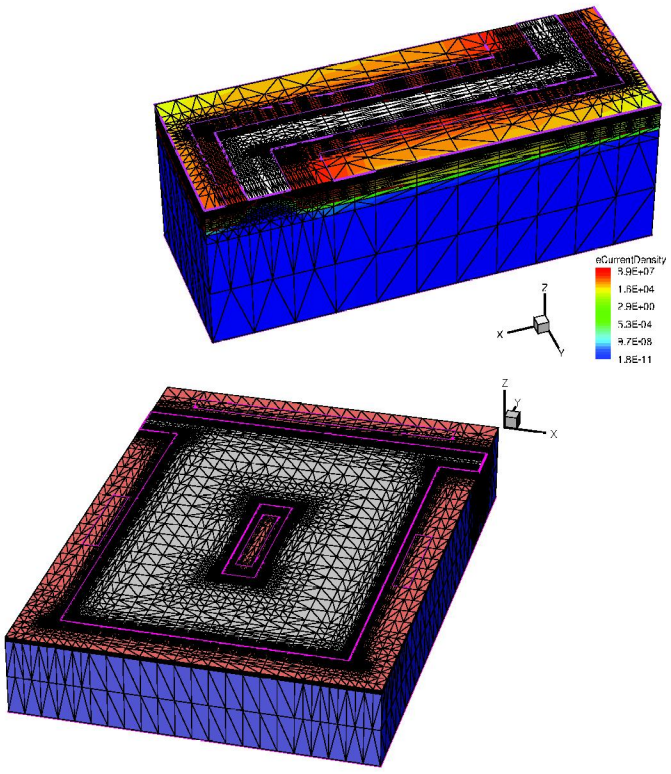

Fig. 5. 3D anisotropic refinement of nMOSFET drivers.

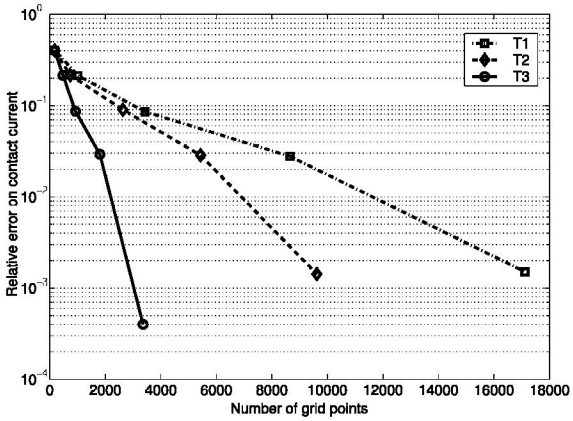

Fig. 6. Example of threshold influence on accuracy and number of vertices ($T1 < T2 < T3$). The higher the threshold, the greater is saving in number of vertices; however, inaccurate (too high) selection causes an unbearable accuracy degradation.

the convergence in reverse bias, even for two-dimensional p-n junction simulations.

VI. Conclusions

The wavelet-based adaptive refinement method already applied to 2D geometries has been extended to deal with three-dimensional device simulations. This extension could not be achieved as a simple generalization of the 2D case because

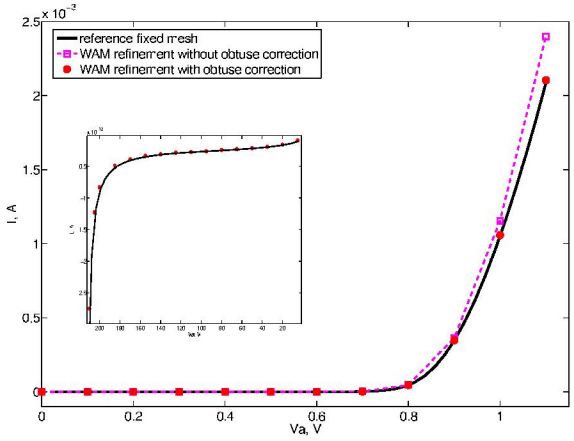

Fig. 7. Comparison of IV curves for a 2D silicon p-n diode with curved junction. The WAM refinement provides a good match with reference characteristics when combined with the obtuse triangle correction: this step is essential to ensure accuracy and even to achieve convergence in the reverse bias.

of some notoriously challenging issues such as redundancy and grid quality. In this paper a modified strategy has been proposed, which strongly improves the selectivity properties of the refinement tool through a two-step wavelet analysis. This also provides an efficient and accurate meshing of the typical anisotropic characteristics of semiconductor device internal quantities. Moreover, the semiregular feature of WAM grids allowed for the implementation of a quality check procedure able to remove undesired mesh patterns affecting simulation convergence and accuracy. The proposed validation tool has been tested on different 3D structures, including a p-n diode and geometrically complex nMOS drivers, to demonstrate the effectiveness of wavelets as a means to guide the automatic refinement of the discretization grid for the simulation of electronic devices and process, preserving the geometrical and physical features of the problem to be solved.

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