

Preconditioned CG-Solvers and Finite Element Grids

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Introduction

To extract parasitic capacitances in wiring structures of integrated circuits we developed the two- and three-dimensional finite element program SCAP (SMART CAPACITANCE ANALYSIS PROGRAM). The program computes the task of the electrostatic field from a solution of Poisson's equation via finite elements and calculates the energies from which the capacitance matrix is extracted. The unknown potential vector, which has for three-dimensional applications 5000 - 50000 unknowns, is computed by a ICCG solver. Currently three- and six-node triangular, four- and ten-node tetrahedral elements are supported.

The capacitance matrix for a charge balanced n -conductor problem has $n(n-1)/2$ entries and can be extracted by $n(n-1)/2$ energy runs. For each run it is necessary to apply a linearly independent potential vector to the contacts and calculate the electrostatic energy. Since the Poisson equation is linear it is only necessary to compute n potential vectors and build up the missing potential vectors from old vectors by superposition.

The variational formulation of the solution of the Euler equation

$$\operatorname{div} \varepsilon(x, y, z) \operatorname{grad} \psi(x, y, z) = 0 \quad (1)$$

is an equivalent formulation of the minimization of the functional

$$I = \varepsilon_0 \int_G \varepsilon_r(x, y, z) \left(\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial \psi}{\partial y} \right)^2 + \left(\frac{\partial \psi}{\partial z} \right)^2 \right) dV \rightarrow \min, \quad (2)$$

which represents exactly twice the electrostatic field energy E_{pot} .

Matrix Assembling

For linear shape functions (only for these) we obtain for the assembled stiffness Matrix an M-Matrix (\mathbf{S} is an M-Matrix if $s_{ii} > 0$, $s_{ij} \leq 0$ for $i \neq j$, \mathbf{S} is nonsingular and $\mathbf{S}^{-1} \geq 0$) based on a Delaunay grid in two dimensions. In [6] it is shown by a counterexample that a three-dimensional Delaunay triangulation does not in general satisfy the condition. Additional boundary nodes have to be inserted to achieve a M-Matrix.

For the following discretization on a triangular partitioning of the domain, using linear shape functions, some criterions have to be satisfied in order to obtain a positive interior connection value between two nodes.

The unknown function ψ is approximated by a combination of linear shape functions for the three triangle corner nodes 1 to 3.

$$\psi(\xi, \eta) = \psi_1 N_1 + \psi_2 N_2 + \psi_3 N_3 \quad N_1 = 1 - \xi - \eta \quad N_2 = \xi \quad N_3 = \eta \quad (3)$$

The transformed formulation for a normalized tirangular element in ξ, η coordinates with inserted shape functions reads

$$I = A \psi^T \int_G \frac{\partial \mathbf{N}}{\partial \xi} \frac{\partial \mathbf{N}^T}{\partial \xi} d\xi d\eta \psi + B \psi^T \int_G \left(\frac{\partial \mathbf{N}}{\partial \xi} \frac{\partial \mathbf{N}^T}{\partial \eta} + \frac{\partial \mathbf{N}}{\partial \eta} \frac{\partial \mathbf{N}^T}{\partial \xi} \right) d\xi d\eta \psi + C \psi^T \int_G \frac{\partial \mathbf{N}}{\partial \eta} \frac{\partial \mathbf{N}^T}{\partial \eta} d\xi d\eta \psi, \quad (4)$$

with the geometric coefficients

$$\begin{aligned} A &= ((y_3 - y_1)^2 + (x_3 - x_1)^2)/J \\ B &= -((y_3 - y_1)(y_2 - y_1) + (x_3 - x_1)(x_2 - x_1))/J \\ C &= ((y_2 - y_1)^2 + (x_2 - x_1)^2)/J \\ J &= (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1) \end{aligned} \quad (5)$$

integration over the elements yields

$$\mathbf{S}_{el} = \frac{1}{2} \begin{pmatrix} A + 2B + C & -A - B & -B - C \\ -A - B & A & B \\ -B - C & B & C \end{pmatrix}. \quad (6)$$

(7)

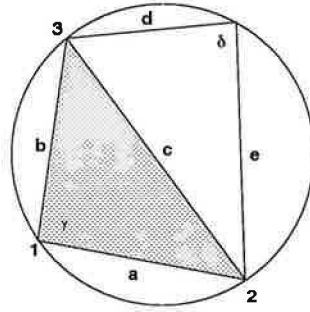


Figure 1: Delaunay criterion

All entries $s_{el\ ii} > 0$ of the stiffness matrix of this element fulfill the M-Matrix criterion. For the off-diagonals, for instance s_{23} the matrix entry in the element matrix becomes positive if the angle opposite two nodes (in this example γ becomes obtuse. For the corresponding in the global stiffness matrix we have to examine the edge c which is shared amongst two triangles. To obtain an M-Matrix the sum of the entries in the global stiffness matrix at each connection has to be negative! Assuming the vertex numbering shown in Fig. 1, we obtain the following criterion for a positive connectivity between nodes 2 and 3.

$$\frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a} \times \mathbf{b}|} + \frac{\mathbf{d} \cdot \mathbf{e}}{|\mathbf{d} \times \mathbf{e}|} > 0 \quad \cot \gamma + \cot \delta > 0 \quad \text{or} \quad \gamma + \delta < \pi \quad (8)$$

This equation assumes that we have the same material for the two adjacent triangles. In the case of different permittivities in different segments we have to rewrite the equation to

$$\varepsilon_1 \cot \gamma + \varepsilon_2 \cot \delta > 0. \quad (9)$$

As a conclusion we can see that for the general case even the Delaunay criterion or sphere criterion in two dimensions does not guarantee an M-Matrix as stiffness matrix. For higher order shape functions, the element stiffness matrix have positive and negative off-diagonal entries and therefore are no M-Matrices.

Preconditioner

For preconditioning the stiffness matrix a CG algorithm an incomplete Cholesky factorization in conjunction with the Eisenstat trick [3] is used. If \mathbf{S} is not an M-Matrix the Cholesky decomposition will certainly not give a regular splitting. As consequence the factorization of \mathbf{S} is not always stable.

This has observed for some examples with quadratic shape functions and bad grid quality. To overcome this non-M-Matrix problem Manteuffel [5] introduced a damping factor for the off diagonal elements for the preconditioner. For the diagonally scaled stiffness matrix

$$\mathbf{S} = \mathbf{I} - \mathbf{B}, \quad \mathbf{S}_d = \mathbf{I} - \frac{1}{1 + \alpha} \mathbf{B} \quad (10)$$

with a sufficiently large α , \mathbf{S}_d will be diagonally dominant. Experiments have shown that an α of 1.5 is an appropriate value for our problems. On the other hand it is evident that the solver loses efficiency by this method.

We observed that only for some nodes in the factorization the recursion starts to get negative

$$\bar{\mathbf{D}} = \mathbf{D} - \text{diag}(\mathbf{L} \cdot \bar{\mathbf{D}}^{-1} \cdot \mathbf{U}) \quad (11)$$

and the CG-Solver diverges. Therefore a simple idea is to eliminate these negative entries which arise from positive off-diagonal entries and to revert the sign of negative $\text{diag}(\mathbf{L} \bar{\mathbf{D}}^{-1} \mathbf{U})$ contributions and proceed. For our examples with the discretized Laplace operator we achieved always convergence. Node ordering for bandwidth reduction improves the solver speed but decreases the overall performance.

Example

The capacitance matrix for the following three-dimensional crosstalk example of two bitlines of a DRAM-Cell can be extracted by three runs with different applied contact potentials. To reduce the crosstalk to other bitlines the trick of twisted pairs will be used here. The disadvantage of the method is that the parasitic capacitances are increased and therefore more line driver current is required. Fig. 2 shows the significant parts of the arrangement: a ground plane (1), the bitline with contact pads (2) and a second bitline (3). The conductors are assumed to have infinite conductivity and are representing Dirichlet boundary conditions. Fig. 3 shows the whole discretized domain. On the outside boundary homogeneous Neumann boundary conditions are assumed except from the bottom plane which is a Dirichlet contact.

On an HP755 we got the following results:

	17673 Tetrahedrons		141384 Tetrahedrons
Shape Functions	linear	quadratic	linear
Matrix size:	(3664, 7.23)	(26480, 13.93)	(26480, 7.56)
Cap ₁₁	$5.81 \cdot 10^{-16} F$	$5.29 \cdot 10^{-16} F$	$5.43 \cdot 10^{-16} F$
Cap ₁₃	$1.64 \cdot 10^{-16} F$	$1.60 \cdot 10^{-16} F$	$1.61 \cdot 10^{-16} F$
Cap ₂₃	$4.11 \cdot 10^{-16} F$	$3.39 \cdot 10^{-16} F$	$3.58 \cdot 10^{-16} F$
CG			
num. iterations	80	186 (186) ¹	162
used time	1.40s	40s (40s)	23.0s
ICCG			
num. iterations	38	92 (77)	83
used time	1.50s	24.0s (21s)	15.0s

References

- [1] BAUER, R., AND SELBERHERR, S. Calculating Coupling Capacitances of Three-Dimensional Interconnections. ICSICT '92 Beijing, China, pp. 697-702.
- [2] BAUER, R., AND SELBERHERR, S. Capacitance Calculation of VLSI Multilevel Wiring Structures. VPAD '93, Nara, Japan, pp. 142-143.
- [3] EISENSTAT, S. C. Efficient Implementation of a Class of Preconditioned Conjugate Gradient Methods. SIAM J. SCI. STAT. COMPUT. Vol. 2, No.1, 1981, pp. 1 - 4.
- [4] BANK, R. E. PLTMG: A Software Package for Solving Elliptic Partial Differential Equations. Users' Guide 6.0 SIAM, ISBN 0898712556.
- [5] MANTEUFFEL T. A. Shifted Incomplete Cholesky-Factorization. Sparse Matrix Proceedings 1978 SIAM, pp. 41-46.
- [6] LETNIEWSKI, F. W. Three-Dimensional Delaunay Triangulations for Finite Element Approximations to a Second-order Diffusion Operator SIAM J. SCI. STAT. COMPUT., Vol. 13, No.3, 1992, pp. 765-770.

¹CutHill-McKee node ordering

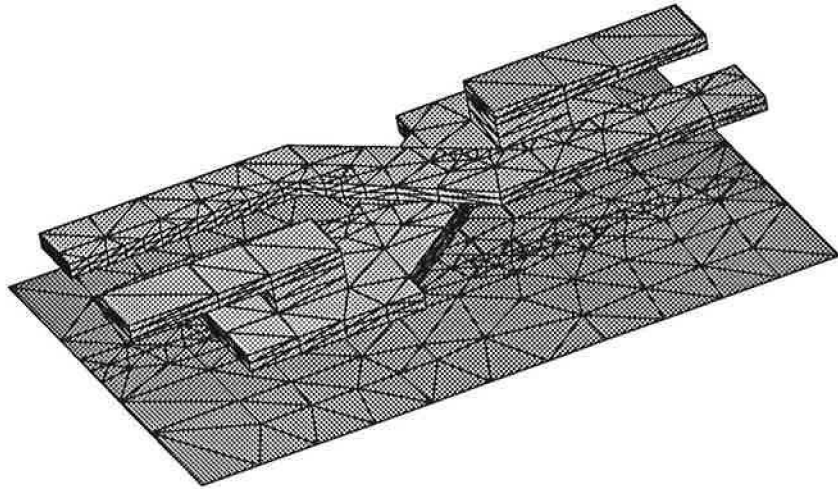


Figure 2: Crossed bitlines with contact pads

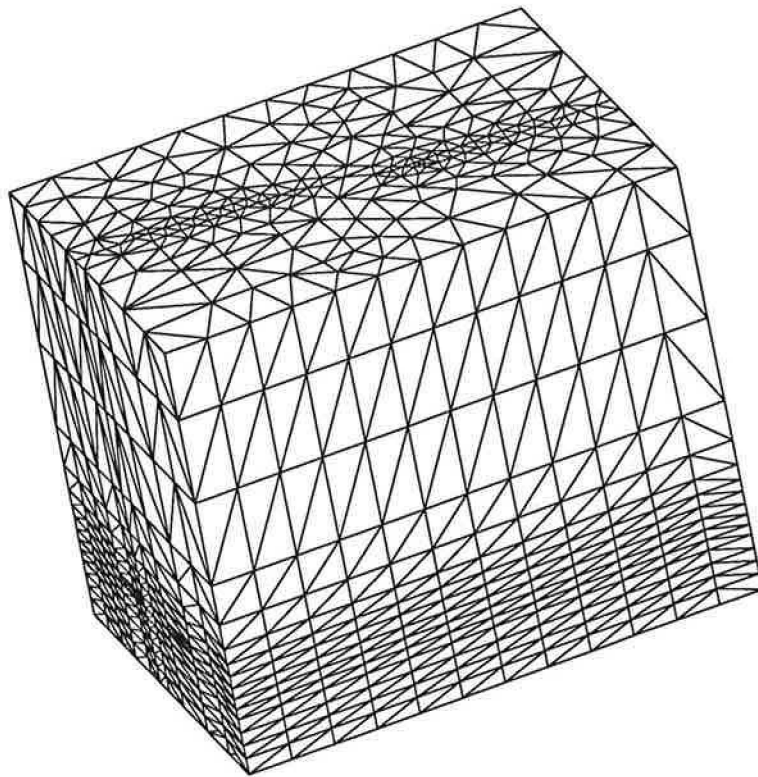


Figure 3: Tetrahedral grid