## On Numerical Methods for PDE-Based Device Simulation: An Introduction

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1. Introduction in discretization and solving procedure for basic drift-diffusion model
2. Mathematical/numerical point of view
3. Interplay between discretization of space (grid) and discretization of differential operators (matrix)
4. Importance of M-matrices

## Content

> Drift-Diffusion Model
An introduction and some analytical properties
> Solving Procedures Nonlinear and linear solvers
> Discretization of Drift-Diffusion Model Some FE examples, the box method, and Scharfetter-Gummel boxmethod
> Grids
Some remarks

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## Drift-Diffusion Model



## Drift-Diffusion Model

Drift-Diffusion Model or van Roosbroeck's equations:

- Describe charge transport in semiconductor devices
- Poisson equation, electron and hole continuity equations (in semiconductors)
- 

$$
\begin{aligned}
& -\nabla \cdot(\varepsilon \nabla \varphi)=q(p-n+C) \\
& \mathrm{q} \frac{\partial n}{\partial t}-\nabla \cdot j_{n}=-q R \\
& q \frac{\partial p}{\partial t}+\nabla \cdot j_{p}=-q R
\end{aligned}
$$

- Completed by electron/hole current equations (using Einstein relation $D=U_{T} \mu$ )

$$
\begin{aligned}
& j_{n}=-q \mu_{n} n \nabla \varphi_{n}=q \mu_{n}\left(U_{T} \nabla n-n \nabla \varphi\right) \\
& j_{p}=-q \mu_{p} p \nabla \varphi_{p}=-q \mu_{p}\left(U_{T} \nabla p+\mathrm{p} \nabla \varphi\right)
\end{aligned}
$$

- Physics: validity of equations, modeling of mobility $\mu$ and recombination $R$

$$
\mu=\mu(x, \nabla \varphi) \quad, \quad R=R(x, n, p, \varphi)
$$

Not topic of this lecture

## DD: Boundary/Interface Conditions

- Domain of equations: distinguish semiconductors, insulators, and metals
- Artificial BCs: artificially introduced borders or the simulation domain

$$
\nabla \varphi \cdot v=j_{n} \cdot v=j_{p} \cdot v=0
$$

- Physical BCs: contact and material interfaces
- Ohmic contacts:

$$
\begin{array}{ll}
n p=n_{i}^{2} & \text { thermodynamic equilibrium } \\
p-n+C=0 & \text { charge neutrality }
\end{array}
$$

result in Dirichlet BCs: $\varphi(x)=\varphi_{0}(x), n(x)=n_{0}(x), p(x)=p_{0}(x)$

- Schottky contacts: ..
- Semiconductor-insulator interfaces:

$$
\begin{aligned}
& \varepsilon_{\text {semi }} \nabla \varphi_{\text {semi }}=\varepsilon_{\text {insu }} \nabla \varphi_{\text {insu }} \\
& j_{n} \cdot v=j_{p} \cdot v=0
\end{aligned}
$$

(neglecting tunneling)

- Heterointerfaces: ...


## Example Structure



Schematic MOSFET model with underlying grid.

## Drift-Diffusion Model

Mathematical View: (only stationary case)
o Task: find functions $\varphi, n, p$ satisfying the above equations
o Simulation domain $\boldsymbol{\Omega}$ : introduce boundary conditions
o Substitute current equations $j_{n, p}$ into DD equations: nonlinearly coupled system of elliptic PDEs (of second order)
o Typical questions:
o Existence of solutions ?
o Uniqueness of solution?
o Is problem well posed (i.e. continuous dependence of solution on 'data') ?
o Nonlinearity:
o drift term in the equations
o Mobility and recombination models

## DD: Some Analytical Properties

1. Existence:

The existence of solutions for the whole system is proven for situations close to equilibrium (assuming certain physical models for the problem).
2. Uniqueness:

In general, uniqueness can not be expected as the experience shows.
3. Layer Behavior:

Scalar diffusion-convection-reaction equations with dominant convection exhibit layer behavior (see Roos,Stynes,Tobiska).
4. Maximum Principle for elliptic PDEs:
coming soon

## DD: Free Energy and Dissipation Rate

## Free Energy:

$$
\begin{aligned}
F(\varphi, n, p) & =\frac{1}{2} \int_{\Omega} \varepsilon\left|\nabla\left(\varphi-\varphi^{*}\right)\right|^{2} d x \\
& +k_{B} T \int_{\Omega} n\left(\ln \left(\frac{n}{n^{*}}\right)-1\right)+n^{*}+p\left(\ln \left(\frac{p}{p^{*}}\right)-1\right)+p^{*} d x
\end{aligned}
$$

Dissipation Rate:

$$
D(\varphi, n, p)=\int_{\Omega} \mu_{n} n\left|\nabla \varphi_{n}\right|^{2} d x+\int_{\Omega} \mu_{p} p\left|\nabla \varphi_{p}\right|^{2}+k_{B} T \int_{\Omega} R \ln \left(\frac{n p}{n^{*} p^{*}}\right) d x
$$

$F$ is Lyapunov function for transient problem under equilibrium boundary conditions and we have:

$$
F(0)-F(t)=\int_{0}^{t} D(\tau) d \tau
$$

## Inverse Monotonicity of Elliptic Operators

Let $L$ be a linear second order elliptic differential operator in divergence form

$$
L u:=-\nabla \cdot[a(x) \nabla u+\boldsymbol{b}(x) u]
$$

Then we have (e.g. Gilbarg, Trudinger, Theorem 9.5):

- Inverse Monotonicity:

$$
\{L u \geq 0 \text { on } \Omega \text { and } u \geq 0 \text { on } \partial \Omega\} \quad \Rightarrow \quad u \geq 0 \text { on } \Omega
$$

- Comparison Theorem:

$$
\{L u \geq L v \text { on } \Omega \text { and } u \geq v \text { on } \partial \Omega\} \quad \Rightarrow \quad u \geq v \text { on } \Omega
$$

- Maximum/Minimum Principle:

$$
\{L u \geq 0 \text { on } \Omega\} \quad \Rightarrow \min _{x \in \Omega}(u(x))=\min _{x \in \partial \Omega}(u(x))
$$

Similar results are valid even for quasilinear operators.

## M-Matrices

Definition (M-Matrix): The real-valued $n x n$-matrix $A$ is M-matrix if

1. $A_{i i}>0$ for all $i$,
2. $A_{i j} \leq 0$ for all $i \neq j$,
3. $\quad A$ is invertible and $A^{-1}$ is nonnegative (i.e. $\left(A^{-1}\right)_{i j} \geq 0$ for all $i$ and $j$ ).

## Remarks:

- Handy sufficient criterion:

If $A$ fulfills the first two conditions and is irreducibly diagonally dominant (i.e. all variables are connected via nonzero offdiagonals, and $\left|A_{i i}\right| \geq \sum_{i \neq j}\left|A_{i j}\right|$, and there exists one $i_{0}$ with strict diagonal dominance), then $A$ is M -matrix.

- $M$-matrices are (positive) stable, i.e. the initial value problem in $\mathbb{R}^{n}$

$$
\dot{x}+A x=0 \quad, \quad x(0)=x_{0}
$$

converges for all initial values $x_{0}$ against 0 .
Stable matrices with nonpositive offdiagonal entries are M-matrices (Horn,Johnson).

- M-matrices are a discrete analogon to the inverse monotonicity of elliptic operators.


## Numerical Discretization

Continuous Problem: formulated in infinite dimensional function spaces

TASK: make finite dimensional

Popular methods:

- Finite differences
- Finite elements
- Box method

Necessary steps:

1. Grid/mesh generation
2. Discretization of the differential operators
3. Solution of nonlinear equations
4. Solution of linear equations

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## Solution Procedures



## Nonlinear Problem

The discretization results in the nonlinear problem in $\mathbb{R}^{n}$

$$
F(u)=\left(\begin{array}{l}
F_{\varphi}(u) \\
F_{n}(u) \\
F_{p}(u)
\end{array}\right)=0 \quad, u=(\varphi, n, p) \in \mathbb{R}^{n}
$$

Nonlinear equations can only be solved iteratively.

## Newton Algorithm

## The well-known Newton iteration:

Given a starting point $u_{0}$, iterate

$$
F^{\prime}\left(u_{n}\right) \cdot\left(u_{n+1}-u_{n}\right)=-F\left(u_{n}\right)
$$

Remarks:

- Quadratic convergence: For sufficiently good starting points (assuming smooth functions $F$ and an isolated root $u^{*}$ ), we have

$$
F\left(u_{n+1}\right)=F\left(u_{n}\right)+F^{\prime}\left(u_{n}\right) \cdot\left(u_{n+1}-u_{n}\right)+O\left(\left|u_{n+1}-u_{n}\right|^{2}\right)
$$

therefore we conclude

$$
\begin{aligned}
& \left|F\left(u_{n+1}\right)\right|=O\left(\left|u_{n+1}-u_{n}\right|^{2}\right)=O\left(\left|F\left(u_{n}\right)\right|^{2}\right) \\
& \left|u_{n+1}-u_{n}\right|=O\left(\left|F\left(u_{n}\right)\right|\right)=O\left(\left|u_{n}-u_{n-1}\right|^{2}\right)
\end{aligned}
$$

- Modifications of pure Newton:
degradation of quadratic convergence, improvement of domain of attraction


## Alternative Nonlinear Solution Procedures

## Gummel Iteration:

- Iteration:

$$
\begin{array}{llll}
\varphi_{k}, n_{k}, p_{k} \text { given: } & & \\
F_{\varphi}\left(\cdot, n_{k}, p_{k}\right)=0 & \rightarrow & & \varphi_{k+1} \\
F_{n}\left(\varphi_{k+1}, \cdot, p_{k}\right)=0 & & \rightarrow & n_{k+1} \\
F_{p}\left(\varphi_{k+1}, n_{k+1}, \cdot\right)=0 & & \rightarrow & p_{k+1}
\end{array}
$$

- Convergence: might converge in case of weak coupling of equations


## Multigrid Procedures:

- Idea: solve problem on different grids with different resolutions, thereby resolving low-frequency components on coarse grids and high-frequency components on fine grids
- Variants: on geometric level (grid) or on the algebraic level (matrix)


## Solution of Linear Equations

Consider the linear equation $\left(A \in M^{n x n}(\mathbb{R}), b \in \mathbb{R}^{n}\right)$ :

$$
A u=b
$$

Remarks:

1. Sparsity: matrices from FD/FE/BM discretizations are sparse, i.e. most entries are zero
2. Nature of Matrix: different procedures for specific sparse matrix problems (e.g. bandstructured, symmetric, diagonally dominant, structurally symmetric, ... )

Two Solver Categories:

- Direct Methods:
- based on Gauss-algorithm, perform LU factorization
- Complexity: dense $O\left(N^{3}\right)$, sparse 2D $O\left(N^{3 / 2}\right)$, sparse 3D $O\left(N^{2}\right)$
- Experimental memory: 2D about 6 times matrix size, 3D about 20 times
- Iterative Methods:
- splitting methods
- Krylov subspace methods (CG, GMRES)
- algebraic multigrid


## Matrix Condition Number

The condition number of a matrix (Golub, van Loan, 'Matrix Computations', 1989)

$$
\kappa(A):=||A \| \cdot|| A^{-1}| |
$$

characterizes the sensitivity of the perturbated equation

$$
(A+\varepsilon F) u_{\varepsilon}=b+\varepsilon f
$$

It can be derived

$$
\frac{\left\|u_{\varepsilon}-u_{0}\right\|}{\left\|u_{0}\right\|} \leq \kappa(A)\left(\varepsilon \frac{\|F\|}{\|A\|}+\varepsilon \frac{\|f\|}{\|b\|}\right)+O\left(\varepsilon^{2}\right)
$$

We have machine precision $\varepsilon \approx 10^{-16}$
(ANSI/IEEE Standard $754-1985$ for 'double floating point numbers'' 64 bit - 1 sign bit, 11 exponent bits, 52 fraction bits)

$$
\text { Maximal number of valid digits of solution } u \approx 16-\log _{10}(\kappa(A))
$$

Device simulation: matrices are stiff, i.e. large condition numbers

## GMRES

## Generalized Minimal Residual (GMRES) Method:

Let $x_{0}, \ldots, x_{k}$ be given, $r_{k}:=b-A x_{k}$ the residuals, and $V_{k+1}:=x_{0}+\left\langle\left\{r_{0}, \ldots, r_{k}\right\}\right\rangle \mathrm{a}$ ( $k+1$ )-dimensional space. Define $x_{k+1}$ by:

$$
\left\|b-A x_{k+1}\right\|_{2}=\min _{x \in V_{k+1}}\left(\|b-A x\|_{2}\right)
$$

## Remarks:

- Detailed algorithm is technical, omitted here.
- Algorithm requires only matrix-vector products $A x$, but not the matrix itself.
- The sequence $\left(x_{k}\right)_{k}$ converges in at most $n$ steps.
- Need to store $k$ vectors to compute $x_{k+1}$.
- GMRES may stagnate (well known, but not really understood).
- A popular variant is the GMRES(m), a restarted GMRES method: stop after $m$ iterations and initialize the procedure again.
- If $A$ is positive definite, GMRES( $m$ ) converges for any $m \geq 1$.
- General convergence results for GMRES(m) are not available.


## Preconditioning

Idea: Instead of solving $A x=b$ we solve

$$
P_{L}^{-1} A x=P_{L}^{-1} b
$$

Remarks:

- $P_{L}$ should be easier to invert than $A$.
- Convergence: If $P_{L}$ is close to $A$, we have $\left\|1-P_{L}^{-1} A\right\|<1$, sufficient for convergence of simple methods.
- Right preconditioning: solve $A P_{R}^{-1} y=b$ for $y$, compute $x=P_{R}^{-1} y$.
- Right vs left preconditioning:

Left preconditioning minimizes the preconditioned residual.
Right preconditioning minimizes the unpreconditioned residual.
For ill-conditioned systems this makes a difference.

Some preconditioning strategies:

- Incomplete LU factorization ILU (with/without threshold).
- Think about physically motivated preconditioners.

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## Discretization of the Drift-Diffusion Model

## BVP: Strong and Weak Formulation

Elliptic boundary value problem (BVP) of the following form:

$$
\begin{array}{rlr}
L u:=-\nabla \cdot(a \nabla u)+b u=f & \text { on } \Omega \\
& a \frac{\partial u}{\partial n}=g & \text { on } \partial \Omega_{N} \\
u=0 & \text { on } \partial \Omega_{\mathrm{D}}
\end{array}
$$

Strong formulation of the problem: Find a function $u \in H$ with the above properties.

Alternative: Choose a test function $v \in H_{0}=\left\{u \in H: u=0\right.$ on $\left.\partial \Omega_{D}\right\}$, multiply the strong problem and integrate by parts.

Weak formulation of the problem:
Find $u \in H_{D}=\left\{u \in H: u\right.$ satisfies Dirichlet BCs on $\left.\partial \Omega_{D}\right\}$ such that for all $v \in H_{0}$ we have

$$
B(u, v):=(a \nabla u, \nabla v)+(b u, v)=(f, v)-\int_{\partial \Omega_{N}} g d S(x)
$$

## 1D Laplace Equation: Standard FE

Laplace equation 1D

$$
\begin{array}{cl}
L u:=-\nabla \cdot(\nabla u)=f & \text { on } \Omega \\
u=0 & \text { on } \partial \Omega
\end{array}
$$

Weak formulation: Find $u \in H_{0}^{1}$ (Sobolev space) with

$$
B(u, v)=\int_{\Omega} \nabla u(x) \cdot \nabla v(x) d x=\int_{\Omega} f v d x=(f, v)
$$

Standard FE on grid $\left(x_{0}, \ldots, x_{N}\right)$ :
Ansatz: $u(x)=\sum_{j} u_{j} \xi_{j}(x)$, where $\xi_{i}$ is hat function at $x_{i}$
Computation per element $K=\left[x_{i}, x_{i+1}\right], h_{i}:=x_{i+1}-x_{i}$

$$
\begin{aligned}
& B^{K}\left(\xi_{i}, \xi_{i}\right)=\int_{K}\left(\frac{1}{h_{i}}\right)^{2} d x=\frac{1}{h_{i}} \\
& B^{K}\left(\xi_{i}, \xi_{i+1}\right)=-\frac{1}{h_{i}}
\end{aligned}
$$

Element matrix: $\quad A^{K}=\left(\begin{array}{cc}1 / h_{i} & -1 / h_{i} \\ -1 / h_{i} & 1 / h_{i}\end{array}\right)$
Global matrix: $\quad A=\operatorname{tridiag}\left(-1 / h_{i-1}, 1 / h_{i-1}+1 / h_{i},-1 / h_{i}\right)$
We get a M-matrix

## 2D Laplace Equation: Standard FE

Laplace equation with homogenous Dirichlet BCs in 2D

$$
B(u, v)=\int_{\Omega} \nabla u(x) \cdot \nabla v(x) d x=\int_{\Omega} f v d x=(f, v)
$$

## Remarks:

1. Bilinear form $B$ can be evaluated on $U^{h} \times U^{h}$, hence $B^{h}$ is uniformly elliptic.
2. The right integral can not be computed exactly for general $f \in L^{2}(\Omega)$ :

Ansatz $f=\sum_{j} f_{j} \xi_{j}(x)$ leads to discrete form $M f$
3. Resulting linear system

$$
A u=M f
$$

4. $A$ is positive definite, hence stable.
5. A is not necessarily M-matrix, but we have in 2D:

For triangulations without obtuse angles, then $A$ is M-matrix.
6. Mesh geometry determines matrix properties.
7. Similar results hold for the Poisson equation

$$
B(u, v)=\int_{\Omega} a(x) \nabla u(x) \cdot \nabla v(x) d x=\int_{\Omega} f v d x=(f, v)
$$

## Box Method (BM)

Assumption: Divergence form of operator

$$
L u(x)=-\nabla \cdot \boldsymbol{F}(x, u)=f(x)
$$

and partition of $\Omega$ into boxes $B_{i}$.
Gauss theorem per box $B_{i}$ :

$$
\int_{\mathrm{B}_{\mathrm{i}}} L u(x) d x=-\int_{B_{i}} \nabla \cdot \boldsymbol{F}(x, u(x)) d x=-\int_{\partial B_{i}} \boldsymbol{F}(x) \cdot v_{i}(x) d S(x)
$$

## Remarks:

- Transform divergence form from volume integral into surface integral
- We need approximation for $\boldsymbol{F}(x) \cdot v_{i}(x)$ on box boundary.
- Form of boxes not yet specified.
- Relation to FE: The test function is the characteristic function of the box, trial functions are not yet specified.


## BM: Voronoi Boxes

Box method with grid vertices ( $\bullet$ ) and dual Voronoi grid (blue)


Voronoi boxes: defined by mid-perpendicular 'planes' of all grid edges:

$$
B_{i}=\left\{x \in \Omega:\left|x-x_{i}\right| \leq\left|x-x_{j}\right| \text { for all } j \neq i\right\}
$$

## BM: Delaunay Property

## Delaunay Property:

The (inner of the) circumsphere/circle of each grid element does not contain any grid point.

## Remarks:

- Delaunay guarantees overlap-free partitioning of $\Omega$ with Voronoi boxes.
- Obtuse angles (i.e $\geq \pi / 2$ ):

$$
s^{T_{1}}{ }_{i, j}<0, \quad s^{T_{2}}{ }_{i, j}>0
$$

Delaunay guarantees

$$
s_{i, j}:=s^{T_{1}}{ }_{i, j}+s^{T_{2}}{ }_{i, j} \geq 0
$$

## BM: Poisson Equation

## Poisson Equation:

$$
L u(x)=-\nabla \cdot(a(x) \nabla u)=g(x)
$$

Mid-perpendicular box method:

$$
\begin{gathered}
-\int_{\mathrm{B}_{\mathrm{i}}} \nabla \cdot(a(x) \nabla u) d x=-\int_{\partial \mathrm{B}_{\mathrm{i}}} a(x) \nabla \mathrm{u}(\mathrm{x}) \cdot v_{i} d S(x) \approx-\sum_{j(i)} a_{i j} \frac{u_{j}-u_{i}}{\left|x_{j}-x_{i}\right|} s_{i j} \\
\int_{B_{-} i} g(x) d x \approx\left|B_{i}\right| g_{i}
\end{gathered}
$$

with $a_{i j}=\left(a\left(x_{j}\right)+a\left(x_{i}\right)\right) / 2$ some average of $a$ on the edge.

## Remarks:

- M-matrix property depends on averaging of $a$.
- Laplace operator: std FE and BM coincide in 2D, but differ in 3D (except for equilateral tetrahedra which do not fill the whole space).


## 1D Drift-Diffusion: Model Problem

Drift-diffusion operator on the interval $[0 ; 1]$ :

$$
\begin{aligned}
& -\left[n^{\prime}-\varphi^{\prime} n\right]^{\prime}=0 \\
& n(0)=0, n(1)=1
\end{aligned}
$$

and assume $\varphi^{\prime}=\beta$ to be constant
o Exact solution: $\quad n(x)=\frac{\exp (\beta x)-1}{\exp (\beta)-1}$
o Solution is strictly monotonously increasing (independent of sign of $\beta$ )
o Well known: large drift causes problems in discretization, leading to instabilities

## 1D Drift-Diffusion: FD Discretization

Equidistant grid: $h=x_{i+1}-x_{i}$
Gradients on intervals left and right: $s_{-}:=\frac{n_{i}-n_{i-1}}{h}$ and $s_{+}:=\frac{n_{i+1}-n_{i}}{h}$

## Equation:

$$
\begin{gathered}
-\frac{s_{+}-s_{-}}{h}+\beta \frac{s_{+}+s_{-}}{2}=0 \\
-\frac{n_{i+1}-n_{i}+n_{i-1}}{h^{2}}+\beta \frac{s_{i+1}-s_{i-1}}{2 h}=0
\end{gathered}
$$

Matrix:

$$
A=\frac{1}{2 h^{2}} \operatorname{tridiag}(-2-h \beta,+4,-2+h \beta)
$$

- We get $\frac{s_{+}}{s_{-}}=\left(1+\frac{h \beta}{2}\right) /\left(1-\frac{h \beta}{2}\right)$ or in words

$$
\text { The solution oscillates if } \boldsymbol{h} \boldsymbol{\beta}>2 \text { !!! }
$$

- The equation poses requirements grid or discretization
- The resulting matrix is not M-matrix
- The characteristic quantity $P=2 / \beta$ is called mesh Peclet number
- Some words: upwinding method, exponential fitting


## 1D Scharfetter-Gummel Discretization

Assumptions: $\left[x_{0}, x_{1}\right]$ interval, $J$ constant current density, and $u:=\exp (-\phi)$ the Slotboom variable, then

$$
J=-\mu n \phi^{\prime}=\mu \exp (\varphi) u^{\prime}
$$

$\mu$ constant, and $\varphi$ linear in $x$, and use notation $\Delta x:=x_{1}-x_{0}$
Solve BVP for u:

$$
\begin{gathered}
\Delta u=\int \frac{J}{\mu} \exp \left(\left[-\varphi_{1}\left(x-x_{0}\right)-\varphi_{0}\left(x_{1}-x\right)\right] / \Delta x\right) d x \\
=\cdots=\frac{J}{\mu} \frac{\Delta x}{\Delta \varphi}\left[\exp \left(-\varphi_{0}\right)-\exp \left(-\varphi_{1}\right)\right]
\end{gathered}
$$

Express J in terms of densities: replace $u_{i}=\exp \left(-\varphi_{i}\right) n_{i}$, then

$$
\begin{gathered}
J=\frac{\mu}{\Delta x} \Delta u \Delta \varphi\left[\frac{1}{\exp \left(-\varphi_{0}\right)-\exp \left(-\varphi_{1}\right)}\right]=\frac{\mu}{\Delta x}\left[\frac{\Delta \varphi}{\exp (\Delta \varphi)-1} n_{1}+\frac{\Delta \varphi}{1-\exp (-\Delta \varphi)} n_{0}\right] \\
=\frac{\mu}{\Delta x}\left[b(\Delta \varphi) n_{1}-b(-\Delta \varphi) n_{0}\right]
\end{gathered}
$$

where we used the Bernoulli function $b(x):=x /(\exp (x)-1)$.

## SG Current Density

Scharfetter-Gummel (SG) approximation

$$
J=\frac{\mu}{\Delta x}\left[b(\Delta \varphi) n_{1}-b(-\Delta \varphi) n_{0}\right]
$$

## Remarks:

- SG reduces for $\Delta \varphi=0$ to pure diffusion.
- Resembles an unsymmetrically weighted diffusion expresion (artificial diffusion).
- BM with this SG approximation for J gives M-matrix independent of $\Delta \varphi$ because

$$
\frac{\partial J}{\partial n_{0}}<0, \quad \frac{\partial J}{\partial n_{1}}>0
$$

## Discretized Equations

Higher dimensions:

- The SG expression is used in the BM, extending to the SG-BM.
- The one-dimensional character along grid edges remains.


## Discretized equations:

$$
\begin{gathered}
\left(F_{\varphi}\right)_{i}=\left[\sum_{j(i)} \varepsilon_{i j} \frac{s_{i j}}{d_{i j}}\left[\varphi_{i}-\varphi_{j}\right]\right]-\left|\mathrm{B}_{\mathrm{i}}\right|\left(p_{i}-n_{i}+C_{i}\right)=0 \\
\left(F_{n}\right)_{i}=\left[\sum_{j(i)} \mu_{i j}^{n} \frac{s_{i j}}{d_{i j}}\left[b\left(\varphi_{i}-\varphi_{j}\right) n_{i}-b\left(\varphi_{j}-\varphi_{i}\right) n_{j}\right]\right]+\left|\mathrm{B}_{\mathrm{i}}\right| R_{i}=0 \\
\left(F_{p}\right)_{i}=\left[\sum_{j(i)} \mu_{i j}^{p} \frac{s_{i j}}{d_{i j}}\left[b\left(\varphi_{j}-\varphi_{i}\right) p_{i}-b\left(\varphi_{i}-\varphi_{j}\right) p_{j}\right]\right]+\left|\mathrm{B}_{\mathrm{i}}\right| R_{i}=0
\end{gathered}
$$

## SG-BM: Discussion

- No closed theory is known for the SG-BM.
- SG-BM guarantees stability on arbitrary boundary Delaunay meshes (extensively used in practice).
- SG-BM as nonconforming Petrov-Galerkin method.
- SG-BM is locally and globally dissipative: the dissipation rate per (non-obtuse) simplex is positive (Gajewski-Gartner).
- Low convergence order is expected: experiments with grid adaptation show $O\left(h^{1 / 2}\right)$.
- The required boundary Delaunay property is quite restrictive (compared to simplex meshes).

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## Grids



## 3D Example



## Quad-Tree vs Normal-Offsetting



Quad-tree and normal-offsetting mesh with current density.

## SG-BM and Current Carrying Edges

## Observations

- BM current along edge with one element

$$
I_{i j}^{E}=s_{i j}^{E} J_{i j}^{E}
$$

- SG-BM: element edge current densities $J_{i j}^{E}$ are not projections of one element vector $\boldsymbol{J}^{E}$
- Large element edge current densities might not be visible on other edges
- Effect on total current: large $J_{i j}^{E}$ with small Voronoi surface $s_{i j}^{E}$ not visible


Edge with Voronoi surface

## Consequences

- Edges should be aligned parallel and orthogonal to the local current density.
- Highly anisotropic grids are desired in such situations (like channel of a MOSFET).


## Grid Effect on Terminal Current



Huge current variations
for a MOSFET structure during automatic grid adaptation.

Filled symbols indicate currents at same bias of AGM simulation.

AGM: grid adapation
REF: fixed grid

## Concluding Remarks

- We gave an introduction into discretization and solution strategies for the DD model.
- We emphasized the importance of the M-matrix property, which seems to be indispensable.
- We illustrated the relation between mesh and matrix properties.
- Properties of the continuous problem are not automatically inherited by the discrete problem.


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Thank you for your attention !


