Control Volume Finite Element Method for Drift-diffusion Equations on General Unstructured Grids

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Numerical Methods for Transport

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Outline

1. Introduction
2. CVFEM Formulation
3. Scharfetter-Gummel Upwinding
4. Selected Computational Results
5. Conclusions

Introduction

Nonlinear coupled drift-diffusion equations for semi-conductors

$$\nabla \cdot (\lambda^2 \mathbf{E}) - (p - n + C) = 0 \quad \text{and} \quad \mathbf{E} = -\nabla\psi \quad \text{in } \Omega \times [0, T]$$

$$\frac{\partial n}{\partial t} - \nabla \cdot \mathbf{J}_n + R(\psi, n, p) = 0 \quad \text{and} \quad \mathbf{J}_n = \mu_n n \mathbf{E} + D_n \nabla n \quad \text{in } \Omega \times [0, T]$$

$$\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{J}_p + R(\psi, n, p) = 0 \quad \text{and} \quad \mathbf{J}_p = \mu_p p \mathbf{E} - D_p \nabla p \quad \text{in } \Omega \times [0, T]$$

E - electric field
n - electron density
ψ - electric potential
p - hole density

Want a numerical scheme that is:

- stable in advection-dominated regime
- locally conservative

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Want a numerical scheme that is: (Standard approach)

- stable in advection-dominated regime $\rightarrow$ Scharfetter-Gummel upwinding
- locally conservative $\rightarrow$ finite volume method

These schemes are typically limited to topologically dual grids

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Want a numerical scheme that is: (Our approach)

- stable in advection-dominated regime $\rightarrow$ multi-dimensional S-G upwinding
- locally conservative $\rightarrow$ control volume finite element method

Stable and robust on unstructured grids

CVFEM Formulation

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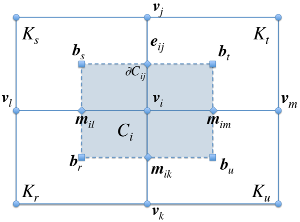
Electron continuity equation

$$\frac{\partial n}{\partial t} - \nabla \cdot \mathbf{J}_n + R(\psi, n, p) = 0$$

$$n = g \quad \text{on} \quad \Gamma_D, \quad \mathbf{J}_n \cdot \mathbf{n} = q \quad \text{on} \quad \Gamma_N$$

$$n(0, \mathbf{x}) = n_0(\mathbf{x}) \quad \text{in} \quad \Omega$$



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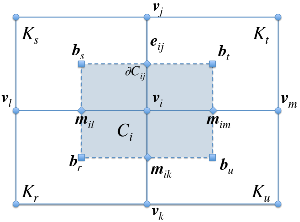

Integrate over control volume C_i and apply divergence theorem

$$\int_{C_i} \frac{\partial n}{\partial t} dV - \int_{\partial \dot{C}_i} \mathbf{J}_n \cdot \vec{\mathbf{n}} dS = - \int_{C_i} R(\psi, n, p) dV + \int_{\partial C_i^N} q dS \quad \forall v_i \in V(\Omega \cup \Gamma_N)$$

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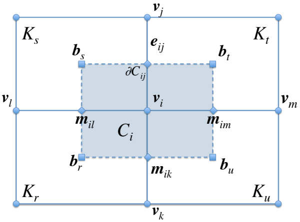

Approximate electron density by $n_h(\mathbf{x}, t) \in \mathbf{G}_D^h(\Omega)$

$$\int_{C_i} \frac{\partial n_h}{\partial t} dV - \int_{\partial \dot{C}_i} \mathbf{J}_n \cdot \vec{\mathbf{n}} dS = -\int_{C_i} R(\psi, n_h, p) dV + \int_{\partial C_i^N} q dS$$

where $\mathbf{J}_n(n_h(\mathbf{x}, t)) = \mu_n n_h(\mathbf{x}, t)\mathbf{E} + D_n \nabla n_h(\mathbf{x}, t)$

and $n_h(\mathbf{x}, t) = \sum_{v_j \in V(\Omega \cup \Gamma_N)} n_j(t) N_j(\mathbf{x}) + \sum_{v_j \in V(\Gamma_D)} g(v_j, t) N_j(\mathbf{x})$

CVFEM Formulation

Electron continuity equation

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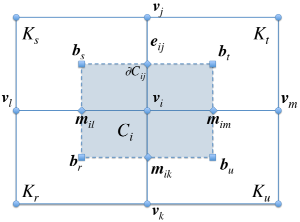


Semi-discrete in space CVFEM formulation

$$\int_{C_i} \frac{\partial n_h}{\partial t} dV - \int_{\partial \dot{C}_i} \mathbf{J}_n \cdot \vec{\mathbf{n}} dS = -\int_{C_i} R(\psi, n_h, p) dV + \int_{\partial C_i^N} q dS$$

$$\text{where} \quad \mathbf{J}_n(n_h(\mathbf{x}, t)) = \sum_{v_j \in V(\Omega \cup \Gamma_N)} n_j(t)(\mu_n N_j \mathbf{E} + D_n \nabla N_j)$$

For advection-dominated problems nodal current density $\mathbf{J}_n$ can develop spurious oscillations. Need some form of stabilization.

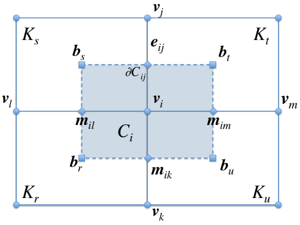
Scharfetter-Gummel Upwinding

- Assume that electric potential varies linearly along $\mathbf{e}_{ij}$

$$E_{ij} = -\frac{(\psi_j - \psi_i)}{h_{ij}}; \quad \psi_i = \psi(v_i); \psi_j = \psi(v_j)$$

- 1-d boundary value problem along primal edge ($\mathbf{e}_{ij}$) for $J_{ij} \approx \mathbf{J}_n \cdot \mathbf{n}_{ij}$

$$\frac{dJ_{ij}}{ds} = 0; \quad J_{ij} = \mu_n E_{ij} n(s) + D_n \frac{dn(s)}{ds}$$
$$n(0) = n_i \quad \text{and} \quad n(h_{ij}) = n_j$$



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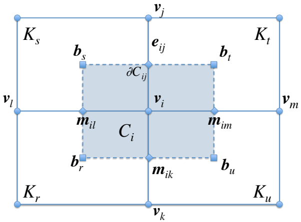

When topologically dual

$$\mathbf{J}_n \cdot \mathbf{n}_{ij}|_{m_{ij}} = \pm \mathbf{J}_n \cdot \mathbf{t}_{ij}|_{m_{ij}}$$

Outgoing flux through control volume boundary

$$\int_{\partial \dot{C}_i} \mathbf{J}_n \cdot \mathbf{n} dS \approx \sum_{\partial C_{ij} \in \partial \dot{C}_i} \frac{a_{ij} D_n}{h_{ij}} \left(n_j \left(\coth(a_{ij}) + 1 \right) - n_i \left(\coth(a_{ij}) - 1 \right) \right) |\partial C_{ij}|$$

where $a_{ij} = \frac{h_{ij} E_{ij}}{2\beta}, \quad \beta = \frac{k_B T}{q}, \quad \mu_n = \frac{D_n}{\beta}$

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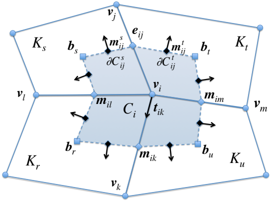

On unstructured grids, J_{ij} not a good estimate of $\mathbf{J}_n \cdot \mathbf{n}_{ij}^t$

Outgoing flux through control volume boundary

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Idea: Use $H(curl)$-conforming finite elements to expand edge currents into primary cell

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Nodal space, $\mathbf{G}_D^h(\Omega)$, and edge element space, $\mathbf{C}_D^h(\Omega)$, belong to an exact sequence

$$\text{given} \quad N_i \in \mathbf{G}_D^h(\Omega), \quad \nabla N_i \in \mathbf{C}_D^h(\Omega)$$

For the lowest order case

$$\nabla N_i = \sum_{e_{ij} \in E(v_j)} \sigma_{ij} \overrightarrow{W}_{ij}, \quad \sigma_{ij} = \pm 1$$

If the carrier drift velocity $\mu_n \mathbf{E} = 0$

$$\mathbf{J}_n(n_h) = \sum_{e_{ij} \in E(v_j)} D_n(n_j - n_i) \overrightarrow{W}_{ij}$$

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Exponentially fitted current density

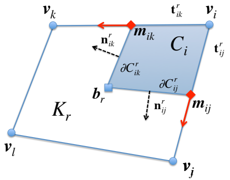
$$\mathbf{J}_E = \sum_{e_{ij} \in E(\Omega)} a_{ij} D_n \left(n_j \left(\coth(a_{ij}) + 1 \right) - n_i \left(\coth(a_{ij}) - 1 \right) \right) \overrightarrow{W}_{ij}$$

Multi-dimensional S-G Upwinding

Standard S-G

$$\int_{\partial \dot{C}_i} \mathbf{J}_n \cdot \mathbf{n} dS \approx \sum_{\partial C_{ij} \in \partial \dot{C}_i} J_{ij} |\partial C_{ij}|$$

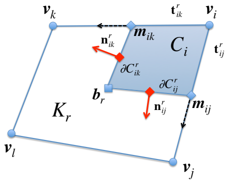
$$= \sum_{\partial C_{ij} \in \partial \dot{C}_i} \sum_{\partial C^r_{ij} \in \partial C_{ij}} J_{ij} \, |\partial C^r_{ij}|$$



Multi-dimensional S-G

$$\int_{\partial \dot{C}_i} \mathbf{J}_n \cdot \mathbf{n} dS \approx \int_{\partial \dot{C}_i} \mathbf{J}_E \cdot \mathbf{n} dS \approx$$

$$\sum_{\partial C_{ij} \in \partial \dot{C}_i} \sum_{\partial C^r_{ij} \in \partial C_{ij}} \left(\sum_{e_{kl} \in K_r} h_{kl} J_{kl} \overrightarrow{W}_{kl}(\mathbf{x}^r_{ij}) \right) \cdot \mathbf{n}^r_{ij} |\partial C^r_{ij}|$$



$$J_{ij} = \frac{a_{ij} D_n}{h_{ij}} \left(n_j \left(\coth(a_{ij}) + 1 \right) - n_i \left(\coth(a_{ij}) - 1 \right) \right)$$

Accuracy Test

Steady-state manufactured solution

$$-\nabla \cdot \mathbf{J}_n + R = 0 \quad \text{in} \quad \Omega$$
$$n = g \quad \text{on} \quad \Gamma_D$$

$$n(x,y) = x^3 - y^2$$
$$\mathbf{u_n} = \mu_n \nabla \psi = (-\sin \pi/6, \cos \pi/6)$$

	CVFEM-SG		FVM-SG		CVFEM-SU	
	L^2 error	H^1 error	L^2 error	H^1 error	L^2 error	H^1 error
Grid	$D_n = 1 \times 10^{-3}$					
32	0.4373E-02	0.7620E-01	0.4364E-02	0.7572E-01	0.5764E-02	0.10270E+00
64	0.2108E-02	0.4954E-01	0.2107E-02	0.4937E-01	0.2712E-02	0.6357E-01
128	0.9870E-03	0.3089E-01	0.9870E-03	0.3084E-01	0.1164E-02	0.3515E-01
Rate	1.095	0.681	1.094	0.679	1.221	0.854
Grid	$D_n = 1 \times 10^{-5}$					
32	0.4732E-02	0.7897E-01	0.4723E-02	0.7850E-01	0.8161E-02	0.1310E+00
64	0.2517E-02	0.5477E-01	0.2515E-02	0.5460E-01	0.4194E-02	0.9312E-01
128	0.1298E-02	0.3834E-01	0.1298E-02	0.3828E-01	0.2122E-02	0.6590E-01
Rate	0.955	0.514	0.955	0.514	0.983	0.499

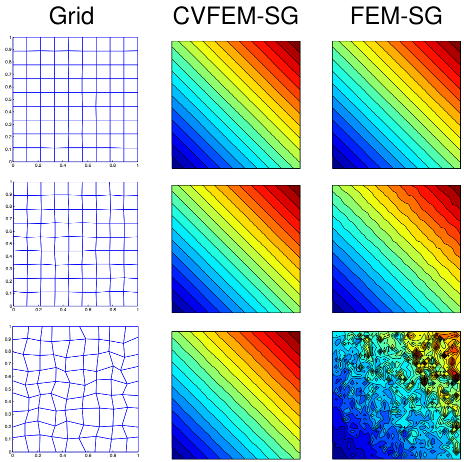
CVFEM-SG	control volume finite element method with multi-dimensional S-G upwinding
FEM-SG	finite volume method with 1-d S-G upwinding
CVFEM-SU	control volume finite element method with streamlined upwind stabilization

Robustness Test

Manufactured solution on randomly perturbed grids

$$-\nabla \cdot \mathbf{J}_n + R = 0 \quad \text{in} \quad \Omega$$
$$n = g \quad \text{on} \quad \Gamma_D$$

$$n(x,y) = x + y$$
$$\mathbf{u_n} = (-\sin \pi/6, \cos \pi/6)$$
$$D_n = 1.0 \times 10^{-5}$$



Application to Semiconductor Devices

- To solve coupled drift-diffusion equations CVFEM-SG has been implemented in Sandia's Charon 2 code
- Charon 2 built with Trilinos libraries (`http://trilinos.sandia.gov/`) that provide
  - Linear and Nonlinear solvers
  - Temporal and spatial discretization
  - Automatic differentiation

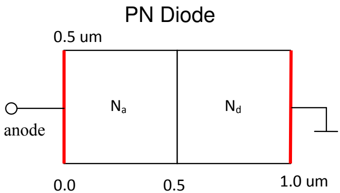
PN Diode Coupled drift-diffusion equations

$$\nabla \cdot (\epsilon_0 \epsilon_{si} \nabla \psi) - (p - n + N_d - N_a) = 0 \quad \text{in } \Omega$$

$$-\nabla \cdot \mathbf{J}_n + R(\psi, n, p) = 0 \quad \text{in } \Omega$$

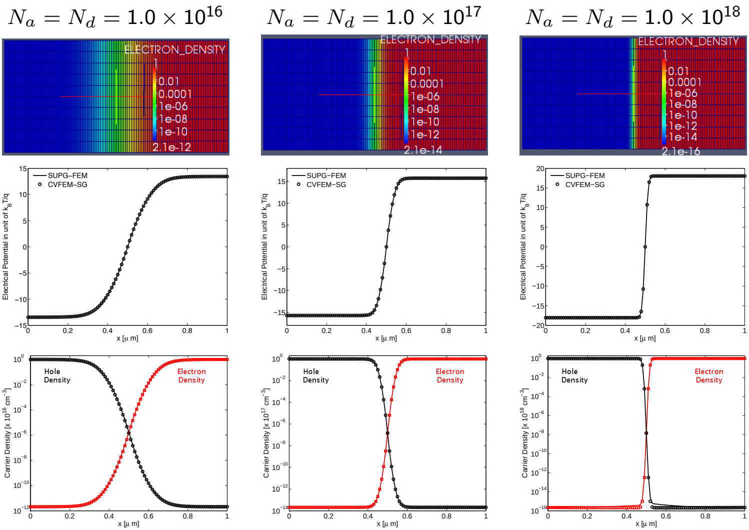
$$-\nabla \cdot \mathbf{J}_p - R(\psi, n, p) = 0 \quad \text{in } \Omega$$

$$R(\psi, n, p) = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)} + (c_n n + c_p p)(np - n_i^2)$$



PN Diode

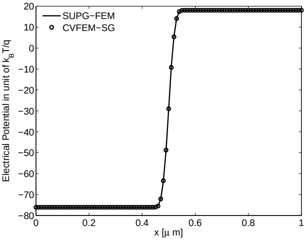
Doping Dependence Test

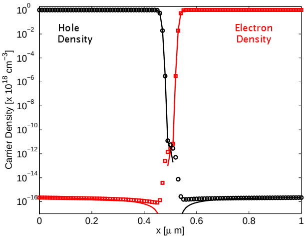


PN Diode

Strong Drift Case

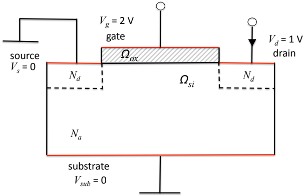
$$N_a = N_d = 1.0 \times 10^{17} cm^{-3}, \quad V_a = -1.5V$$





FEM-SUPG solution develops undershoots and becomes negative in junction region, while CVFEM-SG exhibits only minimal undershoots and values remain positive.

N-Channel MOSFET



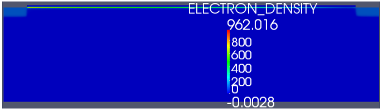
MOSFET coupled drift-diffusion equations

$$\nabla \cdot (\epsilon_0 \epsilon_{ox} \nabla \psi) = 0 \quad \text{in} \quad \Omega_{ox}$$

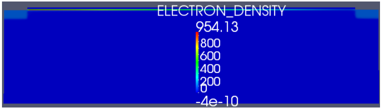
$$\nabla \cdot (\epsilon_0 \epsilon_{si} \nabla \psi) = -q \left(n_i \exp\left(\frac{-q\psi}{k_B T} \right) - n + N_d - N_a \right) \quad \text{in} \quad \Omega_{si}$$

$$\nabla \cdot (n \mu_n \nabla \psi - D_n \nabla n) = 0 \quad \text{in} \quad \Omega_{si}$$

FEM-SUPG



CVFEM-SG



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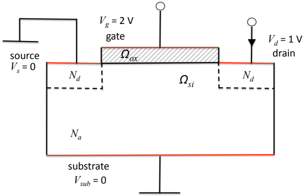

MOSFET coupled drift-diffusion equations

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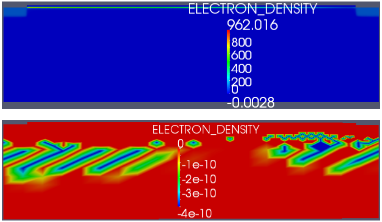
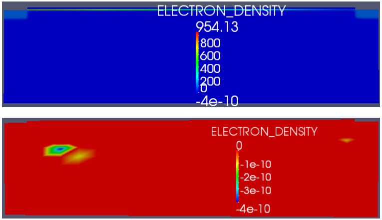
$$\nabla \cdot (\epsilon_0 \epsilon_{si} \nabla \psi) = -q \left(n_i \exp\left(\frac{-q\psi}{k_B T}\right) - n + N_d - N_a \right) \quad \text{in} \quad \Omega_{si}$$

$$\nabla \cdot (n \mu_n \nabla \psi - D_n \nabla n) = 0 \quad \text{in} \quad \Omega_{si}$$

FEM-SUPG



CVFEM-SG



Conclusions

- CVFEM with the edge-element extension of classical S-G upwinding offers a stable and robust method for solving the semiconductor drift-diffusion equations
- Performs well on unstructured grids
- Does not require heuristic stabilization parameters
- Although scheme is not provably monotone, violations of solution bounds are lower than for comparable schemes with SUPG stabilization

More details in:

Bochev, Peterson, Gao (2013) "A new control volume finite element method for the stable and accurate solution of the drift-diffusion equations on general unstructured grids",*CMAME* 254, 126-145.