

SAND2017 - 3512C

Multiscale Stabilized Control Volume Finite Element Method for Advection-Diffusion

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Sandia National Laboratories

FEF 2017



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Outline

- Motivation
- Stabilized CVFEM for drift-diffusion
 - Review of classical Scharfetter-Gummel upwinding
 - Multi-dimensional extension of S-G upwinding for non-uniform grids
 - 2nd-order multi-scale CVFEM
- Conclusions

Application Driver

Semiconductor electrical transport simulation

Scaled semiconductor drift-diffusion equations

Poisson equation $\nabla \cdot (\lambda^2 \nabla \phi) + (p - n + C) = 0$

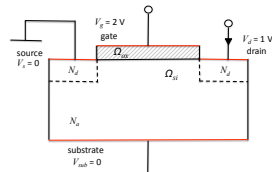
Electron continuity equation $\frac{\partial n}{\partial t} - \nabla \cdot \mathbf{J}_n + R(\phi, n, p) = 0$

Hole continuity equation $\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{J}_p + R(\phi, n, p) = 0$

Electric field $\mathbf{E} = -\nabla \phi$

Electron current density $\mathbf{J}_n = \mu_n \mathbf{E} n + D_n \nabla n$

Hole current density $\mathbf{J}_p = \mu_p \mathbf{E} p - D_p \nabla p$



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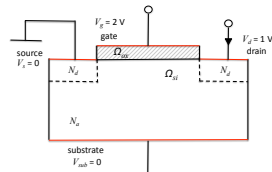
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↑ ↑
drift diffusion



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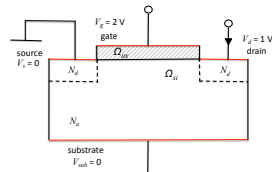
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$\uparrow$ $\uparrow$
 drift diffusion



Require a numerical scheme that is accurate and stable in the strong drift regime

$$(D_n \ll \mu_n \mathbf{E}, D_p \ll \mu_p \mathbf{E})$$

Numerical Discretization

Control Volume Finite Element Method (CVFEM)

Electron continuity equation

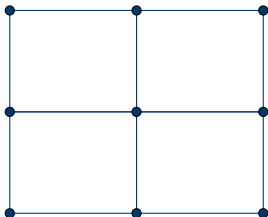
$$\frac{\partial n}{\partial t} - \nabla \cdot \mathbf{J} + R = 0$$

$$\mathbf{J} = \mathbf{u}n + D\nabla n$$

$$\mathbf{u} = \mu\mathbf{E}$$

- Finite element approximation of the electron density

$$n^h(\mathbf{x}, t) = \sum_j n_j(t) N_j(\mathbf{x})$$



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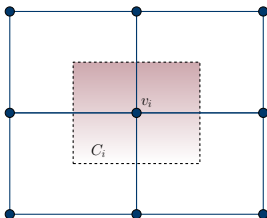
$$\mathbf{u} = \mu \mathbf{E}$$

- Finite element approximation of the electron density

$$n^h(\mathbf{x}, t) = \sum_j n_j(t) N_j(\mathbf{x})$$

- Integrate over control volume and apply the divergence theorem

$$\int_{C_i} \frac{\partial n^h}{\partial t} dV - \int_{\partial C_i} \mathbf{J}(n^h) \cdot \mathbf{\bar{n}} dS + \int_{C_i} R(n^h) dV = 0$$



Numerical Discretization

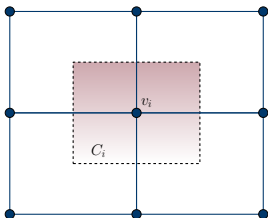
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$$\mathbf{J}(n^h) = \sum_j n_j(t) (\mu \mathbf{E} N_j + D \nabla N_j)$$

Nodal approximation for $\mathbf{J}(n^h)$ can lead to instabilities in strong drift regime.

Numerical Discretization

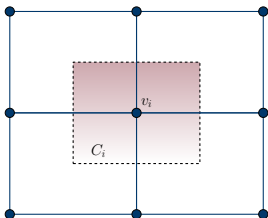
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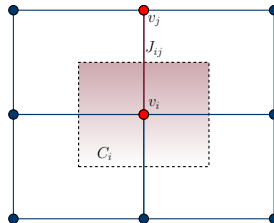
Want a stabilized approximation for $\mathbf{J}$ that includes information on drift.

Scharfetter-Gummel Upwinding

On edge e_{ij} solve 1-d boundary value problem for constant J_{ij}

$$\frac{dJ_{ij}}{ds} = 0; \quad J_{ij} = \mu E_{ij} n(s) + D \frac{dn(s)}{ds}$$

$$n(0) = n_i \quad \text{and} \quad n(h_{ij}) = n_j$$



D. L. Scharfetter and H. K Gummel, Large-signal analysis of a silicon read diode oscillator, *IEEE Transactions on Electron Devices* 16, 64-77, 1969.

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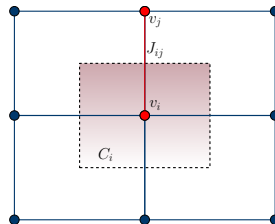
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$$n(0) = n_i \quad \text{and} \quad n(h_{ij}) = n_j$$

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

$$\text{where} \quad a_{ij} = \frac{h_{ij} E_{ij} \mu}{2D}, \quad E_{ij} = -\frac{(\psi_j - \psi_i)}{h_{ij}}$$



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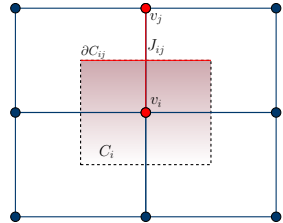
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$$\int_{\partial C_i} \mathbf{J}_n \cdot \vec{\mathbf{n}} dS \approx \sum_{\partial C_{ij} \in \partial C_i} J_{ij} |\partial C_{ij}|$$



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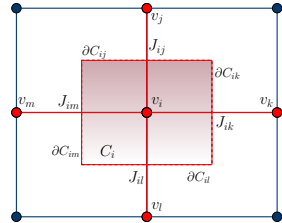
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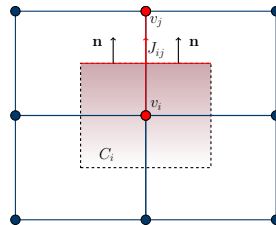
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On structured grids, J_{ij} is a good estimate of $\mathbf{J} \cdot \vec{n}$ on ∂C_{ij}

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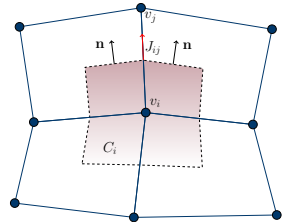
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On unstructured grids, J_{ij} is no longer a good estimate of $\mathbf{J} \cdot \vec{n}$

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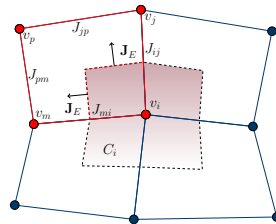
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Multi-dimensional S-G Upwinding

Idea: Use $H(\text{curl})$ -conforming finite elements to expand edge current density into primary cell

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

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

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

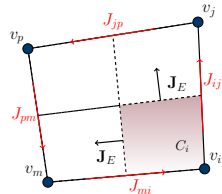
In the limit carrier drift velocity $\mu \mathbf{E} = 0$,

$$\lim_{\mu \mathbf{E} \rightarrow 0} J_{ij} = \frac{D(n_j - n_i)}{h_{ij}}$$

$$\mathbf{J}_E = \sum_{e_{ij} \in E(\Omega)} D(n_j - n_i) \vec{W}_{ij} = \sum_{v_i \in V(\Omega)} D n_i \nabla \phi_i = \mathbf{J}(n^h)$$

Exponentially fitted current density

$$\mathbf{J}_E(\mathbf{x}) = \sum_{e_{ij}} h_{ij} J_{ij} \vec{W}_{ij}(\mathbf{x})$$



$$\int_{e_{ij}} \vec{W}_{ij} \cdot \mathbf{t}_{rs} dl = \delta_{ij}^{rs}$$

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

Convergence on Structured Grids

Steady-state manufactured solution

$$-\nabla \cdot \mathbf{J} + R = 0 \quad \text{in } \Omega$$

$$n = g \quad \text{on } \Gamma_D$$

$$n(x, y) = x^3 - y^2$$

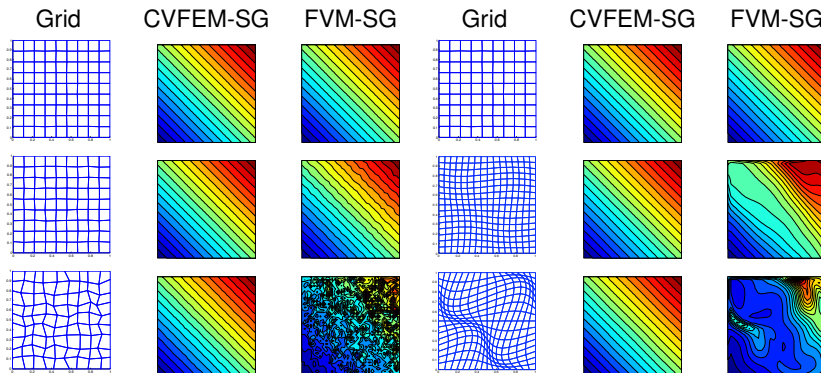
$$\mu \mathbf{E} = (-\sin \pi/6, \cos \pi/6)$$

	CVFEM-SG		FVM-SG	
	L^2 error	H^1 error	L^2 error	H^1 error
Grid	$D = 1 \times 10^{-3}$			
32	0.4373E-02	0.7620E-01	0.4364E-02	0.7572E-01
64	0.2108E-02	0.4954E-01	0.2107E-02	0.4937E-01
128	0.9870E-03	0.3089E-01	0.9870E-03	0.3084E-01
Rate	1.095	0.681	1.094	0.679
Grid	$D = 1 \times 10^{-5}$			
32	0.4732E-02	0.7897E-01	0.4723E-02	0.7850E-01
64	0.2517E-02	0.5477E-01	0.2515E-02	0.5460E-01
128	0.1298E-02	0.3834E-01	0.1298E-02	0.3828E-01
Rate	0.955	0.514	0.955	0.514

CVFEM-SG control volume finite element method with multi-dimensional S-G upwinding
 FVM-SG finite volume method with 1-d S-G upwinding

Robust on Unstructured Grids

Manufactured linear solution



Charon

To solve coupled drift-diffusion equations CVFEM-SG has been implemented in Sandia's Charon code

- Electrical transport simulation code for semiconductor devices, solving PDE-based nonlinear equations
- Built with Trilinos libraries (<https://github.com/trilinos/Trilinos>) that provide
 - Framework and residual-based assembly (Panzer, Phalanx)
 - Linear and Nonlinear solvers (Belos, Nox, ML, etc)
 - Temporal and spatial discretization (Tempus, Intrepid, Shards)
 - Automatic differentiation (Sacado)
 - Advanced manycore performance portability (Kokkos)



Developers: Suzey Gao, Gary Hennigan, Larry Musson, Andy Huang

PN Diode

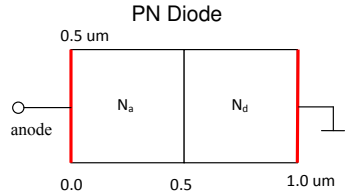
PN Diode coupled drift-diffusion equations

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

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

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

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



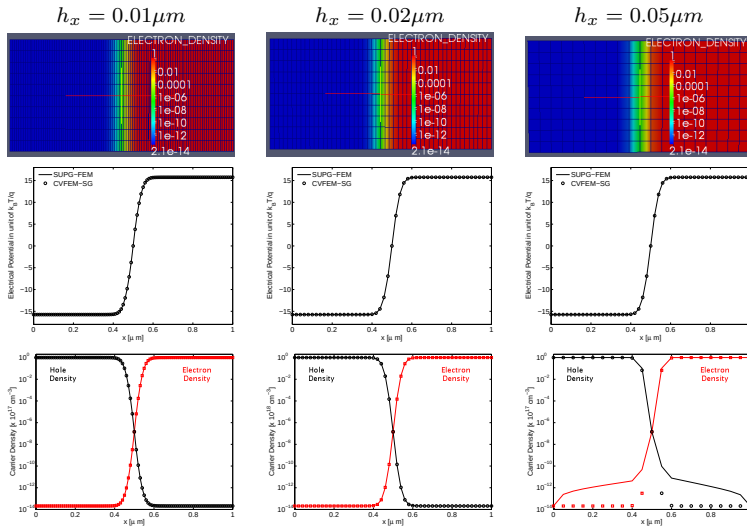
Compare with SUPG Stabilized FEM

$$\int_{\Omega} (\mu \mathbf{E} + D \nabla n) \cdot \nabla \psi dV + \int_{\Omega} R \psi dV + \int_{\Omega} \tau (\mu \mathbf{E} \cdot \nabla n) (\mu \mathbf{E} \cdot \nabla \psi) dV = 0 \quad \forall \psi$$

$$\tau = \frac{1}{\sqrt{\mathbf{u}^T \mathbf{G} \mathbf{u}}} \left(\coth \alpha - \frac{1}{\alpha} \right) \quad \alpha = \frac{\sqrt{\mathbf{u}^T \mathbf{G} \mathbf{u}}}{D \|\mathbf{G}\|} \quad \mathbf{u} = \mu \mathbf{E}$$

PN Diode

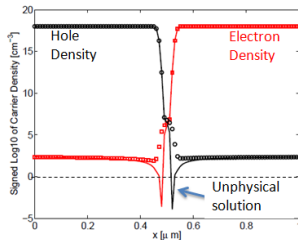
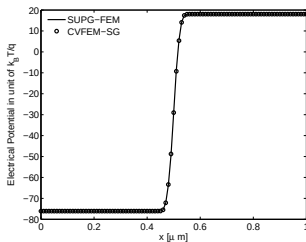
Mesh Dependence Study



PN Diode

Strong Drift Case

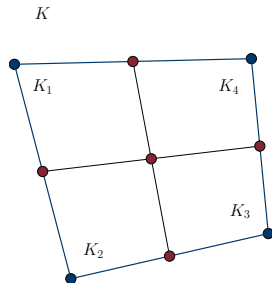
$$N_a = N_d = 1.0 \times 10^{18} \text{ cm}^{-3}, \quad V_a = -1.5 \text{ V}$$



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

Multi-scale Stabilized CVFEM

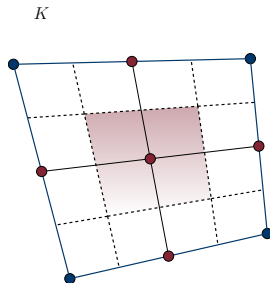
- Divide each element into 4 bilinear (Q1) sub-elements



Bochev, Peterson, Perego "A multi-scale control-volume finite element method for advection-diffusion equations", *IJNMF* Vol. 77, Issue 11, pp. 641-667 (2015).

Multi-scale Stabilized CVFEM

- Divide each element into 4 bilinear (Q1) sub-elements
- Define control volumes around each sub-cell node

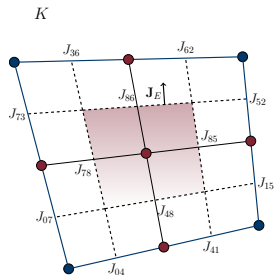


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Multi-scale Stabilized CVFEM

- Divide each element into 4 bilinear (Q1) sub-elements
- Define control volumes around each sub-cell node
- Compute 2nd order J_{ij} at each macro element edge
- Use 2nd order $H(curl)$ basis to evaluate $\mathbf{J}_E$ at control volume integration points

$$\mathbf{J}_E(n_h) = \sum_{e_{ij} \in E(\Omega)} h_{ij} J_{ij} \vec{W}_{ij}$$



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Multi-scale Stabilized CVFEM

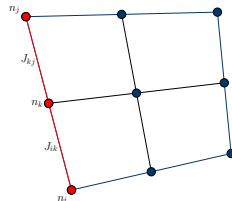
2nd Order Edge Current Density

- Solve 1-d boundary value problem along a compound edge for a linear $J(s) = a + bs$

$$J(s) = \mu \mathbf{E}_s n(s) + D \frac{dn}{ds}$$

$$n(0) = n_i, \quad n(h_s/2) = n_k \quad \text{and} \quad n(h_s) = n_j$$

$$J_{ik} = J(h_s/4) \quad J_{kj} = J(3h_s/4)$$



Multi-scale Stabilized CVFEM

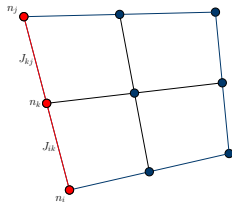
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$$J_{ik} = J(h_s/4) \quad J_{kj} = J(3h_s/4)$$



- Edge current density

$$J_{ik} = \Phi(n_i, n_k) + \gamma(n_i, n_j, n_k)$$

$$J_{kj} = \Phi(n_k, n_j) + \gamma(n_i, n_j, n_k)$$

Multi-scale Stabilized CVFEM

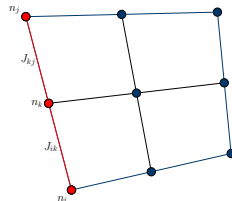
2nd Order Edge Current Density

- Solve 1-d boundary value problem along a compound edge for a linear $J(s) = a + bs$

$$J(s) = \mu \mathbf{E}_s n(s) + D \frac{dn}{ds}$$

$$n(0) = n_i, \quad n(h_s/2) = n_k \quad \text{and} \quad n(h_s) = n_j$$

$$J_{ik} = J(h_s/4) \quad J_{kj} = J(3h_s/4)$$



- Edge current density

$$J_{ik} = \Phi(n_i, n_k) + \gamma(n_i, n_j, n_k)$$

$$J_{kj} = \Phi(n_k, n_j) + \gamma(n_i, n_j, n_k)$$

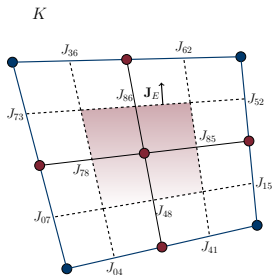
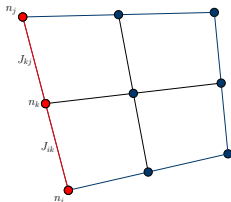
$$\Phi(n_i, n_k) = \frac{aD}{h} (n_k (\coth(a) + 1) - n_i (\coth(a) - 1))$$

$$\gamma(n_i, n_j, n_k) = \frac{D}{h} (a \coth(a) - 1) \left(n_i (\coth(a) - 1) - 2n_k \coth(a) + n_j (\coth(a) + 1) \right)$$

Multi-scale Stabilized CVFEM

- Subedge fluxes are a sum of Scharfetter-Gummel fluxes and a higher-order correction term
- High-order correction contributes an anti-diffusive flux
- In pure advection limit ($D \rightarrow 0$) method only modifies downstream segment

$$J_{ik} = \Phi(n_i, n_k) + \gamma(n_i, n_j, n_k)$$



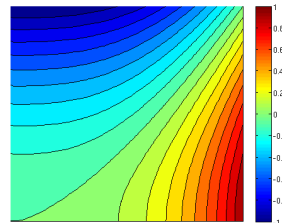
- For assembly, edge basis functions are used only locally so no global edge data structures are required

$$\mathbf{J}_E(n_h) = \sum_{e_{ij} \in E(\Omega)} h_{ij} J_{ij} \vec{W}_{ij}$$

Manufactured Solution

$$\begin{aligned}
 -\nabla \cdot \mathbf{J}(n) &= R \quad \text{in } \Omega \\
 \mathbf{J}(n) &= (D\nabla n + \mu \mathbf{E}n) \quad \text{in } \Omega \\
 n &= g \quad \text{on } \Gamma
 \end{aligned}$$

$$\begin{aligned}
 n(x, y) &= x^3 - y^2 \\
 \mu \mathbf{E} &= (-\sin \pi/6, \cos \pi/6)
 \end{aligned}$$



	CVFEM-MS		CVFEM-SG		FEM-SUPG	
	L^2 error	H^1 error	L^2 error	H^1 error	L^2 error	H^1 error
Grid*	$\epsilon = 1 \times 10^{-3}$					
32	1.57e-3	6.05e-2	4.24e-3	7.48e-2	2.09e-4	3.61e-2
64	3.93e-4	2.89e-2	2.07e-3	4.91e-2	4.85e-5	1.80e-2
128	8.98e-5	1.24e-2	9.78e-4	3.07e-2	1.11e-5	9.02e-3
Rate	2.06	1.14	1.06	0.642	2.12	1.00
Grid	$\epsilon = 1 \times 10^{-5}$					
32	1.69e-3	6.60e-2	4.73e-3	7.90e-2	2.30e-4	3.61e-2
64	4.54e-4	3.45e-2	2.52e-3	5.48e-2	5.78e-5	1.80e-2
128	1.18e-4	1.76e-2	1.30e-3	3.83e-2	1.45e-5	9.02e-3
Rate	1.92	0.955	0.933	0.521	1.99	1.00

* For CVFEM-MS the size corresponds sub-elements rather than macro-elements.

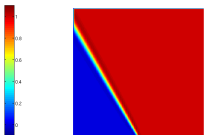
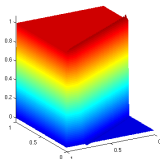
Skew Advection Test

$$\begin{aligned} -\nabla \cdot \mathbf{J}(n) &= R & \text{in } \Omega \\ \mathbf{J}(n) &= (D\nabla n + \mu \mathbf{E}n) & \text{in } \Omega \\ n &= g & \text{on } \Gamma \end{aligned}$$

$$g = \begin{cases} 0 & \text{on } \Gamma_L \cup \Gamma_T \cup (\Gamma_B \cap \{x \leq 0.5\}) \\ 1 & \text{on } \Gamma_R \cup (\Gamma_B \cap \{x > 0.5\}) \end{cases}$$

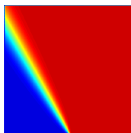
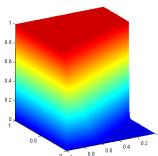
$$\mu \mathbf{E} = (-\sin \pi/6, \cos \pi/6) \quad D = 1.0 \times 10^{-5}$$

CVFEM-MS



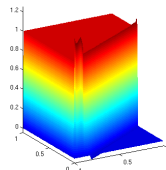
min = -0.0445
max = 1.077

CVFEM-SG



min = 0.00
max = 1.004

SUPG



min = -0.0459
max = 1.251

Double Glazing Test

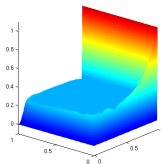
$$\begin{aligned} -\nabla \cdot J(n) &= R & \text{in } \Omega \\ J(n) &= (D\nabla n + \mu \mathbf{E}n) & \text{in } \Omega \\ n &= g & \text{on } \Gamma \end{aligned}$$

$$D = 1.0 \times 10^{-5}$$

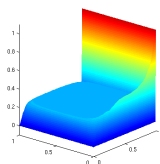
$$g = \begin{cases} 0 & \text{on } \Gamma_L \cup \Gamma_T \cup (\Gamma_B \cap \{x \leq 0.5\}) \\ 1 & \text{on } \Gamma_R \cup (\Gamma_B \cap \{x > 0.5\}) \end{cases}$$

$$\mu \mathbf{E} = \begin{pmatrix} 2(2y-1)(1-(2x-1)^2) \\ -2(2x-1)(1-(2y-1)^2) \end{pmatrix}$$

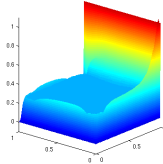
CVFEM-MS



CVFEM-SG



SUPG



Conclusions

Stabilization using an edge-element lifting of edge current densities offers a stable and robust method for solving drift-diffusion equations

- Works on unstructured grids
- Does not require heuristic stabilization parameters
- Although not provably monotone, violations of solution bounds are less than for a comparable scheme with SUPG stabilization
- Can achieve 2nd-order convergence with multi-scale approach
- Future work
 - Investigate modifications to achieve a monotone scheme
 - Implement 2nd-order scheme in Charon
 - More detailed comparison of methods for full drift-diffusion equations