Discretization Tool Use in Charon
A Case Study: CVFEM-SG Implementation in Charon2

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What is Charon

• **Charon** is Sandia’s electrical transport simulation code for semiconductor devices, which solves PDE-based nonlinear equations.

• 1st-generation Charon relies on Nevada framework and has a number of limitations.

• 2nd-generation Charon (**Charon2**) is built upon the **Panzer** toolkit and has many advantages.

• **Charon2** currently contains SUPG-FEM, EFFPG-FEM and **CVFEM-SG** discretized implementations of the semiconductor **drift-diffusion** equations (the latter two schemes are both proposed by Pavel Bochev).
Semiconductor Drift-Diffusion Equations

\[
\begin{align*}
\nabla \cdot (\lambda^2 \mathbf{E}) - (p - n + C) &= 0 \\
\frac{\partial n}{\partial t} - \nabla \cdot \mathbf{J}_n + R(\phi, n, p) &= 0 \\
\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{J}_p + R(\phi, n, p) &= 0
\end{align*}
\]

Poisson equation
Electron continuity equation
Hole continuity equation

\[
\begin{align*}
\mathbf{E} &= -\nabla \phi \\
\mathbf{J}_n &= n\mu_n \mathbf{E} + D_n \nabla n \\
\mathbf{J}_p &= p\mu_p \mathbf{E} - D_p \nabla p
\end{align*}
\]

Stabilized finite element method such as SUPG-FEM can lead to unphysical oscillatory solutions in the strong drift regime.
Therefore, Pavel’s CVFEM-SG scheme \[1\] (Control Volume Finite Element Method with Scharfetter Gummel upwinding)

\[1\] P. Bochev, K. Peterson, and X. Gao, CMAME, accepted.
For any vertex $v_i$ in the primary mesh:

- Integrate the equation in the shaded subcontrol volume
- Convert the divergence volume integral to flux surface integral using divergence theorem
- Compute current (e.g., $J_n$) using the SG upwinding and edge basis vectors

$$\frac{\partial n}{\partial t} - \nabla \cdot J_n + R(\phi, n, p) = 0$$

$J_n = \sum_{e_{ij} \in K_r} J_{ij} \mathbf{W}_{ij}$

Edge basis vectors

Edge current by the SG method, a function of nodal quantities

CVFEM-SG is a finite-volume-based discretization scheme!
Panzer is a flexible toolkit that integrates all the necessary components from Trilinos for easy development of application codes. However, the toolkit has been designed mostly for FEM-based applications.

To implement the finite-volume-based CVFEM-SG in Panzer / Charon2, we identified three main requirements that are different from FEM:

- Require subcontrol volume information
- Require edge basis vectors
- Require modification to equation residual assembly

Intrepid

Can be done in Intrepid in principle
FEM assembly in Panzer is done in residual form through loops over elements. The residual form allows the use of automatic differentiation in Sacado.

It turned out that we can also form a residual for the CVFEM-SG scheme and use element loops.

\[
\int_{C_i} \left( \frac{\partial n}{\partial t} + R \right) dV - \int_{\partial C_i} J_n \cdot \hat{n} dS = 0
\]

For every node in every element:

- Compute integration of scalars over subcv \( C_i \)
- Assign the value to the nodal residual
CVFEM-SG Residual Assembly

\[
\int_{C_i} \left( \frac{\partial n}{\partial t} + R \right) dV - \int_{\partial C_i} J_n \cdot n dS = 0
\]

Element loop

Edge loop

Compute flux \( J_n \cdot n_{r_{ij}} \) at the subcv edge \( \partial C_{r_{ij}} \) associated with a primary edge

Assign residual contribution to the two nodes of a primary edge (+ for \( \nu_i \) and – for \( \nu_j \))

End edge loop

End element loop
Charon2
• Construct subcv
• Obtain edge basis
• Compute residual
\[ \int_{c_i} \left( \frac{\partial n}{\partial t} + R \right) dV - \int_{\partial c_i} J_n \cdot \hat{n} dS \]

Panzer

Shards

Phalanx

Other Trilinos Packages

Intrepid
In the strong drift case, CVFEM-SG continues to yield physically correct solutions and performs better than the SUPG-FEM.
Summary

• **Take home message**: one can in principle implement a finite-volume-based discretization scheme using the Panzer toolkit, as demonstrated by the implementation of CVFEM-SG in Charon2.