Discretization Tool Use in Charon

A Case Study: CVFEM-SG Implementation in Charon2

Trilinos User Group Meeting 2012

Suzey Gao, Pavel Bochev, Kara Peterson, Eric Cyr, Roger Pawlowski,
Gary Hennigan, Larry Musson

Sandia National Laboratories

SAND 2012-8985C

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

$$\left\{\begin{array}{ll} \nabla\cdot(\lambda^2\mathbf{E})-(p-n+C)=0 & \text{Poisson equation} \\ \dfrac{\partial n}{\partial t}-\nabla\cdot\mathbf{J}_n+R(\phi,n,p)=0 & \text{Electron continuity equation} \\ \dfrac{\partial p}{\partial t}+\nabla\cdot\mathbf{J}_p+R(\phi,n,p)=0 & \text{Hole continuity equation} \end{array}\right.$$

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

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

$$\mathbf{J}_p=\underbrace{p\mu_p\mathbf{E}}_{\text{Drift}}-\underbrace{D_p\nabla p}_{\text{Diffusion}}$$

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.

CVFEM-SG Scheme

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

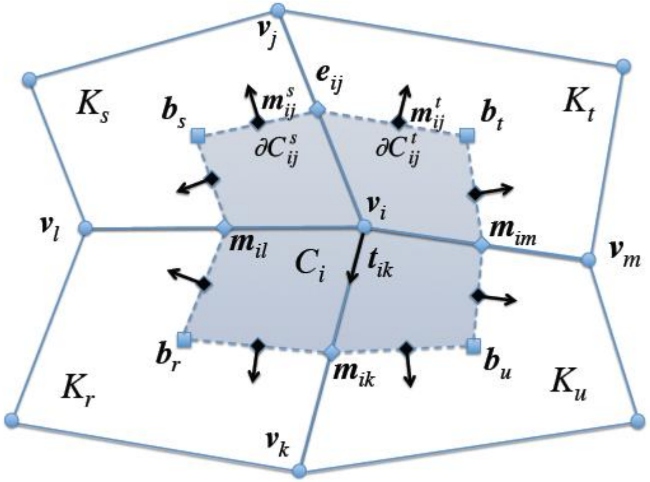
For any vertex $\mathbf{v}_\mathrm{i}$ in the primary mesh:

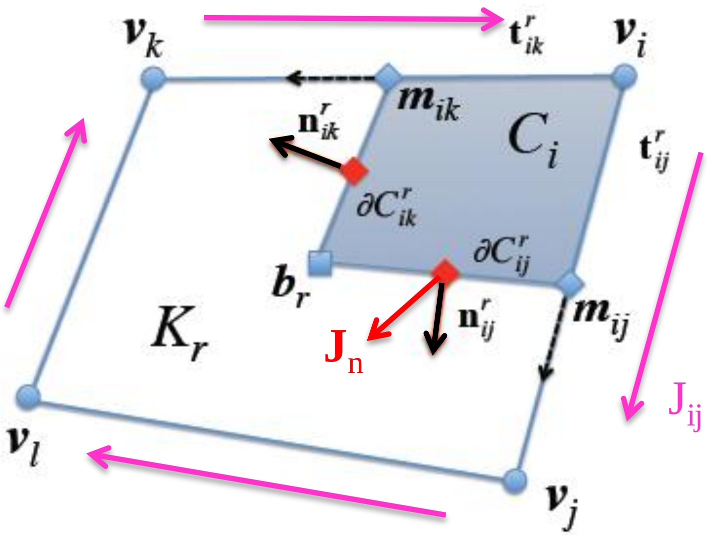
- Integrate the equation in the shaded subcontrol volume
- Convert the divergence volume integral to flux surface integral using divergence theorem
- Compute current (e.g., $\mathbf{J}_\mathrm{n}$) using the SG upwinding and edge basis vectors

$$\boldsymbol{J}_n = \sum_{\boldsymbol{e}_{ij} \in K_r} J_{ij} \, \vec{W}_{ij}$$

Edge basis vectors

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





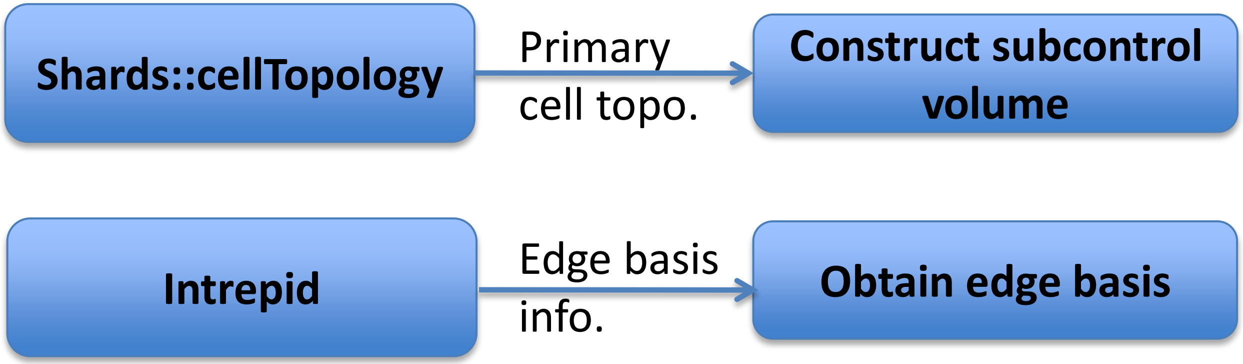
CVFEM-SG is a finite-volume-based discretization scheme !

CVFEM-SG Implementation Requirements

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



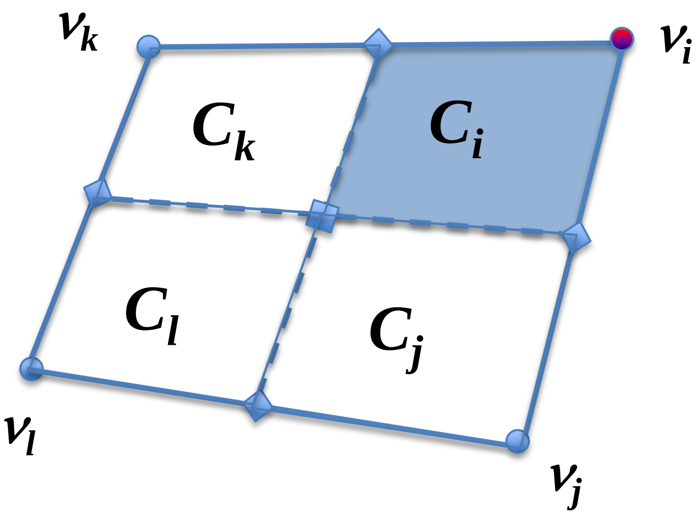
Can be done in Intrepid in principle

CVFEM-SG Residual Assembly

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**.

$$\underbrace{\int_{C_i}\left(\frac{\partial n}{\partial t}+R\right)dV}_{} - \int_{\partial C_i} \mathrm{J}_n \cdot \hat{\mathrm{n}}\, dS = 0$$



For every node in every element:

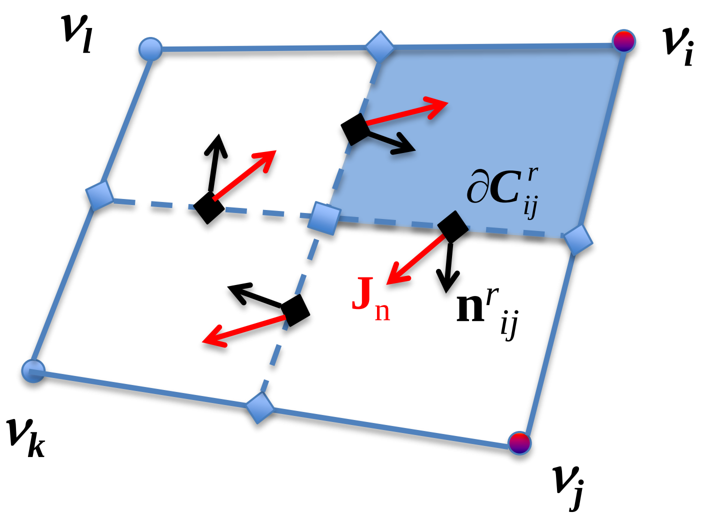
Compute integration of scalars over subcv C_i

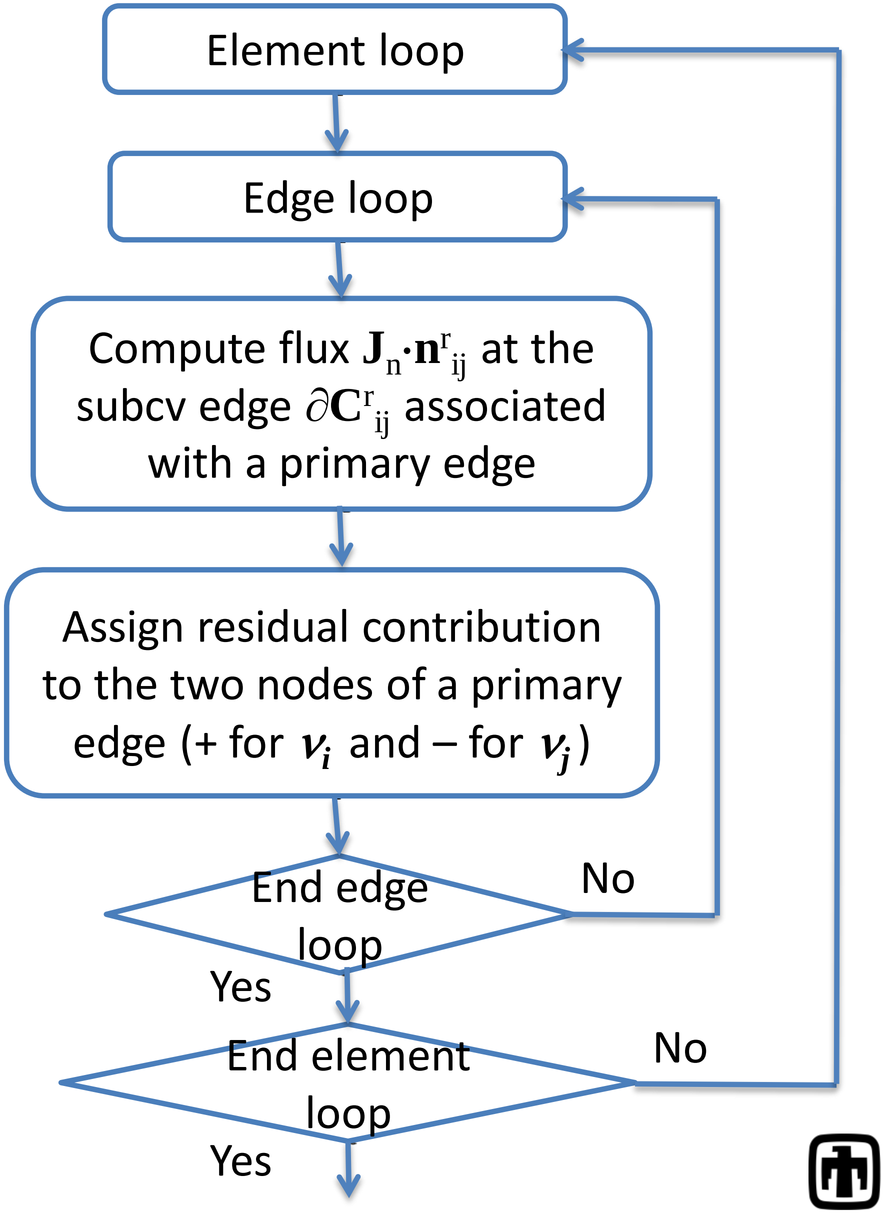
↓

Assign the value to the nodal residual

CVFEM-SG Residual Assembly

$$\int_{C_i}\left(\frac{\partial n}{\partial t}+R\right)dV-\underbrace{\int_{\partial C_i}\mathrm{J}_n\cdot\hat{\mathrm{n}}\,dS}_{}=0$$





Element loop

Edge loop

Compute flux $\mathbf{J}_\mathrm{n}\cdot\mathbf{n}^\mathrm{r}_\mathrm{ij}$ at the subcv edge $\partial\mathbf{C}^\mathrm{r}_\mathrm{ij}$ associated with a primary edge

Assign residual contribution to the two nodes of a primary edge (+ for v_i and – for v_j)

End edge loop

No

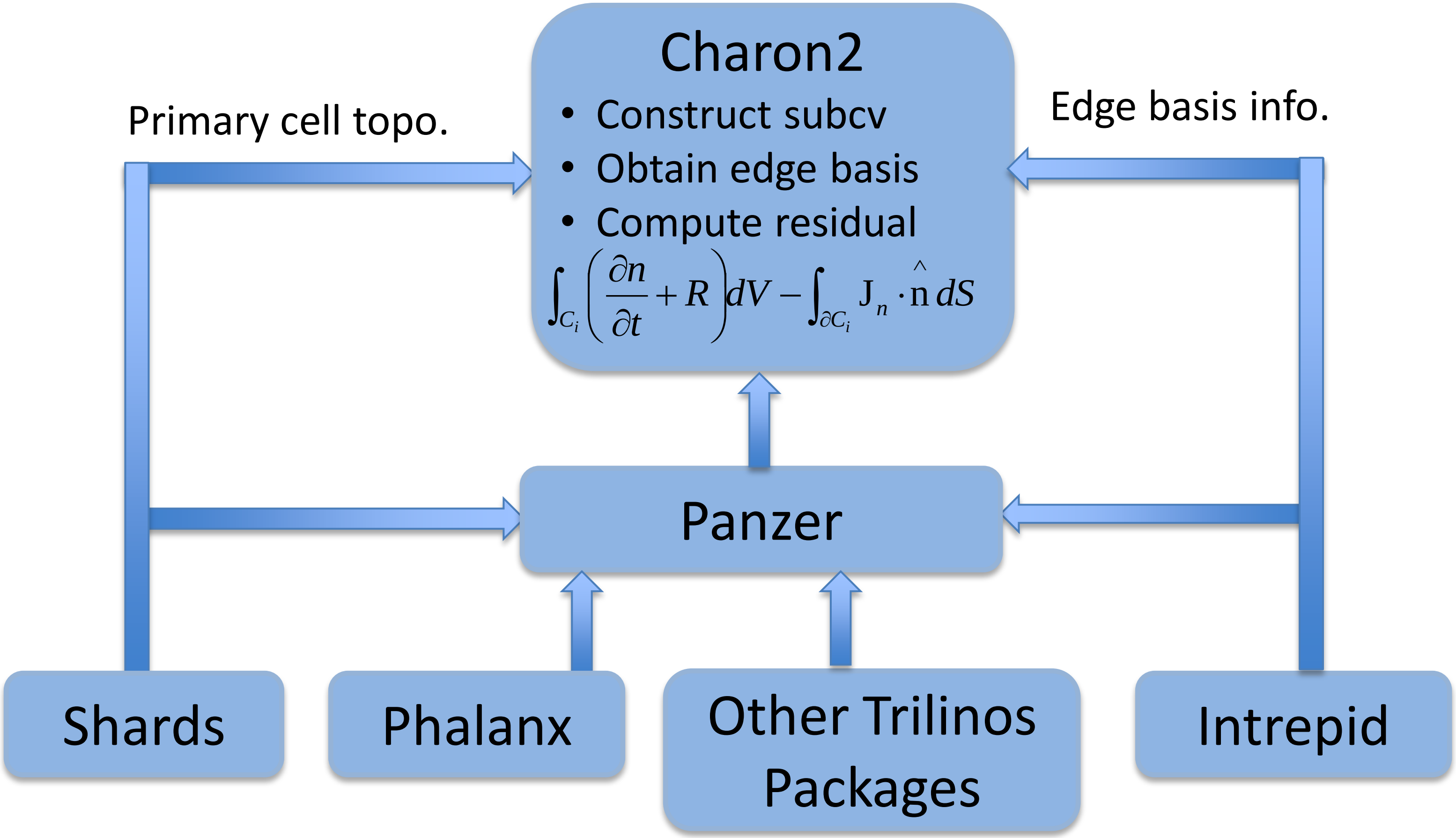
Yes

End element loop

No

Yes

Implementation Diagram



Primary cell topo.

Charon2

- Construct subcv
- Obtain edge basis
- Compute residual

$$\int_{C_i}\left(\frac{\partial n}{\partial t}+R\right)dV-\int_{\partial C_i}\mathrm{J}_n\cdot\hat{\mathrm{n}}\,dS$$

Edge basis info.

Panzer

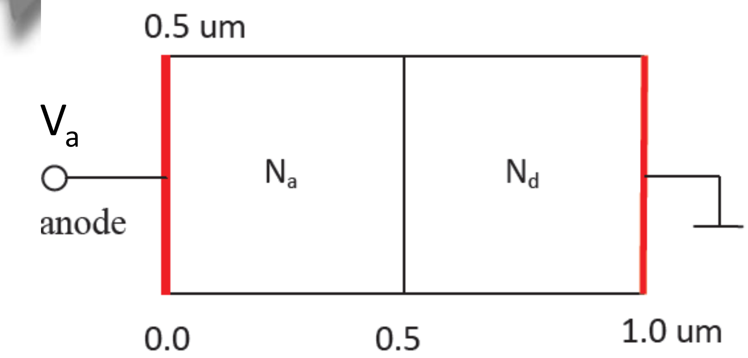
Shards

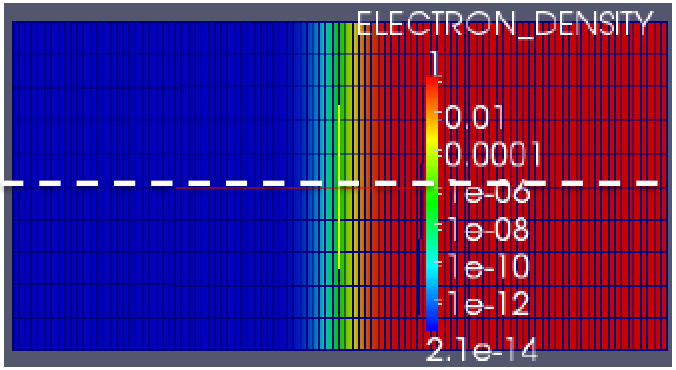
Phalanx

Other Trilinos Packages

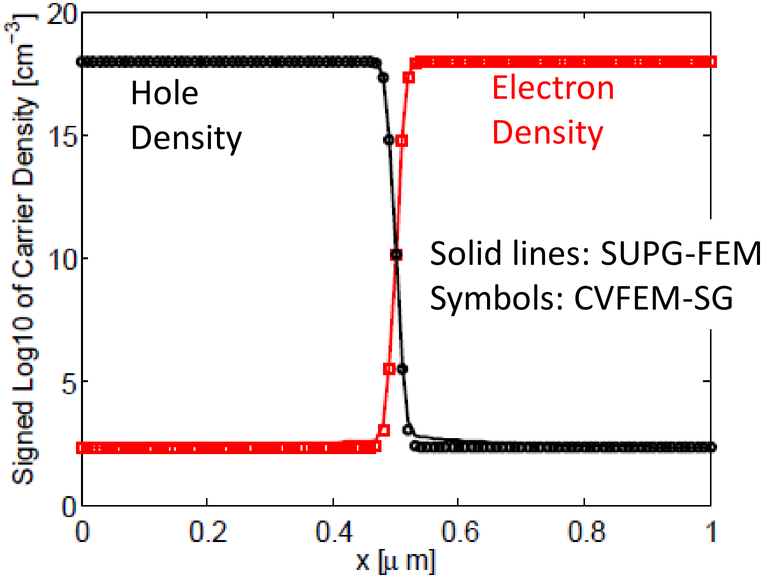
Intrepid

PN Diode Example Results



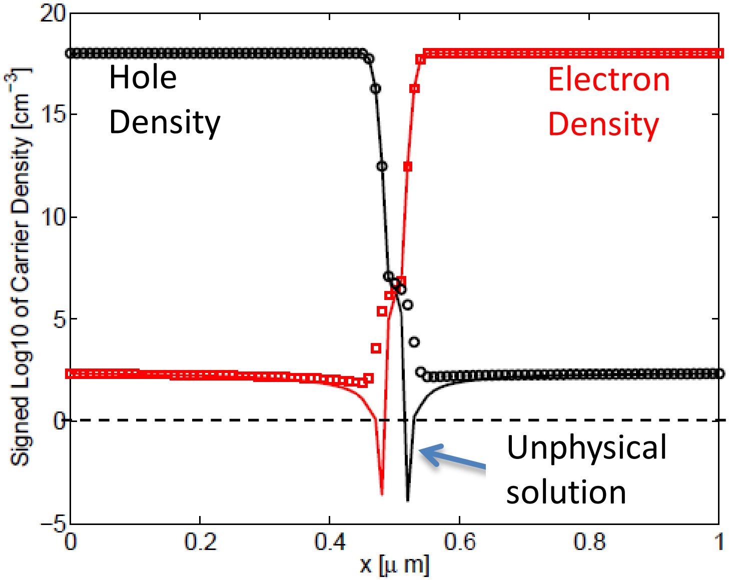


V_a = 0 (moderate drift)



Solid lines: SUPG-FEM
Symbols: CVFEM-SG

V_a = -1.5V (strong drift)



Unphysical solution

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.

Sandia
National
Laboratories