

# Discretization Tool Use in Charon

## A Case Study: CVFEM-SG Implementation in Charon2

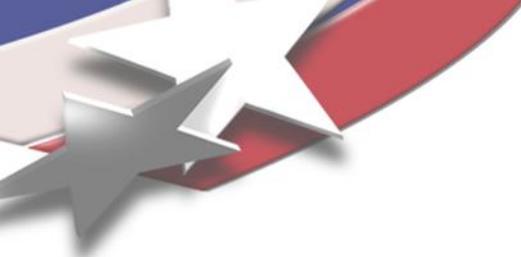
Trilinos User Group Meeting 2012

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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

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

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

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

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

Drift

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 <sup>[1]</sup> (Control Volume Finite Element Method with Scharfetter Gummel upwinding)

[1] P. Bochev, K. Peterson, and X. Gao, CMAME, accepted.

# CVFEM-SG Scheme

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

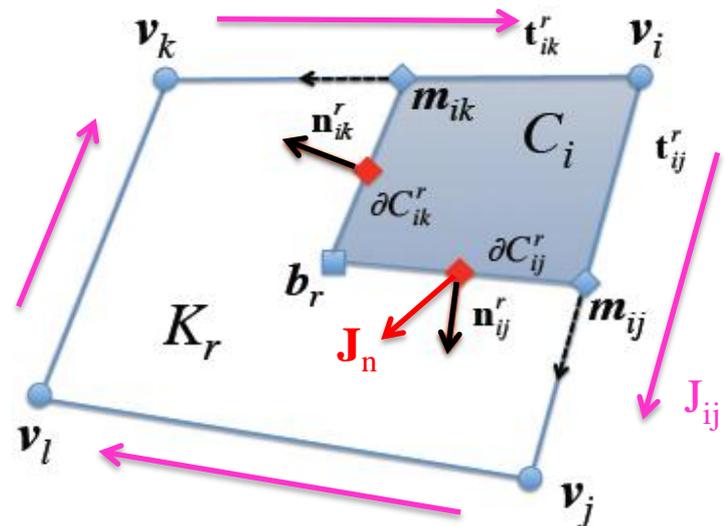
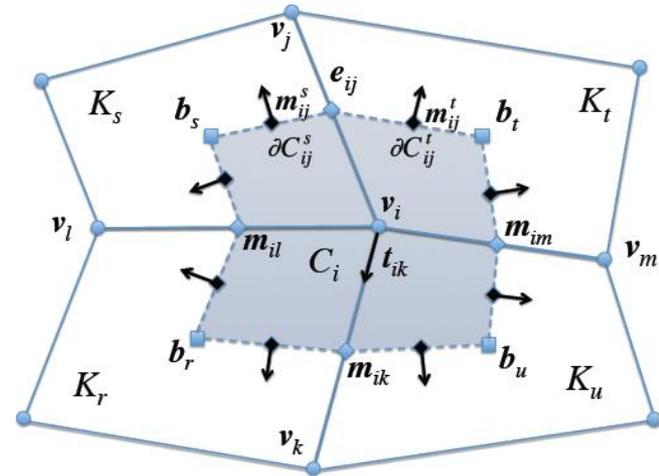
For any vertex  $v_i$  in the primary mesh:

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

$$\mathbf{J}_n = \sum_{e_{ij} \in K_r} J_{ij} \vec{W}_{ij}$$

Edge basis vectors

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



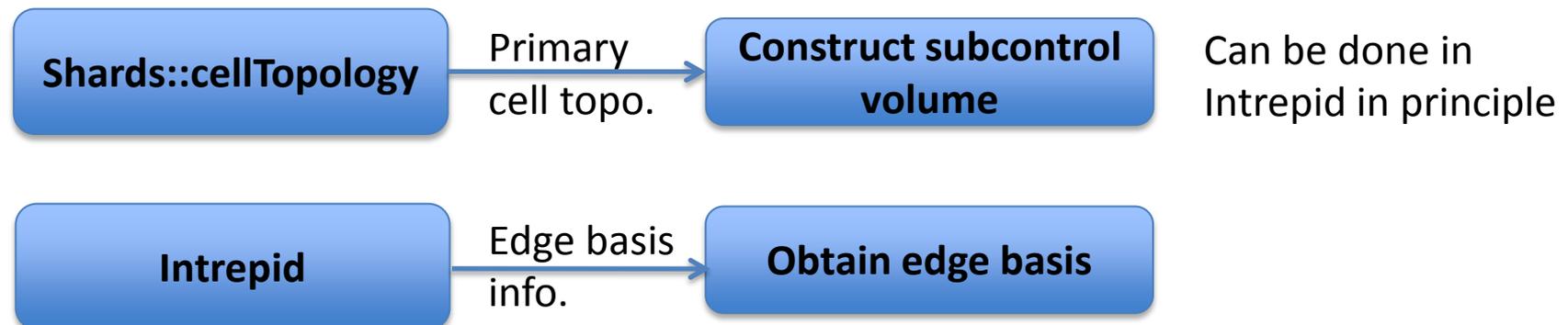
CVFEM-SG is a finite-volume-based discretization scheme !

# 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**



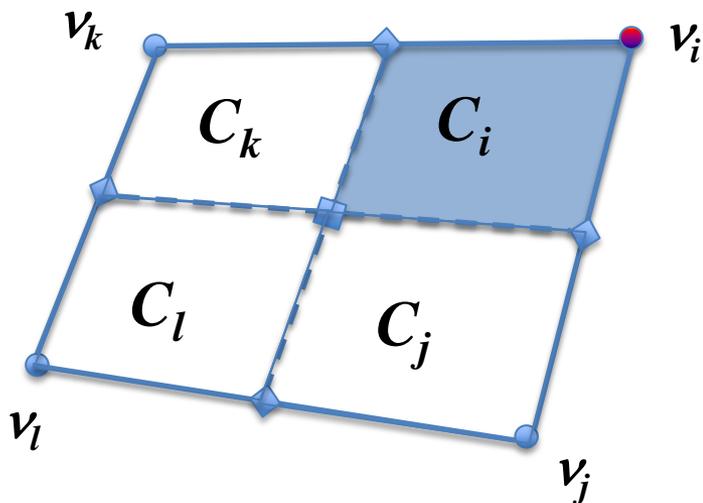
# CVFEM-SG Residual Assembly

**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**.

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

For every node in every element:

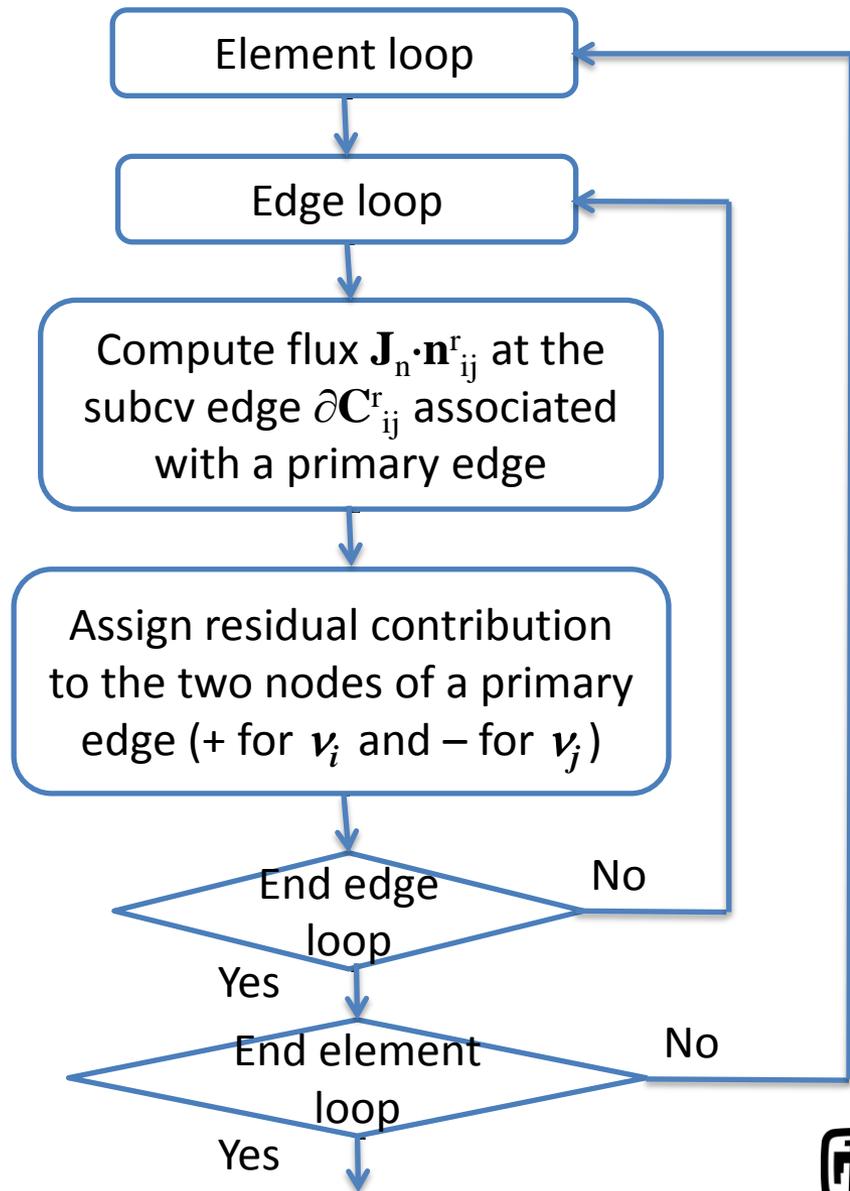
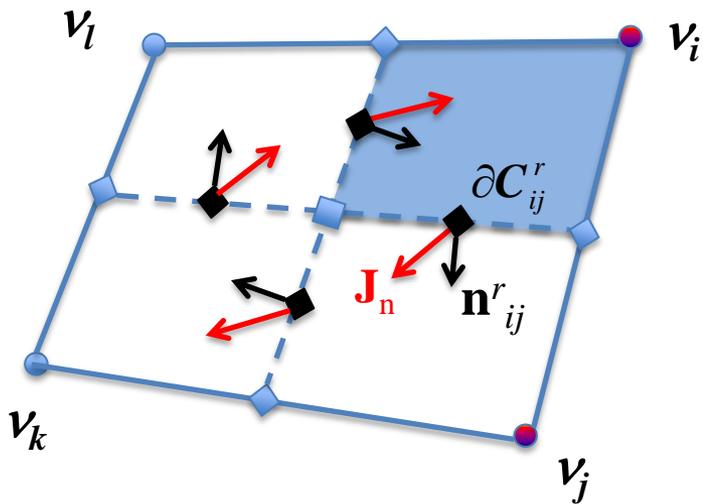


Compute integration of scalars over subcv  $C_i$

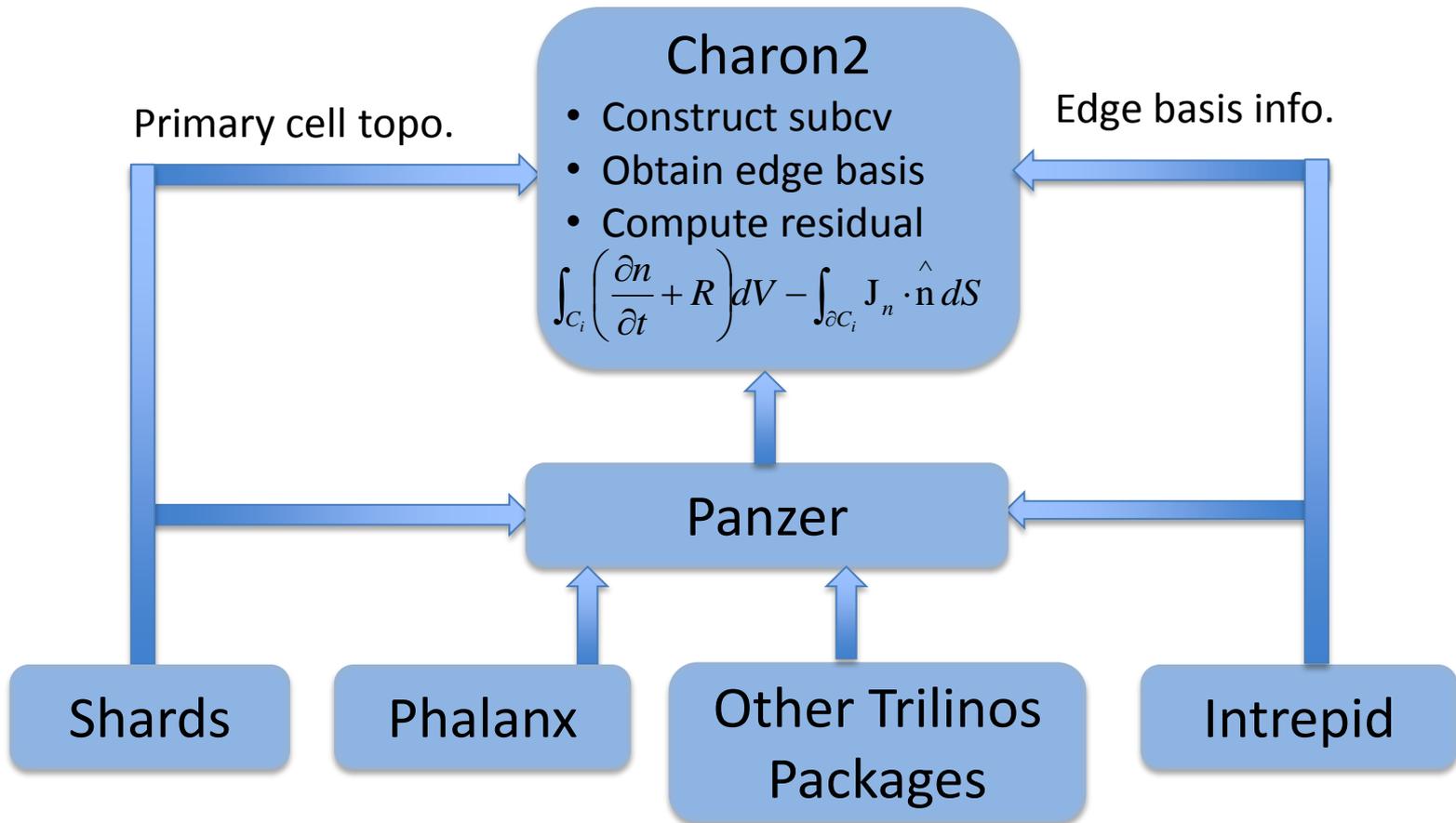
Assign the value to the nodal residual

# CVFEM-SG Residual Assembly

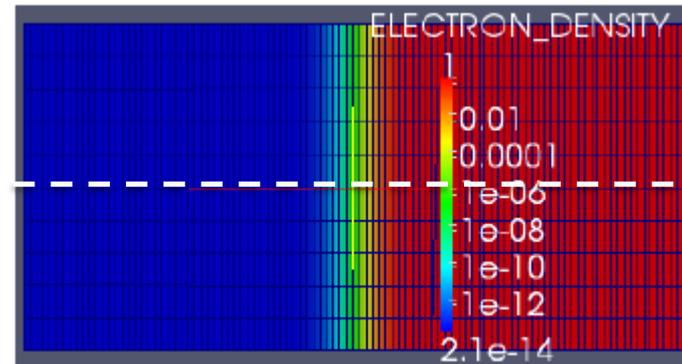
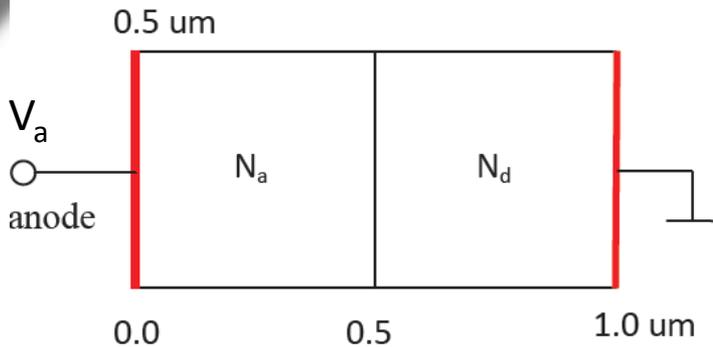
$$\int_{C_i} \left( \frac{\partial n}{\partial t} + R \right) dV - \underbrace{\int_{\partial C_i} \mathbf{J}_n \cdot \hat{\mathbf{n}} dS}_{\text{Flux}} = 0$$



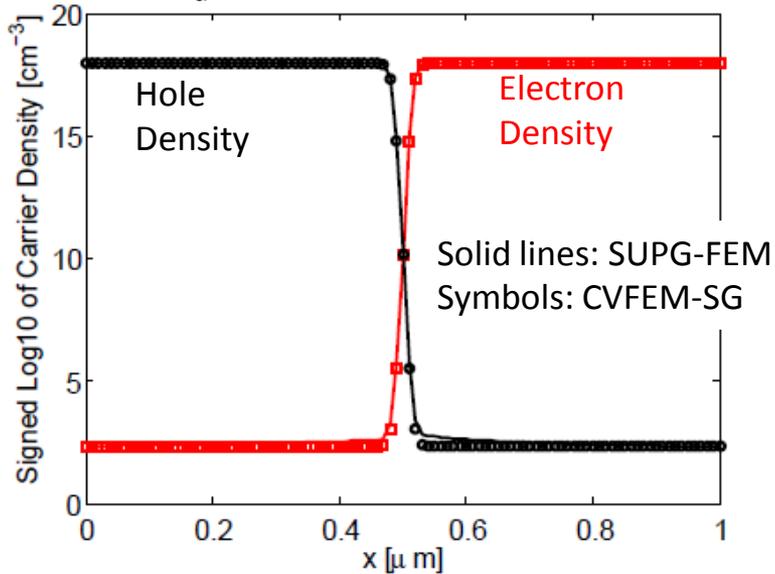
# Implementation Diagram



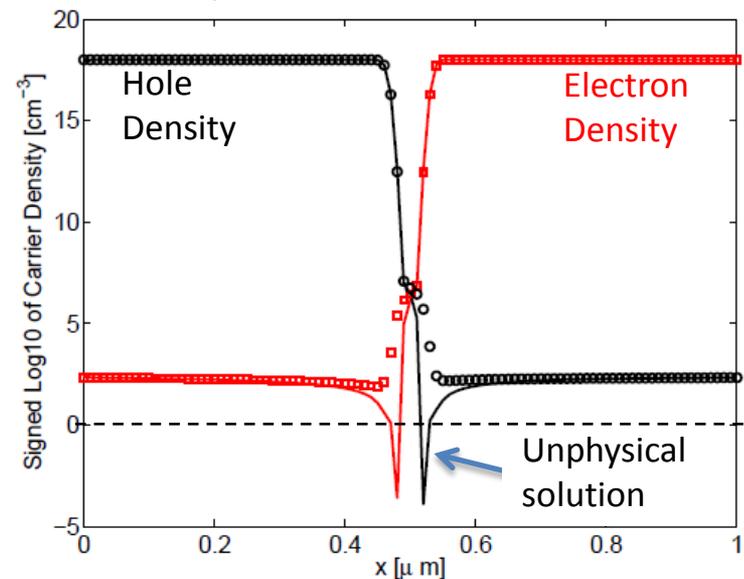
# PN Diode Example Results



$V_a = 0$  (moderate drift)



$V_a = -1.5V$  (strong drift)



**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.