CVFEM and Climate Visualization Applications Using Intrepid

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Outline

1. Intrepid Functionality
2. Control Volume Finite Element Method
3. Parallel Analysis and Visualization for Ultra-Large Climate Data Sets
Intrepid Functionality

- Cell geometry
  - maps to and from reference cells
  - Jacobians
  - surface normals and line tangents

- Integration on cells
  - cubature points and weights
  - up to high degree

- Discrete spaces
  - basis functions evaluated at points in cell
  - differential operators

- Discrete operators and functionals

\[
K_{i,j}^\kappa = \int_\kappa \mathcal{L}\phi_i(x)\mathcal{L}\phi_j(x)dx
\]

\[
\approx \sum_{p=1}^{N} \Phi^* (\mathcal{L}\hat{\phi}_i(\hat{x}_p))\Phi^* (\mathcal{L}\hat{\phi}_j(\hat{x}_p))J(\hat{x}_p)\omega_p
\]
Nonlinear coupled drift-diffusion equations for semi-conductors

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

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

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

\( E \) - electric field
\( \psi \) - electric potential
\( n \) - electron concentration
\( p \) - hole concentration
Drift-Diffusion Equations

Nonlinear coupled drift-diffusion equations for semi-conductors

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\[ E - \text{electric field} \]
\[ \psi - \text{electric potential} \]
\[ n - \text{electron concentration} \]
\[ p - \text{hole concentration} \]
Integrate over control volume \((C_i)\) to get weak form

\[
\int_{C_i} \frac{\partial n}{\partial t} dV - \int_{\partial C_i} \mathbf{J} \cdot \mathbf{n} dS = \int_{C_i} R(\psi, n, p) dV + \int_{\partial C_i^N} h dS
\]

Express in terms of nodal coefficients \((n_j)\)

\[
\sum_{j \in \Omega \cup \Gamma_N} \frac{\partial n_j(t)}{\partial t} \int_{C_i} N_j dV - \int_{\partial C_i} \mathbf{J}_h \cdot \mathbf{n} dS = \int_{C_i} R(\psi, n_h, p) dV + \int_{\partial C_i^N} h dS
\]
Control Volume Finite Element Method
with Scharfetter-Gummel Upwinding

Scharfetter-Gummel Upwinding

Assume \( \psi \) varies linearly along \( e_{ij} \)

\[ E_{ij} = - \frac{(\psi_j - \psi_i)}{|e_{ij}|} \quad \psi_i = \psi(v_i); \quad \psi_j = \psi(v_j) \]

Solve simplified ODE on edge to get

\[ J_{ij} = \frac{D_n}{|e_{ij}|} \left[ n_j B(-2a_{ij}) - n_i B(2a_{ij}) \right] \]

where \( a_{ij} = - \frac{(\psi_j - \psi_i)}{2\beta} \) and \( B(x) = \frac{x}{\exp(x)-1} \)

Approximation of Integral over \( \partial C_{ij} \)

\[ \int_{\partial C_{ij}} J \cdot \vec{n} dS \approx \frac{D_n}{|e_{ij}|} \left[ n_j B(-2a_{ij}) - n_i B(2a_{ij}) \right] \left( |\partial C_{ij}^s| + |\partial C_{ij}^t| \right) \]

Control Volume Finite Element Method
with Multi-Dimensional Scharfetter-Gummel Upwinding

Multi-Dimensional Scharfetter-Gummel Upwinding

\[ \hat{J}_h = \sum_{e_{kl} \in E(K_s)} \alpha_{kl} \mathbf{W}_{kl}(x) \]
\[ \alpha_{kl} = \frac{D_n}{|e_{kl}|} \left[ n_l B(-2a_{kl}) - n_k B(2a_{kl}) \right] \]

CVFEM with Multi-Dimensional Scharfetter-Gummel Upwinding

\[ \sum_{j \in \partial \Omega \cup \Gamma_N} \frac{\partial n_j(t)}{\partial t} \int_{C_i} N_j dV - \]
\[ \sum_{e_{kl} \in E(\Omega)} \left[ \frac{D_n}{|e_{kl}|} \left[ n_l B(-2a_{kl}) - n_k B(2a_{kl}) \right] \int_{\partial C_i} \mathbf{W}_{kl} \cdot \mathbf{n} dS \right] \]
\[ = \int_{C_i} R(\psi, n_h, p) dV + \int_{\partial C_i^N} h dS \]

CVFEM with SG Upwinding

Patch Test Results

CVFEM with SG Upwinding

Pseudo-1D Example Results

CVFEM M-D SG

CVFEM SUPG

FEM SUPG

CVFEM with SG Upwinding

N-Channel MOSFET

Scaled Continuity Equation

$$\nabla \cdot J_n = 0, \quad J_n = \bar{n} \mu_n \nabla \bar{\psi} - \bar{D}_n \nabla \bar{n}$$

Figure provided by Suzey Gao, SNL

Electron Density from CVFEM Using Intrepid

Figure provided by Suzey Gao, SNL
Parvis
Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets

**Motivation**
Climate models produce huge amounts of data and efficient, parallel algorithms for processing this data are required.

**Approach**
- Use NCAR Command Language (NCL) as the framework for the new capability
- Replace functions inside of NCL with parallel equivalents to speed up calculations
- Create Parallel Climate Analysis Library (ParCAL)
  - MOAB for mesh management
  - Intrepid for interpolation, cell operations
  - PNetcdf for parallel I/O
- Joint work with ANL(lead), NCAR, PNNL, UC-Davis
Given zonal and meridional velocity components \((u, v)\) and grid in longitude and latitude coordinates \((\lambda, \phi)\)

1. Compute gradients of basis functions on reference element

\[ \hat{\nabla} \hat{\phi}_i (\xi, \eta) \]

2. Map basis derivatives to element in \((\lambda, \phi)\) space and compute approximate \((u, v)\) gradients

\[ \nabla u = \sum_i u_i DF^{-T} \hat{\nabla} \phi_i, \quad \nabla v = \sum_i v_i DF^{-T} \hat{\nabla} \phi_i, \]

3. Combine partial derivatives and metric terms for vorticity in physical space

\[ \text{vorticity} = \frac{1}{r \cos \phi} \frac{\partial v}{\partial \lambda} - \frac{1}{r} \frac{\partial u}{\partial \phi} + \frac{u}{r} \tan \phi \]
Calculated locally on each element
- Easily parallelizable
- Global data not required

Calculated with spherical harmonics
- Requires global data

\[
vorticity = \frac{1}{r \cos \phi} \frac{\partial v}{\partial \lambda} - \frac{1}{r} \frac{\partial u}{\partial \phi} + \frac{u}{r} \tan \phi
\]
Calculating Divergence of a Vector Field with Intrepid

- Calculated locally on each element
- Easily parallelizable
- Global data not required

\[
\text{divergence} = \frac{1}{r \cos \phi} \frac{\partial u}{\partial \lambda} + \frac{1}{r} \frac{\partial v}{\partial \phi} - \frac{v}{r} \tan \phi
\]
Other Grid Operations Using Intrepid

- Bilinear interpolation from one grid to another
- Velocity potential ($\chi$) or stream function ($\psi$)

\[ \nabla^2 \chi = \text{divergence} \]

\[ \nabla^2 \psi = \text{vorticity} \]

Source Mesh

Target Mesh

Velocity Potential via Spherical Harmonics

www.ncl.ucar.edu
Conclusion

- Intrepid can be used for more than just standard finite element assembly

  - Multidimensional Edge Element
  - Scharfetter-Gummel upwinding
  - Calculating vorticity and divergence for climate data analysis
  - Interpolating values from one grid to another