CVFEM and Climate Visualization Applications Using Intrepid

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Numerical Analysis and Applications

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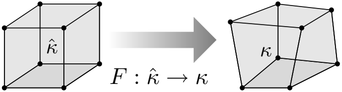
Outline

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



$$\mathbf{K}^{\kappa}_{i,j} = \int_{\kappa} \mathcal{L}\phi_i(x)\mathcal{L}\phi_j(x)dx$$
$$\approx \sum_{p=1}^{N} \Phi^*(\mathcal{L}\hat{\phi}_i(\hat{x}_p))\Phi^*(\mathcal{L}\hat{\phi}_j(\hat{x}_p))J(\hat{x}_p)\omega_p$$

Drift-Diffusion Equations

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
ψ - electric potential
n - electron concentration
p - hole concentration

Drift-Diffusion Equations

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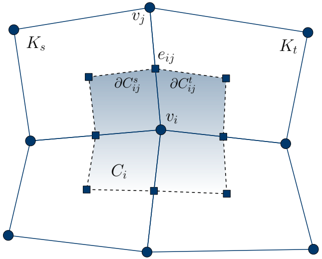
Control Volume Finite Element Method



Integrate over control volume (C_i) to get weak form

$$\int_{C_i} \frac{\partial n}{\partial t} dV - \int_{\partial \dot{C}_i} \mathbf{J} \cdot \vec{\mathbf{n}} dS = \int_{C_i} R(\psi, n, p) dV + \int_{\partial C_i^N} h dS$$

Express in terms of nodal coefficients (n_j)

$$\sum_{j \in \dot{\Omega} \cup \Gamma_N} \frac{\partial n_j(t)}{\partial t} \int_{C_i} N_j dV - \int_{\partial \dot{C}_i} \mathbf{J}_h \cdot \vec{\mathbf{n}} dS = \int_{C_i} R(\psi, n_h, p) dV + \int_{\partial C_i^N} h dS$$

Control Volume Finite Element Method

with Scharfetter-Gummel Upwinding

Scharfetter-Gummel Upwinding

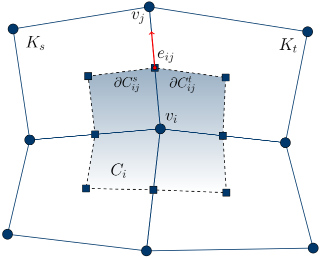
Assume ψ varies linearly along e_{ij}

$$\mathbf{E}_{ij} = -\frac{(\psi_j - \psi_i)}{|\mathbf{e}_{ij}|} \quad \psi_i = \psi(v_i); \psi_j = \psi(v_j)$$

Solve simplified ODE on edge to get

$$\mathbf{J}_{ij} = \frac{D_n}{|\mathbf{e}_{ij}|}\left[n_j B(-2a_{ij}) - n_i B(2a_{ij})\right]$$

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



Approximation of Integral over ∂C_{ij}

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

P. Bochev, "Control Volume Finite Element Method with Multidimensional Edge Element Scharfetter-Gummel upwinding. Part 1. Formulation", SAND 2011-3865, (2011).

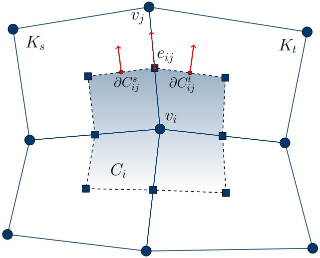
Control Volume Finite Element Method

with Multi-Dimensional Scharfetter-Gummel Upwinding

Multi-Dimensional Scharfetter-Gummel Upwinding

$$\widehat{\mathbf{J}}_h = \sum_{\mathbf{e}_{kl} \in E(K_s)} \alpha_{kl} \mathbf{W}_{kl}(\mathbf{x})$$

$$\alpha_{kl} = \frac{D_n}{|\mathbf{e}_{kl}|} \Big[n_l B(-2a_{kl}) - n_k B(2a_{kl}) \Big]$$



CVFEM with Multi-Dimensional Scharfetter-Gummel Upwinding

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

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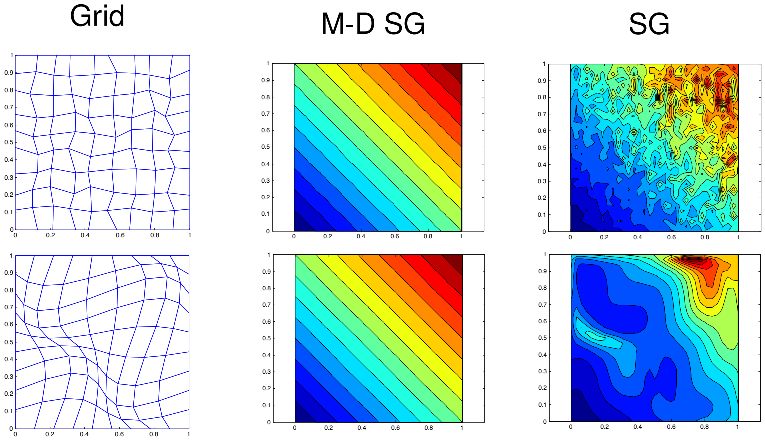
CVFEM with SG Upwinding

Patch Test Results



P. Bochev, K. Peterson, "Control Volume Finite Element Method with Multidimensional Edge Element Scharfetter-Gummel upwinding. Part 2. Computational Study", SAND 2011-5395, (2011).

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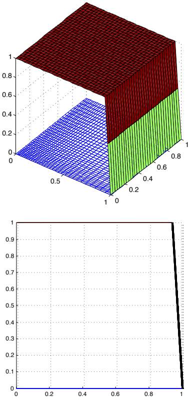
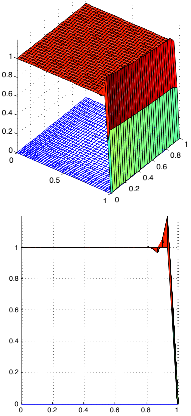
CVFEM with SG Upwinding

Pseudo-1D Example Results

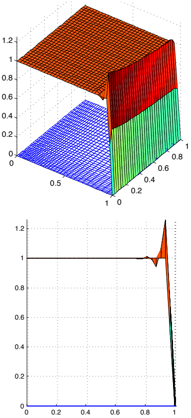
CVFEM M-D SG



CVFEM SUPG



FEM SUPG



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CVFEM with SG Upwinding

N-Channel MOSFET

Scaled Continuity Equation

$$\nabla \cdot \mathbf{J}_n = 0, \quad \mathbf{J}_n = \bar{n}\bar{\mu}_n \nabla \bar{\psi} - \bar{D}_n \nabla \bar{n}$$

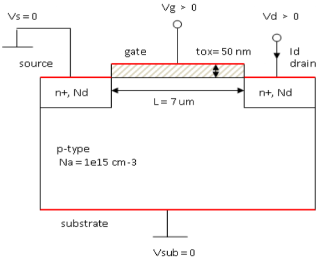
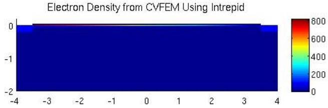
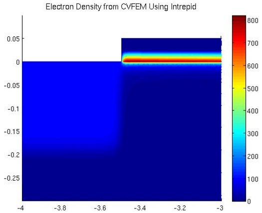


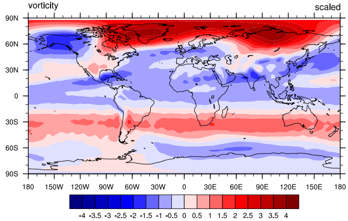
Figure provided by Suzey Gao, SNL





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

Parvis

Calculating Vorticity of a Vector Field with Intrepid

Given zonal and meridional velocity components (u, v) and grid in longitude and latitude coordinates (λ, ϕ)

1. Compute gradients of basis functions on reference element

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

2. Map basis derivatives to element in (λ, ϕ) space and compute approximate (u, v) gradients

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

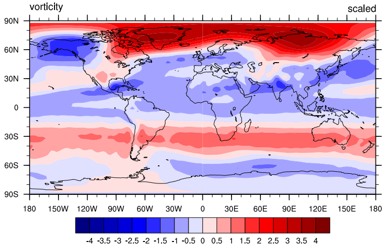
3. Combine partial derivatives and metric terms for vorticity in physical space

$$vorticity = \frac{1}{r\cos\phi}\frac{\partial v}{\partial \lambda} - \frac{1}{r}\frac{\partial u}{\partial \phi} + \frac{u}{r}\tan\phi$$

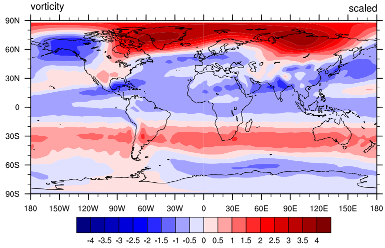
Parvis

Calculating Vorticity of a Vector Field with Intrepid

Intrepid



NCL



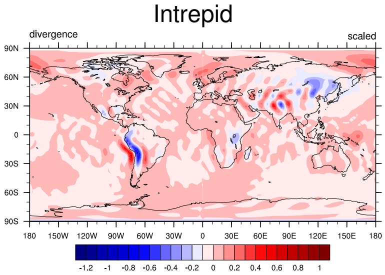
- Calculated locally on each element
- Easily parallelizable
- Global data not required

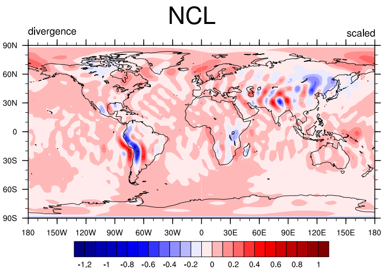
- Calculated with spherical harmonics
- Requires global data

$$vorticity = \frac{1}{r\cos\phi}\frac{\partial v}{\partial \lambda} - \frac{1}{r}\frac{\partial u}{\partial \phi} + \frac{u}{r}\tan\phi$$

Parvis

Calculating Divergence of a Vector Field with Intrepid





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

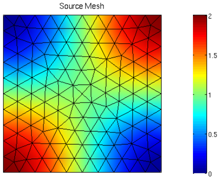
- Calculated with spherical harmonics
- Requires global data

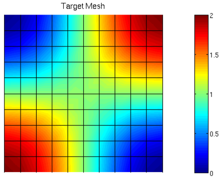
$$divergence = \frac{1}{r\cos\phi}\frac{\partial u}{\partial \lambda} + \frac{1}{r}\frac{\partial v}{\partial \phi} - \frac{v}{r}\tan\phi$$

Parvis

Other Grid Operations Using Intrepid

- Bilinear interpolation from one grid to another

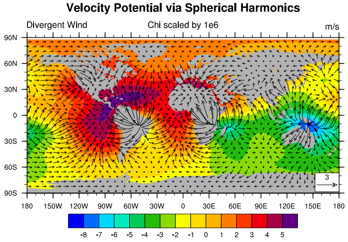




- Velocity potential (χ) or stream function (ψ)

$$\nabla^2 \chi = divergence$$

$$\nabla^2 \psi = vorticity$$



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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