Simulation Overview
FLOORS
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Outline

• Modeling Overview
• Device Simulation Development
• Directions
FLOOPS / FLOODS / FLOORS

- Object-oriented codes
- Multi-dimensional
- \( P = \text{Process} / D = \text{Device} \) 90% code shared
- Scripting capability for PDE’s - Alagator

- Commercialized - ISE / Synopsis
  - Sentaurus - Process is based on FLOOPS
- Licensed at over 400 sites world-wide
  - 2008 release
  - Manual is online (building a wiki manual)
What is Alagator?

- Scripting language for PDE’s
- Parsed into an expression tree
- Assembled using FV / FE techniques
- Stored in hierarchical parameter data base

- Models are accessible, easily modified
What is Alagator?

<table>
<thead>
<tr>
<th>Operator</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>“ddt”</td>
<td>Time derivative</td>
</tr>
<tr>
<td>“grad”</td>
<td>Spatial derivative</td>
</tr>
<tr>
<td>“sgrad”</td>
<td>Scharfetter / Gummel Discretization Operator</td>
</tr>
<tr>
<td>“dot”</td>
<td>Returns the dot product of the gradient of two field – electric field in direction of current flow</td>
</tr>
<tr>
<td>“elastic”</td>
<td>Compute elastic forces - FEM balance</td>
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</tbody>
</table>

- Example use of operators for diffusion equation
  
  - Fick’s Second Law of Diffusion
    - \( \text{ddt}(\text{Boron}) - 9.0 \times 10^{-16} \times \text{grad}(\text{Boron}) - K \times (\text{Boron} - \text{Trap}) \)
    - \( \partial C(x,t) / \partial t = D \partial^2 C(x,t) / \partial x^2 - K \times C(x,t) \times C_T \)
Discretization – Current Density

Quasi-Fermi Current Density
\[
J_n = -q \mu_n n \nabla \phi_n \\
J_p = -q \mu_p p \nabla \phi_p
\]

Boltzmann Relations
\[
\phi_n = \psi - \frac{kT}{q} \ln \left( \frac{n}{n_i} \right) \\
\phi_p = \psi + \frac{kT}{q} \ln \left( \frac{p}{n_i} \right)
\]

Drift-Diffusion Current Density
\[
J_n = q n \mu_n E + q D_n \nabla n \\
J_p = q p \mu_p E - q D_p \nabla p
\]

- To obtain a closed system of equations, current densities written as function quasi-Fermi levels.
- Using Boltzmann relations, current density can be written in the familiar relationship as the sum of drift and diffusion components.
- Drift-Diffusion subtracting large numbers is not a good recipe with finite precision arithmetic.
Finite Volume Scharfetter-Gummel (FVSG)

- Each PDE is integrated over a control volume $A$
- $A$ is defined by the perpendicular bisectors of mesh elements
- PDEs integrated using Green’s formula
- Current $J_{n,p}$ evaluated using the Scharfetter-Gummel
- Scharfetter Gummel
  - Assume field and current constant
  - Solve resulting equation
  - $J_n/q = D \left( B(t) n_i^+ - B(-t) n_i^- \right)/l_i$
  - $t = \mu E/D$
  - $B(t) = t/(e^t - 1)$ Bernoulli Function

- Advantages:
  - Commonly used “proven” method
  - Assembly time, each edge assembled once

- Disadvantages
  - Current defined only on edges, not continuous in space
  - Impact Ionization, Joule Heating more difficult
  - Works best when grid is aligned with current flow

\[
\begin{align*}
J_n &= qn\mu E + qD_n\nabla n \\
\frac{dn}{dt} &= \frac{1}{q} \nabla \cdot J_n - U_n \\
\frac{1}{q} \sum_i J_i \left( h_i^+ + h_i^- \right) - A \left( U_n + \frac{dn}{dt} \right) &= 0
\end{align*}
\]
Finite Element Quasi-Fermi (FEQF)

- \( \phi_{n,p} \) defined at grid nodes
- Use shape function in an element
  - Piecewise linear most common
  - Can be higher order
- Integrate equations and minimize error

- Advantages:
  - Current is a continuous function over each element
  - Easier to compute Joule Heating, Impact Ionization
  - Compatible with strain calculations

- Disadvantages
  - Not as stable
  - Convergence issues

\[
J_n = -q\mu_n n \nabla \varphi_n
\]

\[
\frac{dn}{dt} = \frac{1}{q} \nabla \cdot J_n - U_n
\]

\[
a(\psi, \nu) \equiv (-\rho, \nu)
\]

\[
a(\psi, \nu) \equiv \iint_{\Omega} \epsilon \nabla \psi \cdot \nabla \nu \, dx \, dy
\]

\[
(-\rho, \nu) \equiv -\iint_{\Omega} \rho \nu \, dx \, dy
\]
Inverse Piezoelectric Effect Calculation

- Electro-Mechanical Simulation with InversePiezo
- 25V Drain - above the del Alamo threshold
Material Flow Simulation

- Crude electromigration simulation
- Density is lowest where field is highest (corner)
- Field driven kickout mechanism
Conclusions / Directions

• Experimentally Integrated
  – Failure Mechanism Identification feeds M&S
  – Electrical Measurement feeds Model Accuracy

• Direction
  – Integrate Pieces Discussed
  – Connect strain calculations to Temp, Traps
  – Work on Trap Generation - Bosman Connection