DG Schemes for Collisional Plasma Models with Insulating BC on Rough Boundaries

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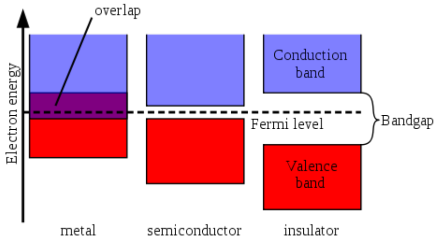
Semiconductors: Energy Bands, Conductivity, Periodicity

METALS: High Conductivity
E_F within one or more energy bands. Many occupied states above E_F, many unoccupied states below.

INSULATORS: Very Low Conductivity
E_F within large band gap between conduction and valence bands. Extremely few electrons and holes.

SEMICONDUCTORS: Intermediate Conductivity
E_F within moderate band gap between conduction and valence bands. A few electrons and holes.

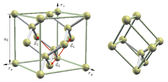


CRYSTAL: Lattice & Atomic Basis.

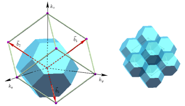
x-space Position Lattice $\leftrightarrow$ k-space reciprocal Lattice (Crystal Momentum - Fourier Transform Wave Vector)

Brillioun Zone (BZ) : Wigner-Seitz Unit Cell of Reciprocal Lattice

Periodic in x-space (FCC-Face Centered Cubic) & in k-space: (BCC-Body Centered Cubic) - Silicon



(a) Conventional cubic cell. (b) Primitive cell.



(a) Reciprocal lattice cell with first Brillouin zone. (b) Brillouin zone cells on every node.

Boltzmann-Poisson Model: *e*-Transport - Conduction Band

Boltzmann Equation for pdf $f(\mathbf{x}, \mathbf{k}, t)$:

$$\underbrace{\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})\cdot\nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E}(\mathbf{x},t)\cdot\nabla_{\mathbf{k}} f}_{\text{Hamiltonian } \textbf{Transport} \text{ along } (\mathbf{x},\mathbf{k})\text{-trajectories}} = \frac{df}{dt} = \underbrace{Q(f)(t,\mathbf{x},\mathbf{k})}_{\textbf{Collisions}\text{: in } \mathbf{k}\text{-space}} ,$$

Collisions: Scattering in **k**-space by Instant Short Range Forces.

$$Q(f)(t,\mathbf{x},\mathbf{k}) = \int_{\Omega_{\mathbf{k}'}} \left[S(\mathbf{k}'\to\mathbf{k})f'(1-f) - S(\mathbf{k}\to\mathbf{k}')f(1-f')\right] d\mathbf{k}'$$

Transport: Boltzmann Conserves Hamiltonian Structure (div.form)

$$\frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})\cdot\nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E}(\mathbf{x},t)\cdot\nabla_{\mathbf{k}} f = \nabla_{(\mathbf{x},\mathbf{k})}\cdot\left(f\left(\nabla_{\mathbf{k}}\varepsilon(\mathbf{k}), -q\mathbf{E}(\mathbf{x},t)\right)\frac{1}{\hbar}\right)$$

Poisson Equation for Electric Field $\mathbf{E} = -\nabla_{\mathbf{x}} V$, V potential:

$$\nabla_{\mathbf{x}}\cdot[\epsilon_r(\mathbf{x})\mathbf{E}(\mathbf{x},t)] = -\frac{q}{\varepsilon_0}\left[\rho(t,\mathbf{x}) - N_D(\mathbf{x})\right], \quad \mathbf{E}(\mathbf{x},t) = -\nabla_{\mathbf{x}} V(\mathbf{x},t)$$

Linear Collision Operator for Electron-Phonon Scattering in Si ($f << 1$)

$$Q(f)(t,\mathbf{x},\mathbf{k}) = \int_{\Omega_{\mathbf{k}'}} \left[S(\mathbf{k}' \to \mathbf{k}) f(t,\mathbf{x},\mathbf{k}') - S(\mathbf{k} \to \mathbf{k}') f(t,\mathbf{x},\mathbf{k}) \right] d\mathbf{k}'$$

Electron - Phonon Scattering in Silicon $S(\mathbf{k} \to \mathbf{k}') = S(\mathbf{k},\mathbf{k}')$

$$S(\mathbf{k},\mathbf{k}') = K_0\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})) + (n_q + 1)\, K\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p) + n_q\, K\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega_p)$$

Phonon Energy $\hbar\omega_p$ & Distribution $n_q = \left[\exp\left(\frac{\hbar\omega_p}{k_B T_L} \right) - 1 \right]^{-1}$.

$$Q(f) = K n_q \left\langle \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p), e^{\frac{\hbar\omega_p}{k_B T_L}} f' - f \right\rangle - K n_q \left\langle \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p), e^{\frac{\hbar\omega_p}{k_B T_L}} f - f' \right\rangle + K_0 \left\langle \delta(\varepsilon' - \varepsilon), f' - f \right\rangle$$

Maxwellian $M(\mathbf{k}) = \exp(-\varepsilon(\mathbf{k})/k_B T_L)$ in Kernel of Collision Op.

Previous Work on Numerical Methods for BP Models

Direct Simulation Monte Carlo (DSMC): Traditional in EE-CE
· Computes moments, noise, hard to resolve **pdf** & transients.
· Contact Boundary Conditions for BP hard to treat in DSMC
Deterministic Solvers: Alternative Method for BP in EE-CE
· No statistical noise, resolution of **pdf** evolution & transients
Previous Work: Parabolic & Kane band model approx.
Upwind finite difference: Fatemi, Odeh. Majorana, Pidatella.
WENO: Carrillo, Gamba, Majorana, Shu
Spherical Harmonics Expansion for pdf - Truncation: TU-Wien
Discontinuous Galerkin (DG): Cheng, Gamba, Majorana, Shu
DG - BP Computational Features:
Boundary Conditions simpler to treat.
Numerical Method adequate for physics of electron transport.
Energy related Coordinates for collisions (Fermi Golden Rule)
Dimension Reduction of Collision Integral by Energy Coordinates

BP model: e^- in Si Kane energy band

$t = \mathrm{t}/t_*$, $(x,y) = \vec{x}/\ell_*$, $\ell_* = 10^{-6}m$, $t_* = 10^{-12}s$, $V_* = 1\mathrm{Volt}$

Kane Energy Band Model:

$$\varepsilon\,(1+\alpha\varepsilon) = \frac{\hbar^2|k|^2}{2m^*}\,, \quad w = \frac{\varepsilon}{K_B T}\,, \quad |\vec{k}| = \frac{\sqrt{2m^* K_B T}}{h}\sqrt{w(1+\alpha_K w)}$$

$\vec{k}$: Description by Kane Energy & Angular Coordinates

$$\vec{k} = \frac{\sqrt{2m^* K_B T}}{h}\sqrt{w(1+\alpha_K w)}\left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi\right),$$

$w \geq 0\,, \mu \in [-1,1]\,, \varphi \in [-\pi,\pi]$.

Transformed Boltzmann for Jacobian DOS weighted pdf

$$\Phi(t,x,y,w,\mu,\varphi) = s(w)f\,, \quad s(w) = \sqrt{w(1+\alpha_K w)}(1+2\alpha_K w)$$

$$\frac{\partial \Phi}{\partial t} + \nabla_{(x,y,w,\mu,\varphi)} \cdot (\,\Phi\,\vec{g}\,) = C(\Phi)$$

BP model: e^- in Si Kane energy band

Transport Terms:

$$(g_1, \mathbf{g_2}) = c_x \left(\frac{\sqrt{w(1+\alpha_K w)}\,\mu}{1+2\alpha_K w}, \quad \frac{\sqrt{\mathbf{w(1+\alpha_K w)}}\sqrt{\mathbf{1-\mu^2}}\cos\varphi}{\mathbf{1+2\alpha_K w}} \right) \tag{1}$$

$$(g_3, g_4, g_5) = -c_k \left(\frac{2\sqrt{w(1+\alpha_K w)}\,\hat{e}_w}{1+2\alpha_K w}, \frac{\sqrt{1-\mu^2}\,\hat{e}_\mu}{\sqrt{w(1+\alpha_K w)}}, \frac{\hat{e}_\varphi / \sqrt{1-\mu^2}}{\sqrt{w(1+\alpha_K w)}} \right) \cdot \vec{E}(\vec{x}, t) \tag{2}$$

Collisions: Electron-Phonon Scattering (Fermi's G. Rule) in Si:

$$C(\Phi)(t,x,y,w,\mu,\varphi) = s(w) \left(c_0 \int_0^\pi d\varphi' \int_{-1}^1 d\mu' \,\Phi(t,x,y,w,\mu',\varphi') + \int_0^\pi d\varphi' \int_{-1}^1 d\mu' \,[c_+ \Phi(t,x,y,w+\gamma,\mu',\varphi') + c_- \Phi(t,x,y,w-\gamma,\mu',\varphi')] \right) - 2\pi[c_0 s(w) + c_+ s(w-\gamma) + c_- s(w+\gamma)]\Phi(t,x,y,w,\mu,\varphi)\,,$$

Poisson Eq: $\frac{\partial}{\partial x}\left(\epsilon_r \frac{\partial \Psi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\epsilon_r \frac{\partial \Psi}{\partial y}\right) = c_p\left[\rho(t,x,y) - N(x,y)\right],$

$\rho(t,x,y) = \int_0^{+\infty} dw \int_{-1}^{1} d\mu \int_0^\pi d\varphi \,\Phi(t,x,y,w,\mu,\varphi)$

DG Formulation for Transformed Boltzmann Eq.

$\Phi_h \in V_h = Q^{1,0}$: PW Linear in $\vec{x}$, PW Constant in $\vec{w}$

$$\Phi_h = \sum_I \chi_I \left[T_I(t) + X_I(t) \frac{(x-x_i)}{\Delta x_i/2} + Y_I(t) \frac{(y-y_j)}{\Delta y_j/2} \right], \; I = ijkmn.$$

$$\Omega_{ijkmn} = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}} \right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}} \right] \times \left[w_{k-\frac{1}{2}}, w_{k+\frac{1}{2}} \right] \times \left[\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}} \right] \times \left[\varphi_{n-\frac{1}{2}}, \varphi_{n+\frac{1}{2}} \right]$$

where $i = 1, \ldots N_x$, $j = 1, \ldots N_y$, $k = 1, \ldots N_w$, $m = 1, \ldots N_\mu$, $n = 1, \ldots N_\varphi$,

DG Formulation for Boltzmann Eq:

Find $\Phi_h \in V_h^k$, s.t. for any test function $v_h \in V_h^k$

$$\int_{\Omega_{ijkmn}} (\Phi_h)_t \, v_h \, d\Omega - \int_{\Omega_{ijkmn}} g_1 \Phi_h \, (v_h)_x \, d\Omega - \int_{\Omega_{ijkmn}} g_2 \Phi_h \, (v_h)_y \, d\Omega$$
$$+ F_x^+ - F_x^- + F_y^+ - F_y^- + F_w^+ - F_w^- + F_\mu^+ - F_\mu^- + F_\varphi^+ - F_\varphi^- =$$
$$\int_{\Omega_{ijkmn}} C(\Phi_h) \, v_h \, d\Omega.$$

$F^{\pm}$'s: Boundary integrals related to Upwind Numerical Fluxes.

DG Solver - Full Band BP Models
Algorithm for DG-BP in Numerical Scheme

Dynamic Extension of Gummel Iteration Map

Starting with an Initial Condition Φ_h, and given the B.C., the **DG-BP algorithm** advances from t^n to t^{n+1} in these steps:

Step 1.- Compute charge density ρ

Step 2.- Use this ρ to solve Poisson (LDG) for potential and electric field, compute then transport g_i's & boundary integrals.

Step 3.- Solve the transport part of Boltzmann Equation by DG, then obtaining a method of line for Φ_h (ODE system).

Step 4.-Evolve ODE system by proper time stepping from t^n to t^{n+1} (If partial time step necessary, repeat Step 1 to 3 as needed).

Boundary Conditions in BP: 2D-$\vec{x}$, 3D-$\vec{k}$

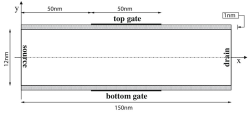


Fig. 4.14. Schematic representation of a 2D double gate MOSFET device.

Neutral Charges BC: Source & Drain
$f_{out}(t,\vec{x},\vec{k})|_\Gamma = N_D(\vec{x}) f_{in}(t,\vec{x},\vec{k})|_\Gamma / \rho_{in}(t,\vec{x})$, $\Gamma \subset \partial\Omega_{\vec{x}} : x = 0, L_x$.
Reflection BC: Silicon Region (Top & Bottom):
$f|_{\Gamma_N^-} = F_R(f|_{\Gamma_N^+})$. Neumann Inflow/Outflow (-/+) Boundary:
$\Gamma_N^\pm = \{(\vec{x},\vec{k}) : \vec{x} \in \Gamma_N, \vec{k} \in \Omega_{\vec{k}}, \pm\eta(\vec{x}) \cdot \nabla_{\vec{k}}\varepsilon(\vec{k}) > 0\}$,
$\eta(\vec{x})$ outward normal. $v(\vec{k}) := \nabla_{\vec{k}}\varepsilon(\vec{k})/\hbar$
Zero Flux Condition at Reflecting Boundary (Pointwise)
$0 = \eta(\vec{x}) \cdot \int_{\Omega_{\vec{k}}} v(\vec{k}) f d\vec{k} = \int_{v\cdot\eta>0} v \cdot \eta f|_+ d\vec{k} + \int_{v\cdot\eta<0} v \cdot \eta F_R(f|_+) d\vec{k}$
Poisson BC Example: 2D Double gated MOSFET
$\Psi = 0.5235$ V at source, $\Psi = 1.5235$ at drain, $\Psi = 1.06$ at gate.
For the rest of boundaries: $\frac{\partial\Psi}{\partial\hat{n}} = 0$ (Homogeneous Neumann BC)

Reflection Boundary Conditions for Boltzmann-Poisson

$\mathbf{f}_- = \mathbf{F}(\mathbf{f}_+)$: Reflection at Inflow − Boundary (Outflow: +)
$\Gamma_N^{\pm} = \{(\vec{x}, \vec{k}) | \pm \nabla_{\vec{k}} \varepsilon(\vec{k}) \cdot \eta(\vec{x}) > 0, \quad \eta(\vec{x}) : \text{outward normal}\}$

Specular Reflection:

$$f(\vec{x}, \vec{k}, t)|_{\Gamma_N^-} = f(\vec{x}, \vec{k}', t)|_{\Gamma_N^+}, \quad \text{for} \quad (\vec{x}, \vec{k}) \in \Gamma_N^-, \quad t > 0,$$

$$\vec{k}' \quad \text{s.t.} \quad \nabla_{\vec{k}} \varepsilon(\vec{k}') = \nabla_{\vec{k}} \varepsilon(\vec{k}) - 2(\nabla_{\vec{k}} \varepsilon(\vec{k}) \cdot \eta(\vec{x}))\eta(\vec{x}), \quad (\vec{x}, \vec{k}') \in \Gamma_N^+.$$

Diffusive Reflection:

$$f(\vec{x}, \vec{k}, t)|_{\Gamma_N^-} = C e^{-\varepsilon(\vec{k})/K_B T} \sigma(\vec{x}, t), \quad (\vec{x}, \vec{k}) \in \Gamma_N^-$$

$$\sigma(\vec{x}, t) = \int_{\nabla_{\vec{k}} \varepsilon(\vec{k}) \cdot \eta > 0} \nabla_{\vec{k}} \varepsilon(\vec{k}) \cdot \eta(\vec{x}) \, f|_{\Gamma_N^+} \, d\vec{k}, \quad C(\eta) \quad \text{s.t. zero flux holds}$$

Mixed Reflection:

$$f(\vec{x}, \vec{k}, t)|_- = p \, f(\vec{x}, \vec{k}', t) + (1 - p) e^{-\frac{\varepsilon(\vec{k})}{K_B T}} C \sigma(\vec{x}, t), \quad (\vec{x}, \vec{k}) \in \Gamma_N^-$$

p : Specularity Parameter, $0 \le p \le 1$. p constant, $p(\vec{k})$...

Reflection BC: A non-exhaustive list of references by topic

Kinetic Theory of Gases:

- Cercignani, The Boltzmann Equation and Its Application (1988)
- Sone, Molecular Gas Dynamics: Theory, Techniques & Applications
- Brull, Charrier, Mieussens, Gas-surface interaction & BC for the Boltzmann equation, Kinetic & Related Models (2014)
- Struchtrup, H. Maxwell boundary condition and velocity dependent accommodation coefficient. Phys. Fluids 25, 112001 (2013):

Electric Conduction Physics & Boltzmann for Semiconductors

- Fuchs' BC for e^- pdf: mixed reflection with constant specularity p.
- Greene: $p(\vec{k})$ BC for metal, semimetal, & semiconductor.
- Soffer, Gaussian models rough surface. $\underline{p(\vec{k}) = exp(-4\eta^2 k^2 \sin^2 \varphi)}$
- Cercignani, Gamba, Levermore, High field approximations to a BP system & BC in a semiconductor. AML '97
- A. Jungel, Transport Eq. for Semiconductors, Springer (2009)

Reflective BC on BP & Zero Flux Condition

Formulation of Reflective BC:

$$f(\vec{x},\vec{k},t)|_{\Gamma_{N^-}} = F(f|_{\Gamma_{N^+}}) \tag{3}$$

s.t. Zero flux condition (Cercignani, Gamba, Levermore) satisfied at reflecting boundaries:

$$0 \;=\; \eta(\vec{x})\cdot J(\vec{x},t) = \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}\, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, F(f|_{\Gamma_{N^+}})\, d\vec{k}$$

For simplicity we write $\vec{v} = \vec{v}(\vec{k}) = \nabla_{\vec{k}}\varepsilon(\vec{k})/\hbar$.

Specular Reflection BC on BP & Zero Flux Condition

$$f(\vec{x},\vec{k},t)|_{\Gamma_N^-} = f(\vec{x},\vec{k}',t)|_{\Gamma_N^+}, \quad \text{for} \quad (\vec{x},\vec{k}) \in \Gamma_N^-, \quad t>0,$$

$$\vec{k'} \quad \text{s.t.} \quad \nabla_{\vec{k}}\varepsilon(\vec{k}') = \nabla_{\vec{k}}\varepsilon(\vec{k}) - 2(\nabla_{\vec{k}}\varepsilon(\vec{k})\cdot\eta(\vec{x}))\eta(\vec{x}), \quad (\vec{x},\vec{k}') \in \Gamma_N^+.$$

Specular BC clearly satisfies zero flux condition at reflecting boundaries:

$$\int_{\eta\cdot\vec{v}>0} |\eta\cdot\vec{v}|\, f(\vec{x},\vec{k},t)|_{\Gamma_{N^+}}\, d\vec{k} + \int_{\eta\cdot\vec{v}<0} -|\eta\cdot\vec{v}|\, f(\vec{x},\vec{k}',t)|_{\Gamma_{N^+}}\, d\vec{k} = 0$$

Diffusive Reflection BC on BP & Zero Flux Condition

$$f(\vec{x},\vec{k},t)|_{\Gamma_N^-} = Ce^{-\varepsilon(\vec{k})/K_BT}\int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta(\vec{x})\,f(\vec{x},\vec{k},t)|_{\Gamma_N^+}\,d\vec{k}, \quad (\vec{x},\vec{k})\in\Gamma_N^-$$

$C\{\eta(x)\}$ independent of $f(\vec{x},\vec{k},t)$, $\vec{k}$, given by zero flux condition:

$$\begin{aligned}
0 &= \int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\, f|_+ d\vec{k} + \int_{\vec{v}\cdot\eta<0}\vec{v}\cdot\eta\left[Ce^{-\frac{\varepsilon}{K_BT}}\int_{v\cdot\eta>0} v\cdot\eta f|_+ d\vec{k}\right] d\vec{k} \\
0 &= \int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\, f|_+\, d\vec{k} + C\int_{\vec{v}\cdot\eta<0}\vec{v}\cdot\eta\, e^{-\frac{\varepsilon}{K_BT_L}}\, d\vec{k}\int_{v\cdot\eta>0} v\cdot\eta f|_+ d\vec{k} \\
0 &= \int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\, f|_+\, d\vec{k}\left(1 - C\int_{\vec{v}\cdot\eta<0}|\vec{v}\cdot\eta|\, e^{-\frac{\varepsilon}{K_BT_L}}\, d\vec{k}\right), \quad \text{so:} \\
C &= \left(\int_{\vec{v}\cdot\eta<0}|\vec{v}\cdot\eta|\, e^{-\varepsilon(\vec{k})/K_BT_L}\, d\vec{k}\right)^{-1}
\end{aligned}$$

Mixed Reflection BC with $p(\vec{k})$ & Zero Flux Condition

For $p(\vec{k})$, the traditional C, σ do not necessarily satisfy zero flux.
C', σ' **for** $p(\vec{k})$ **should be derived from zero flux condition.**
Problem: Find C', σ' s.t. zero flux holds for $p(\vec{k})$ Mixed Reflection
Solution:

$$
\begin{aligned}
0 &= \eta(\vec{x}) \cdot J(\vec{x}, t) = \int_{\vec{v}\cdot\eta>0} \vec{v} \cdot \eta \, f|_{\Gamma_{N^+}} \, d\vec{k} \\
&+ \int_{\vec{v}\cdot\eta<0} \vec{v} \cdot \eta \left[p(\vec{k}) f(\vec{x}, \vec{k}', t)|_{\Gamma_{N^+}} + (1 - p(\vec{k})) C' e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}} \sigma'(\vec{x}, t) \right] d\vec{k} \\
0 &= \underbrace{\int_{\vec{v}\cdot\eta>0} \vec{v} \cdot \eta \, f|_{\Gamma_{N^+}} \, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v} \cdot \eta \, p(\vec{k}) \, f(\vec{k}')|_{\Gamma_{N^+}} \, d\vec{k}}_{\sigma'(\vec{x},t)} \\
&- \sigma'(\vec{x}, t) \cdot C' \underbrace{\int_{\vec{v}\cdot\eta<0} |\vec{v} \cdot \eta| (1 - p(\vec{k})) e^{\frac{-\varepsilon}{K_B T_L}} d\vec{k}}_{1/C'} \quad .
\end{aligned}
$$

Mixed Reflection BC with $p(\vec{k})$ & Zero Flux Condition

Solution: Defining the integrals

$$\begin{aligned} \sigma'(\vec{x},t) &= \int_{\vec{v}\cdot\eta>0} |\vec{v}\cdot\eta|\, f|_{\Gamma_{N^+}}\, d\vec{k} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta| p(\vec{k})\, f(\vec{k}')|_{\Gamma_{N^+}}\, d\vec{k} \\ &= \int_{\vec{v}\cdot\eta>0} |\vec{v}(\vec{k})\cdot\eta| \left(1-p(\vec{k}')\right) f(\vec{x},\vec{k},t)|_{\Gamma_{N^+}}\, d\vec{k}\,, \qquad (4) \\ C'(\eta(\vec{x})) &= \left(\int_{\vec{v}\cdot\eta<0} \left(1-p(\vec{k})\right) |\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}\right)^{-1}, \qquad (5) \end{aligned}$$

the Mixed Reflection BC for $p(\vec{k})$ is given in terms of $\sigma'\{f|_+\}$, C', such that the zero flux condition is satisfied, as:

$$f(\vec{x},\vec{k},t)|_{\Gamma_N^-} = p(\vec{k}) f|_+(\vec{x},\vec{k}',t) + \left(1-p(\vec{k})\right) e^{\frac{-\varepsilon(\vec{k})}{K_B T}} C'\sigma'\{f|_+\}(\vec{x},t)$$

$p(\vec{k})$ Mixed Reflex. BC in DG-FEM & Numeric. Zero Flux

$$f_h(\vec{x},\vec{k},t)|_{\Gamma_N^-} = \Pi_h \left\{ p(\vec{k}) f_h|_+(\vec{x},\vec{k}',t) + \left(1-p(\vec{k})\right) e^{\frac{-\varepsilon(\vec{k})}{K_B T}} C'\sigma'_h(\vec{x},t) \right\}$$

Find C', σ'_h s.t. zero flux holds for BC, $V_h = Q^{1,0} = P^1(\vec{x}) \times P^0(\vec{k})$

$$\begin{aligned} 0 &= \eta(\vec{x}) \cdot J_h(\vec{x},t) = \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f_h|_{\Gamma_{N^+}}\, d\vec{k} \\ &+ \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, \Pi_h \left\{ p(\vec{k}) f'_h|_{\Gamma_{N^+}} + (1-p(\vec{k})) C' e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}} \sigma'_h(\vec{x},t) \right\} d\vec{k} \\ 0 &= \underbrace{\int_{\vec{v}\cdot\eta>0} |\vec{v}\cdot\eta|\, f_h|_{\Gamma_{N^+}}\, d\vec{k} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, \Pi_h\{p(\vec{k})\, f_h(\vec{x},\vec{k}',t)|_{\Gamma_{N^+}}\} d\vec{k}}_{\sigma'_h(\vec{x},t)} \\ &- \sigma'_h(\vec{x},t) \cdot \underbrace{\left(C' \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta| \Pi_h\{(1-p(\vec{k})) e^{\frac{-\varepsilon}{K_B T_L}} d\vec{k}\} \right)} \quad . \end{aligned}$$

Numerical Implementation of Reflection BC in DG-BP

Specular Reflection BC (Approximating $\vec{v}(\vec{k}) = \vec{k}$) $y_{1/2} = 0$:

$\hat{\Phi}(t, x, y_{1/2}, w, \mu, \varphi) = \hat{\Phi}(t, x, y_{1/2}, w, \mu, \pi - \varphi)$. $n' = N_\varphi - n + 1$:

$(x, y_{1/2}, w, \mu, \varphi) \in \Omega_{i0kmn}$, $(x, y_{1/2}, w, \mu, \pi - \varphi) \in \Omega_{i1kmn'}$, $y_{\frac{1}{2}} = 0$

$T_{10kmn} = T_{i1kmn'}$, $X_{10kmn} = X_{i1kmn'}$, $Y_{10kmn} = -Y_{i1kmn'}$

Diffusive Reflection BC. Project Φ from BC in V_h^1 for Φ_h:

$\Phi_h \in V_h$, $\quad \sigma_h(x, y, t) = \int_{\pm \cos\varphi \geq 0} |g_2| \, \hat{\Phi}_h|_+ \, dw d\mu d\varphi =$

$\sigma_I^0(t) + \sigma_I^x(t) \frac{2(x - x_i)}{\Delta x_i} + \sigma_I^y(t) \frac{2(y - y_j)}{\Delta y_j} = \sigma_h \in V_h^1$, $y_b = 0, L_y$.

$\Phi|_- = C \, \sigma_h(x, y, t) \, e^{-w} s(w) \to \hat{\Phi}_h|_- = \Pi_h \{\Phi|_-\} |_{y_b} \in V_h^1$

Mixed Reflection BC:

$\Phi_h = p \, \Phi_h^{spec} + (1 - p) \Phi_h^{diff}$. p constant

Mixed Reflection BC in DG-BP Numerics

$\hat{\Phi}_h(\vec{x}, \vec{w}, t)|_{\Gamma_N^-} =$
$\Pi_h \left\{ p(\vec{w})\hat{\Phi}_h(\vec{x}, \vec{w}', t)|_+ \, + \, (1 - p(\vec{w}))s(w)e^{-w}C'\sigma' \left\{ \hat{\Phi}_h|_+ \right\}(\vec{x}, t) \right\}$

Example of parameter $p(\vec{w})$:

$p(\vec{k}) = e^{-4l_r^2|k|^2\cos^2\Theta} = \exp(-4l_r^2 w(1 + \alpha_K w)\sin^2\varphi) = p(w, \varphi)$,
l_r: rms height of rough interface (Soffer's $p(\vec{k})$ parameter).

Mixed Reflection - $p(\vec{w})$ **BC.** Project Φ from BC in V_h for $\hat{\Phi}_h|_-$:

$\sigma_h'(x, y, t) =$
$\int_{\vec{w}\cdot\eta>0} \vec{w}\cdot\eta\, \hat{\Phi}_h|_+ d\vec{w} - \int_{\vec{w}\cdot\eta<0} |\vec{w}\cdot\eta| \Pi_h \left\{ p(\vec{w})\hat{\Phi}_h|_+(\vec{x}, \vec{w}', t) \right\} d\vec{w} =$
$\sigma_I'^0(t) + \sigma_I'^x(t)\frac{2(x-x_i)}{\Delta x_i} + \sigma_I'^y(t)\frac{2(y-y_j)}{\Delta y_j} = \sigma_h' \in V_h^1 \,,\; y = 0, L_y.$

Numerical Results

Simulation: 2D n bulk Silicon. 3D in $\underline{k}(w,\mu,\varphi)$

Initial Condition: $\Phi(w)|_{t=0} = \Pi\left\{Ne^{-w}s(w)\right\}$. Final Time: 1.0ps

Boundary Conditions (BC):

$\vec{k}$-space: Cut-off - at $w = w_{max}$, Φ is machine zero.
Only needed BC in (w,μ,φ): transport normal to the boundary analitically zero at 'singular points' boundaries:
At $w = 0$, $g_3 = 0$. At $\mu = \pm 1$, $g_4 = 0$. At $\varphi = 0, \pi$, $g_5 = 0$.

$\vec{x}$-space: Charge Neutrality at boundaries $x = 0$, $x = 0.15\mu m$.
Bias - Potential: $V|_{x=0} = 0.5235$ V, $V|_{x=0.15\mu m} = 1.5235$ V.
Neumann BC for Potential at $y = 0$, $L_y = 12nm$: $\partial_y V|_{y=0,\,L_y} = 0$
Reflection BC at $y = 0, y = 12nm$: Specular, Diffusive, Mixed

Density

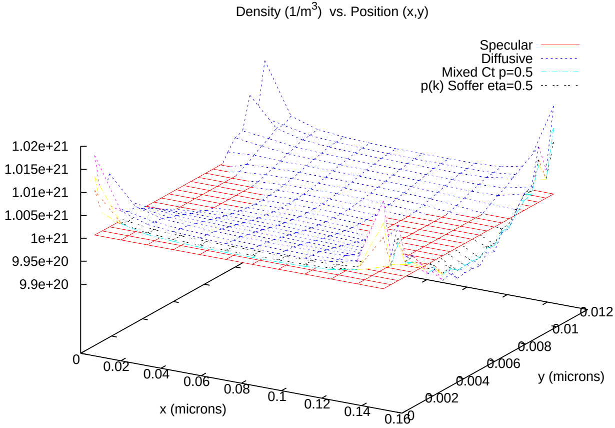


Figure : Density ρ (m^{-3}) vs Position (x, y) in (μm) plot for Specular, Diffusive, & Mixed Reflection.

Total Mass

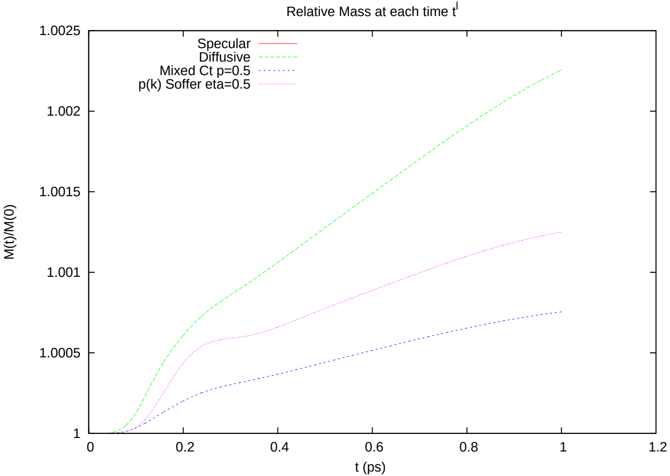


Figure : Total Mass $M(t)$) vs time t plot for Specular, Diffusive, & Mixed Reflection.

Average Velocity Components

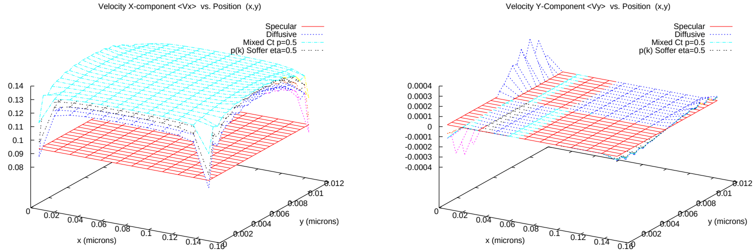


Figure : Mean Velocity (Vx, Vy) vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed Reflection.

Average Energy

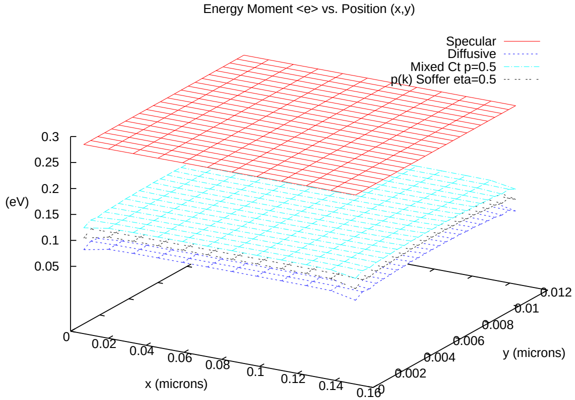


Figure : Mean energy $e(eV)$ vs. Position (x, y) in (μm) plots for Specular, Diffusive, & Mixed Reflection.

Electric Potential

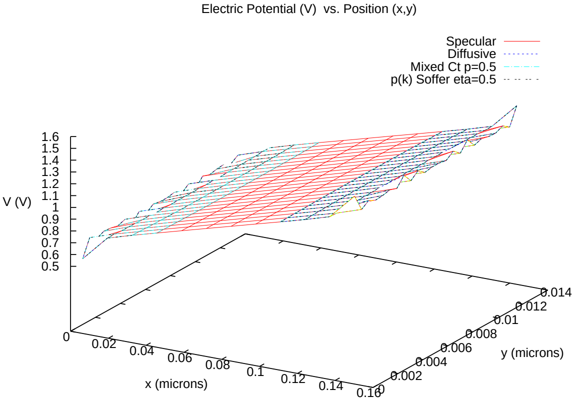
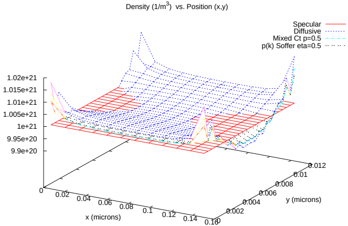
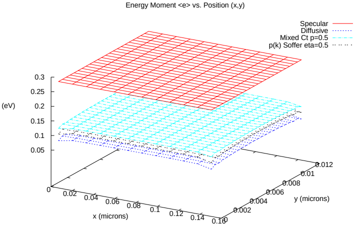
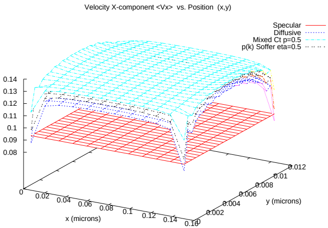


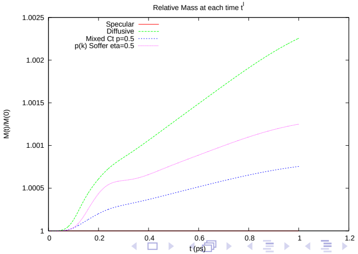
Figure : Potential $V(Volts)$ vs. Position (x, y) (μm) plot for Specular, Diffusive & Mixed Reflection

Si e-phonon collisions with Reflection & Neutral Charge BC

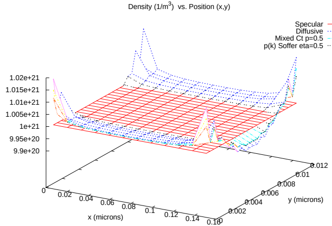


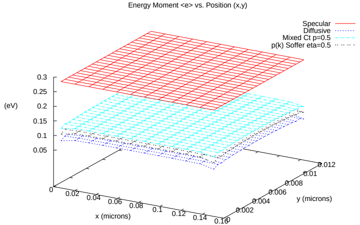


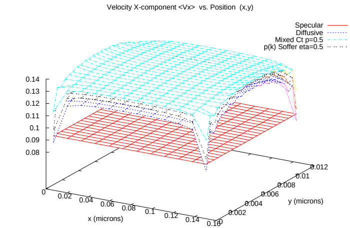


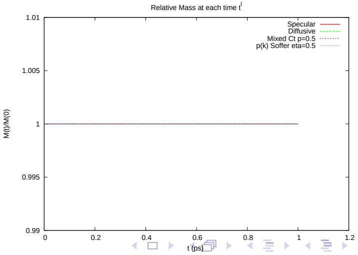


Si e-phonon collisions with Reflection & Periodic BC

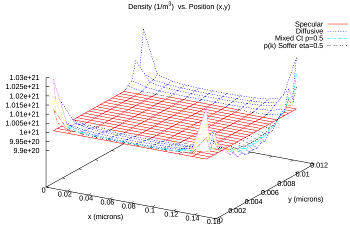


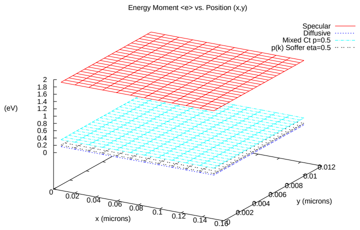


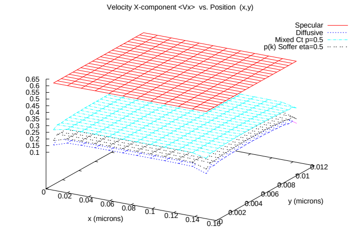


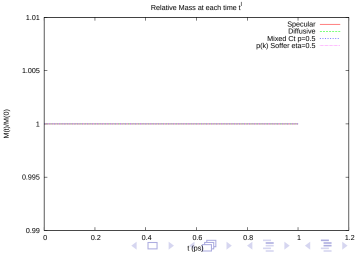


Collisionless e^{-} Transport with Reflection & Periodic BC









Conclusions:

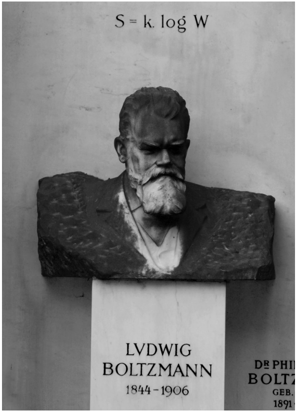
- Formulation of Numerical Boundary Conditions for Diffusive and General Mixed Reflection that satisfy a Numerical Equivalent of a Zero Flux Condition at Insulating Boundaries
- Diffusive Reflection Numerical BC, compared to Specular, contributes to:
  - Increase density profile close to reflecting boundaries (decreasing it at the center due to mass conservation)
  - Decrease Average Energy over the domain
  - Without collisions, it decreases the average velocity, but...
  - Collisions (energy transitions) with diffusive BC for momentum give average velocity greater than specular. More complex.

Work in Progress:

- Boundary Layer Homogenization in BP - Heitzinger & Degond Half Domain with Periodic Cells horizontally.
  BC: Periodic Charge & Surface Roughness Reflection.

The End

Thanks!



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