Boundary Conditions in DG Methods for Boltzmann - Poisson Models of Electron Transport in Semiconductors

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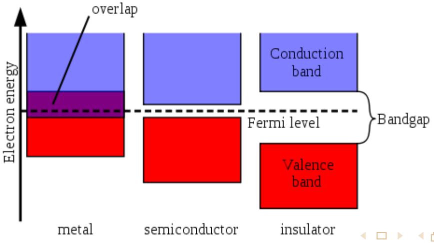
Electron Transport in Semiconductors Physics: Energy Bands and Conductivity

METALS: High Conductivity
E_F (Fermi Level: $f(E_F) = 1/2$) 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 vacancies (holes).

SEMICONDUCTORS: Low to Intermediate Conductivity
E_F within moderate band gap between conduction and valence bands.
A few electrons and vacancies (holes).



Semiconductors with Periodic Crystal Structure

Crystal: Lattice & Atomic Basis.

Position x-space Lattice $\leftrightarrow$ Fourier k-space reciprocal Lattice

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

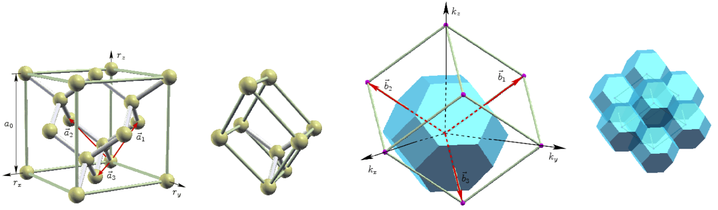


Figure : Periodicity in x-space (FCC - Face Centered Cubic) and in Crystal Momentum k-space (BCC - Body Centered Cubic) for Silicon

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)

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

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

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

BP Model : Macroscopic Quantities & Conservation Prop.

- Macroscopic quantities of Boltzmann Eq: (Moments)

  Electron Density: $\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{k}, t) d\mathbf{k}$

  Mean Velocity: $v(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x},t)} \int f(\mathbf{x}, \mathbf{k}, t) \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon(\mathbf{k}) d\mathbf{k}$

  Avg. Momentum (Current):
  $v(\mathbf{x}, t)\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{k}, t) \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon(\mathbf{k}) d\mathbf{k}$

  Mean Energy Density: $e(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x},t)} \int f(\mathbf{x}, \mathbf{k}, t) \varepsilon(\mathbf{k}) d\mathbf{k}$

- Conservation Properties:

  Mass Conservation: holds for previous collision operators.
  $\int Q(f) d\mathbf{k} = 0$

  However, $\int Q(f) \varepsilon(\mathbf{k}) d\mathbf{k} = 0$ is true only for elastic collisions

  (momentum and Energy Conservation do not hold in general).

Previous Work on Numerical Methods for BP Models

Direct Simulation Monte Carlo (DSMC): Traditional in EE-CE
· Statistical noise, hard to resolve 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 transients and kinetic moments
Previously: Based on Parabolic and 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 Features: Boundary Conditions simpler to treat.
Numerical Method adequate for physics of electron transport.
Analytical treatment of Dirac delta related to Fermi's Golden Rule

Computational challenges of Boltzmann - Poisson:
High dimensional space. Cost of Collisional Integrals.

DG-FEM: Discontinuous Galerkin Finite Element Methods

Example: 1st Order Transport Equation in 1D with Constant Coeff.

$$u_t + u_x = 0 \tag{1}$$

DG FEM Semi-discrete Formulation of the Problem:
Let $V_h = span\{\phi_i(x)\}_{j=1}^{n}$ piecewise continuous polynomial space.
Find $u \in V_h$ s.t. $\forall v \in V_h$ (2) holds:

$$\int_I u_t v dx - \int_I u v_x dx + \hat{u} v^-|_{x_R} - \hat{u} v^+|_{x_L} = 0 \tag{2}$$

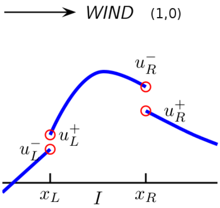
Functions are discontinuous across neighbor elements.

$v^-|_{x_R}$, $v^+|_{x_L}$: Values at boundary from the interior of the element.

How to choose the value of $\hat{u}$ on the boundary of the elements?

Discontinuous Galerkin (DG) Methods: Formulation

DG-FEM Semi-Discrete Formulation:



Find $u \in V_h$= piecewise polynomial space, s.t. for any $v \in V_h$,

$$\int_I u_t v\, dx - \int_I u v_x\, dx + \hat{u}v^-(x_R) - \hat{u}v^+(x_L) = 0.$$

Numerical Fluxes $\hat{u}$ **:** Represent Physics of Transport. I.E.:
Upwind Flux: $\hat{\mathbf{u}} = \mathbf{u}^-$ if Wind: $(1,0)$, $\hat{\mathbf{u}} = \mathbf{u}^+$ if Wind: $(-1,0)$.
ODE system. Example: $du_I/dt = L(u_I, u_{I-1})$, V_h : PW Constant.

DG: Why is it convenient for Boltzmann - Poisson ?

- Physics of Electron transport captured in Numerical Method (Fluxes)
- Basis Functions Discontinuous: Adequate for transport eq. Flexibility with Mesh (h) at different elements possible
- Polynomials of different degrees in different elements possible
- Non-polynomial basis possible in principle as well.
- Compact Scheme, Local Data Structure $\rightarrow$ Parallelizable Communication among Immediate Neighbors

BP model: e^- in Si Kane energy band

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

Kane Band Model: $\varepsilon(1 + \alpha\varepsilon) = \frac{\hbar^2|k|^2}{2m^*}$, $\quad w = \varepsilon/K_B T$

$\vec{k}$: 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:

$$g_1 = c_x \frac{\mu\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}, \quad \mathbf{g_2} = \mathbf{c_x} \frac{\sqrt{\mathbf{w}(\mathbf{1}+\alpha_{\mathbf{K}}\mathbf{w})}\sqrt{\mathbf{1}-\mu^{\mathbf{2}}}\cos\varphi}{\mathbf{1}+\mathbf{2}\alpha_{\mathbf{K}}\mathbf{w}}, \tag{3}$$

$$(g_3, g_4, g_5) = -c_k \left(\frac{2\sqrt{w(1+\alpha_K w)}\,\hat{e}_w}{1+2\alpha_K w}, \frac{\sqrt{1-\mu^2}\,\hat{e}_\mu}{\sqrt{w(1+\alpha_K w)}}, \frac{\hat{e}_\varphi/\sqrt{1-\mu^2}}{\sqrt{w(1+\alpha_K w)}} \right) \cdot \vec{E} \tag{4}$$

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

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

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.

$\Phi_h \in V_h$: 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.

Poisson Equation in 2D - Local Discontinuous Galerkin

Example: 2D Double Gated MOSFET
(Cheng, Gamba, Majorana, Shu, CMAME 2009).

The Poisson equation: rewriting it as

$$\begin{cases} q = \dfrac{\partial \Psi}{\partial x}, \qquad s = \dfrac{\partial \Psi}{\partial y} \\ \dfrac{\partial}{\partial x}(\epsilon_r q) + \dfrac{\partial}{\partial y}(\epsilon_r s) = R(t,x,y) = c_p\left[\rho(t,x,y) - \mathcal{N}_D(x,y)\right] \end{cases}$$

Grid $I_{ij} = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}\right]$, $i = 1, \dots, N_x$,
$j = 1, \dots, N_y + M_y$, $j = N_y + 1, \dots, N_y + M_y$ oxide-silicon region,
$j = 1, \dots, N_y$ consistent with grid for Boltzmann in silicon region.
Test function space $W_h^k = \{v : v|_{I_{ij}} \in P^k(I_{ij})\}$.

Poisson Equation - Local Discontinuous Galerkin: LDG

LDG - Poisson: Find $q_h, s_h, \Psi_h \in V_h^k$, s.t. for any $v_h, w_h, p_h \in W_h^k$:

$$\int_{I_{i,j}} q_h v_h dxdy + \int_{I_{i,j}} \Psi_h (v_h)_x dxdy - \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \hat{\Psi}_h v_h^-(x_{i+\frac{1}{2}}, y)dy + \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \hat{\Psi}_h v_h^+(x_{i-\frac{1}{2}}, y)dy = 0,$$

$$\int_{I_{i,j}} s_h w_h dxdy + \int_{I_{i,j}} \Psi_h (w_h)_y dxdy - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tilde{\Psi}_h w_h^-(x, y_{j+\frac{1}{2}})dx + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tilde{\Psi}_h w_h^+(x, y_{j-\frac{1}{2}})dx = 0,$$

$$- \int_{I_{i,j}} \epsilon_r q_h (p_h)_x dxdy + \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \widehat{\epsilon_r q}_h p_h^-(x_{i+\frac{1}{2}}, y)dy - \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \widehat{\epsilon_r q}_h p_h^+(x_{i-\frac{1}{2}}, y)dy$$

$$- \int_{I_{i,j}} \epsilon_r s_h (p_h)_y dxdy + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \widetilde{\epsilon_r s}_h p_h^-(x, y_{j+\frac{1}{2}})dx - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \widetilde{\epsilon_r s}_h p_h^+(x, y_{j-\frac{1}{2}})dx = \int_{I_{i,j}} R(t,x,y) p_h dxdy$$

Flux in x-direction: $\hat{\Psi}_h = \Psi_h^-$, $\widehat{\epsilon_r q}_h = \epsilon_r q_h^+ - [\Psi_h]$.
Flux in y-direction: $\tilde{\Psi}_h = \Psi_h^-$, $\widetilde{\epsilon_r s}_h = \epsilon_r s_h^+ - [\Psi_h]$.
Flux flip in x for Dirichlet BC: $\hat{\Psi}_h(x_{i+\frac{1}{2}}, y) = \Psi_h^+(x_{i+\frac{1}{2}}, y)$ and $\widehat{\epsilon_r q}_h(x_{i+\frac{1}{2}}, y) = \epsilon_r q_h^-(x_{i+\frac{1}{2}}, y) - [\Psi_h](x_{i+\frac{1}{2}}, y)$, if $(x_{i+\frac{1}{2}}, y)$ at drain.
Flip flux in y-direction for Neumann BC: $\tilde{\Psi}_h = \Psi_h^+$, $\widetilde{\epsilon_r s}_h = \epsilon_r s_h^-$.

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

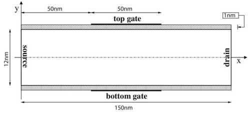


Fig. 4.14. Schematic representation of a 2D double gate MOSFET device.

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 Boundary Points

$0 = \eta(\vec{x}) \cdot \int_{\Omega_{\vec{k}}} v(\vec{k}) f d\vec{k} = \int_{v\cdot\eta>0} v \cdot \eta f|_+ d\vec{k} + \int_{v\cdot\eta<0} v \cdot \eta F_R(f|_+) d\vec{k}$

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:

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

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

Mixed Reflection:

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

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

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

Kinetic Theory of Gases:
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A. Jungel, Transport Eq. for Semiconductors, Springer (2009)

Reflective BC on BP & Zero Flux Condition

Formulation of Reflective BC:

$$f(\vec{x},\vec{k},t)|_{\Gamma_{N^-}} = F(f|_{\Gamma_{N^+}}) \tag{5}$$

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

$$\begin{aligned} 0 &= \eta(\vec{x})\cdot J(\vec{x},t) = \eta(\vec{x})\cdot\int_{\Omega_{\vec{k}}} \vec{v}(\vec{k})\, f(\vec{x},\vec{k},t)\, d\vec{k} \qquad (6) \\ &= \int_{\eta\cdot\vec{v}>0} \eta(\vec{x})\cdot\vec{v}(\vec{k})\, f|_{\Gamma_{N^+}}\, d\vec{k} + \int_{\eta\cdot\vec{v}<0} \eta(\vec{x})\cdot\vec{v}(\vec{k})\, f|_{\Gamma_{N^-}}\, d\vec{k} \\ 0 &= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}\, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, F(f|_{\Gamma_{N^+}})\, d\vec{k} \end{aligned}$$

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

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

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

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

Mixed Reflection BC - constant p & Zero Flux Condition

$$f(\vec{x},\vec{k},t)|_{\Gamma_N^-} = pf(\vec{x},\vec{k}',t) \,+\, (1-p)Ce^{-\frac{\varepsilon(\vec{k})}{K_B T}} \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}} d\vec{k}\,,$$

Zero flux with previous C, specular & diffusive convex combination:

$$\eta\cdot J = \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, \left[pf(\vec{x},\vec{k}',t)|_+ + (1-p)Ce^{-\frac{\varepsilon(\vec{k})}{K_B T_L}}\sigma(\vec{x},t)\right] \, d\vec{k}$$

$$+ \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+ \, d\vec{k} \,=\, \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+ \, d\vec{k} \,+$$

$$+\, p\int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, f(\vec{x},\vec{k}',t)|_+ \, d\vec{k} + (1-p)\sigma C \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}} \, d\vec{k} =$$

$$\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+ \, d\vec{k} \,+\, p\int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, f(\vec{x},\vec{k}',t)|_+ \, d\vec{k} \,-(1-p)\sigma(\vec{x},t)$$

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

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

For $p(\vec{k})$ the previous $C(\eta)$ does not necessarily satisfy zero flux. Proper C for $p(\vec{k})$ case should be derived from zero flux condition:

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

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

For mixed reflection with $p(\vec{k})$, it can be derived that:

$$C\{\eta, f\}(\vec{x}, t) = \frac{\int_{\vec{v}\cdot\eta>0}(1 - p(\vec{k}'))|\vec{v}\cdot\eta|\, f|_{\Gamma_{N^+}}\, d\vec{k}}{\int_{\vec{v}\cdot\eta>0} |\vec{v}\cdot\eta|\, f|_{\Gamma_{N^+}}\, d\vec{k} \int_{\vec{v}\cdot\eta<0}(1 - p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}}$$

C above depends on $f|_{\Gamma_{N^+}}$ cumbersomely. However, note that:

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

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

We can define the following integrals:

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

$$C'(\eta(\vec{x})) = \left(\int_{\vec{v}\cdot\eta<0} (1 - p(\vec{k})) |\vec{v} \cdot \eta| \, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}} \, d\vec{k} \right)^{-1}$$

C' does not depend on $f(\vec{x}, \vec{k}, t)$. Since $C \cdot \sigma(\vec{x}, t) = C' \cdot \sigma'(\vec{x}, t)$, the mixed reflection BC for the general case $p(\vec{k})$ can be expressed in terms of σ', C' , satisfying the zero flux condition, as:

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

C' and σ' more convenient for computational implementation.

Numerical Scheme: RK-DG-BP Algorithm

Dynamic Extension of Gummel Iteration Map

Starting with an Initial Condition Φ_0 , and given the B.C., the DG-BP algorithm advances from t^n to t^{n+1} in these steps:

1. Compute charge density ρ
2. Use this ρ to solve Poisson Eq. (LDG) for the potential and electric field, and compute then transport g_i's.
3. Solve the transport part of Boltzmann Equation by DG, then obtaining a method of lines for Φ_h (ODE system).
4. Evolve ODE system in time by Runge - Kutta method from t^n to t^{n+1} (If partial time step necessary, repeat Steps 1 to 3 as needed).

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:

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

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

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

Mixed Reflection BC:

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

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

Diffusive Reflection BC in DG-BP Numerics

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

$\Phi_h \in V_h \to \sigma_h(x,y,t) = \int_{\pm \cos\varphi \geq 0} |g_2|\, \hat{\Phi}_h|_+ \, dw d\mu d\varphi = \sigma_I^0(t) + \sigma_I^x(t) \frac{2(x-x_i)}{\Delta x_i} + \sigma_I^y(t) \frac{2(y-y_j)}{\Delta y_j} \in V_h^1$

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

Ex: Boundary $y_{N_y+1/2} = L_y$: $\eta \cdot \vec{g} = +\hat{y} \cdot \vec{g} = +g_2 \propto +\cos\varphi$. **Outflow:** $j = N_y$. **Inflow:** $j = N_y + 1$.

$$\sigma_h = \int_{\cos\varphi \geq 0} \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} \sqrt{1-\mu^2} \cos\varphi\, \hat{\Phi}_h|^+_{I(j=N_y)}\, dw d\mu d\varphi$$

$$\sigma_I^0 = \sum_{k,m,n \leq N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi\, T_I(t)$$

$$\sigma_I^x = \sum_{k,m,n \leq N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi X_I(t)$$

$$\sigma_I^y = \sum_{k,m,n \leq N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi Y_I(t).$$

$\hat{\Phi}_h|^-_{I(j=N_y+1)}(x, y_{N_y+1/2}, w) = \Pi_h\{C\,\sigma_h(x,y,t)\, e^{-w} s(w)\}|_{y_{N_y+1/2}} \in V_h,$ with coefficients:

$$T_{I(j=N_y+1)} = C\sigma_I^0 \frac{\int_k e^{-w} s(w) dw}{\int_k dw},\ X_{I(j=N_y+1)} = C\sigma_I^x \frac{\int_k e^{-w} s(w) dw}{\int_k dw},\ Y_{I(j=N_y+1)} = (-1)C\sigma_I^y \frac{\int_k e^{-w} s(w) dw}{\int_k dw},$$

$$C^{-1} = \int_{\cos\varphi \leq 0} \Pi_h \left\{ s(w) e^{-w} \right\} |g_2|\, dw d\mu d\varphi =$$

$$C^{-1} = \sum_{k,m,n \geq N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} \Pi_h \left\{ s(w) e^{-w} \right\} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi$$

Mixed Reflection BC with constant p: DG-BP Numerics

$$\hat{\Phi}_h^{mixed}|_{\Gamma_{N^-}} = p\,\hat{\Phi}_h^{spec}|_{\Gamma_{N^-}} + (1-p)\hat{\Phi}_h^{diff}|_{\Gamma_{N^-}}$$

p **constant:**

$$I = (i,j,k,m,n),\ j = 0\,,\ N_y + 1$$

$$T_I^{mixed} = p\,T_I^{spec} + (1-p)\,T_I^{diff}$$
$$X_I^{mixed} = p\,X_I^{spec} + (1-p)X_I^{diff}$$
$$Y_I^{mixed} = p\,Y_I^{spec} + (1-p)\,Y_I^{diff}$$

Convex combination of previous specular and diffusive coefficients.

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 $\hat{\Phi}_h|_-$:

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

Code Implementation: Work in Progress.

Numerical BC: General Mixed Reflection and Zero Flux

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

$$\vec{w} = (w,\mu,\varphi), \quad d\vec{w} = dw\, d\mu\, d\varphi\,, \quad \vec{w}' = (w,\mu,\pi-\varphi). \tag{8}$$

$$\begin{aligned} 0 &= \eta(\vec{x}) \cdot \int_{\Omega_{\vec{w}}} \vec{w}\, \hat{\Phi}_h d\vec{w} = \int_{\vec{w}\cdot\eta>0} \vec{w}\cdot\eta\, \hat{\Phi}_h|_+ d\vec{w} + \int_{\vec{w}\cdot\eta<0} \vec{w}\cdot\eta\, \hat{\Phi}_h|_- d\vec{w} \\ &= \int_{\vec{w}\cdot\eta>0} \vec{w}\cdot\eta\, \hat{\Phi}_h|_+ d\vec{w} + \int_{\vec{w}\cdot\eta<0} \vec{w}\cdot\eta\, \Pi_h \left\{ p(\vec{w})\hat{\Phi}_h|_+(\vec{x},\vec{w}',t) + (1-p(\vec{w}))C'\sigma_h'(\vec{x},t)e^{-w}s(w) \right\} d\vec{w} \\ &= \int_{\vec{w}\cdot\eta>0} \vec{w}\cdot\eta\, \hat{\Phi}_h|_+ d\vec{w} - \int_{\vec{w}\cdot\eta<0} |\vec{w}\cdot\eta|\, \Pi_h \left\{ p(\vec{w})\hat{\Phi}_h|_+(\vec{x},\vec{w}',t) \right\} d\vec{w} \\ &- \sigma_h' C' \sum_{k,m,n}^{\vec{w}\cdot\eta<0} \int_{K_{kmn}} |\vec{w}\cdot\eta|\, d\vec{w}\, \frac{\int_{K_{kmn}} (1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\Delta w_k}\,, \end{aligned}$$

in V_h space of PW-linear in $\vec{x}$ and PW-constant in $\vec{w}$.

Numerical equivalent of Zero Flux condition with:

$$\sigma_h'(\vec{x},t) = \int_{\vec{w}\cdot\eta>0} \vec{w}\cdot\eta\, \hat{\Phi}_h|_+ d\vec{w} - \int_{\vec{w}\cdot\eta<0} |\vec{w}\cdot\eta|\, \Pi_h \left\{ p(\vec{w})\hat{\Phi}_h|_+(\vec{x},\vec{w}',t) \right\} d\vec{w} = \sigma_h' \left\{ \hat{\Phi}_h|_+ \right\} \tag{9}$$

$$\left(C' \{\eta\} \right)^{-1} = \sum_{k,m,n,\ \vec{w}\cdot\eta<0} \frac{\int_{K_{kmn}} |\vec{w}\cdot\eta|\, d\vec{w}\ \int_{K_{kmn}} (1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\Delta w_k} \tag{10}$$

General Mixed Reflection BC in DG-BP Numerics

Ex: Boundary $y_{N_y+1/2} = L_y \, : \, \eta \cdot \vec{g} = +\hat{y} \cdot \vec{g} = +g_2 \propto + \cos\varphi$. **Outflow:** $j = N_y$. **Inflow:** $j = N_y + 1$.

$\sigma_h = \int_{\cos\varphi>0} g_2 \, \hat{\Phi}_h|_+ d\vec{w} \; - \int_{\vec{w}\cdot\eta<0} |g_2| \, \Pi_h \left\{ p(\vec{w})\hat{\Phi}_h|_+(\vec{x},\vec{w}',t) \right\} d\vec{w}$. $I' = (iN_y kmn'), \; n' = N'_\varphi - n + 1$

$$\sigma_I^0 = \sum_{k,m,n\le N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi \; T_I(t)$$
$$- \sum_{k,m,n\ge N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi \frac{\int_{kmn} \Pi_h p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \; T_{I'}(t)$$
$$\sigma_I^x = \sum_{k,m,n\le N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi X_I(t)$$
$$- \sum_{k,m,n\ge N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi \frac{\int_{kmn} \Pi_h p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \; X_{I'}(t)$$
$$\sigma_I^y = \sum_{k,m,n\le N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi Y_I(t).$$
$$- \sum_{k,m,n\ge N_p/2} \int \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int \sqrt{1-\mu^2} d\mu \int \cos\varphi d\varphi \frac{\int_{kmn} \Pi_h p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \; Y_{I'}(t)$$

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

$$T_{I(j=N_y+1)} = T_{I'} \frac{\int_{kmn} \Pi_h\{p(\vec{w})\} d\vec{w}}{\int_{kmn} d\vec{w}} + C'\sigma'^0_I \frac{\int_{kmn} \Pi_h \left\{ (1-p(\vec{w}))e^{-w} s(w) \right\} d\vec{w}}{\int_{kmn} d\vec{w}},$$
$$X_{I(j=N_y+1)} = X_{I'} \frac{\int_{kmn} \Pi_h\{p(\vec{w})\} d\vec{w}}{\int_{kmn} d\vec{w}} + C'\sigma'^x_I \frac{\int_{kmn} \Pi_h \left\{ (1-p(\vec{w}))e^{-w} s(w) \right\} d\vec{w}}{\int_{kmn} d\vec{w}},$$
$$Y_{I(j=N_y+1)} = -\left(Y_{I'} \frac{\int_{kmn} \Pi_h\{p(\vec{w})\} d\vec{w}}{\int_{kmn} d\vec{w}} + C'\sigma'^y_I \frac{\int_{kmn} \Pi_h \left\{ (1-p(\vec{w}))e^{-w} s(w) \right\} d\vec{w}}{\int_{kmn} d\vec{w}} \right), \; I' = (i, N_y, k, m, n').$$

Preliminary Numerical Results

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

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

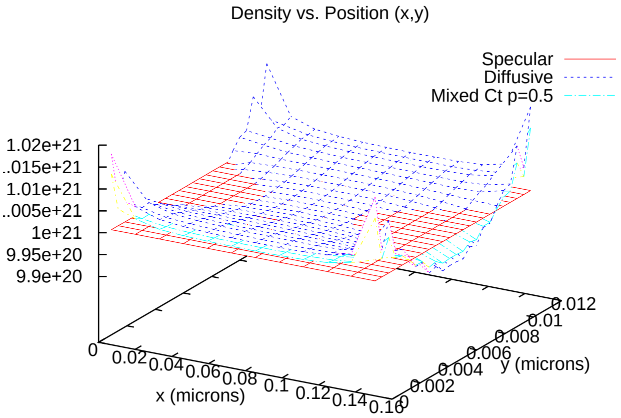
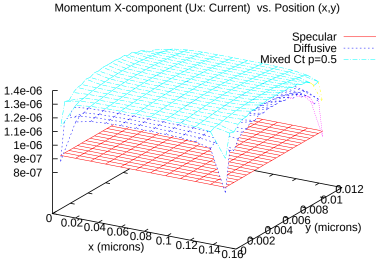


Figure : Density ρ (m^{-3}) vs Position (x, y) in (μm) plot for Specular, Diffusive, & Mixed $p = 0.5$ Reflection.

Momentum Components



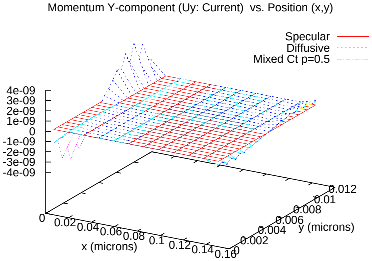


Figure : Momentum $(Ux, Uy)\,(10^{28}\,\frac{cm^{-2}}{s})$ vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed $p = 0.5$ Reflection.

Average Velocity Components

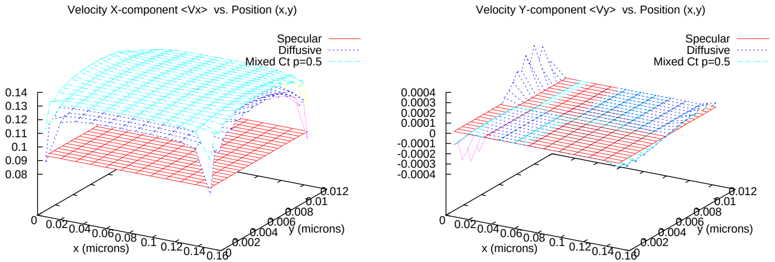


Figure : Mean Velocity (Vx, Vy) vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed $p = 0.5$ Reflection.

Average Energy

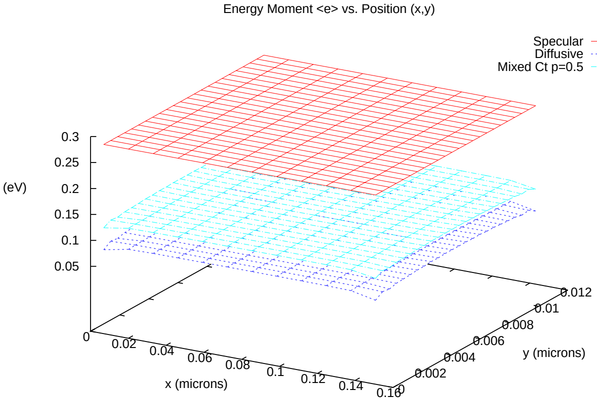


Figure : Mean energy $e(eV)$ vs. Position (x, y) in (μm) plots for Specular, Diffusive, & Mixed $p = 0.5$ Reflection.

Electric Potential

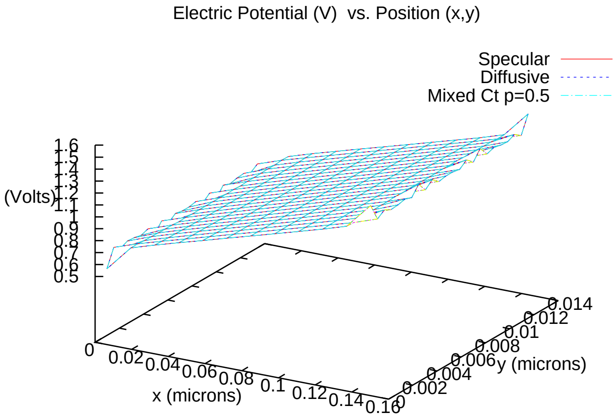


Figure : Potential $V(Volts)$ vs. Position (x, y) (μm) plot for Specular, Diffusive & Mixed $p = 0.5$ Reflection

Electric Field

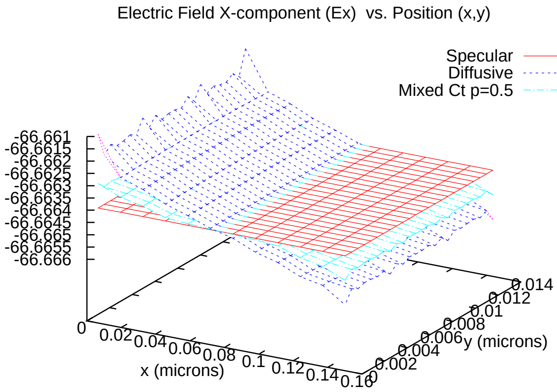


Figure : Electric Field Component Ex vs. Position (x, y) in (μm) for Specular, Diffusive & Mixed $p = 0.5$ Reflection

Conclusions, Work in Progress & Future Research

Conclusions:

Influence of Diffusive and Mixed Reflection in Macroscopic Observables, as noticed in the Kinetic Moments.

- Distribution of Charges slightly increases with Diffusive Reflection close to reflecting boundaries (and alters density profile over domain due to mass conservation).
- Momentum & Velocity increase with Diffusive Reflex. over domain
- Energy is decreased by Diffusive Reflection over domain

Work in Progress:

Mixed Reflection $p(\vec{w})$: Computational Implementation in Progress.
Reflective BC in 2D double gate MOSFET device.

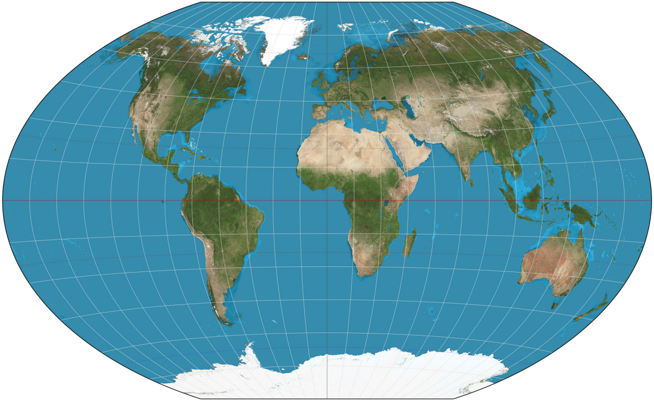
Future Research:

Reflective BC with EPM-DG-BP Full Band Model

Inclusion of additional scattering mechanisms

The End

Thanks!



KI-Net YRW, CSCAMM, U. Maryland - College Park, MD 2015.