A Self-Consistent Event Biasing Scheme for Statistical Enhancement

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- Motivation: faster convergence of the stochastic process;
  - Useful when rare events govern the transport process;
  - Population control versus Event biasing;
  - Splitting particles entering Ω versus Guiding particles towards Ω by biasing the classical transport probabilities;
- History: When proposed? Who is the Godfather of event biasing?
- Event Biasing: from frozen field to self-consistent algorithms;
- Simulation Results;

History: Statistical enhancement

Particle splitting: Single Particle MC

- A. Phillips, P. Price,"MC calculus of hot electron tails",*Appl. Phys. Lett.*, 1977.

Event biasing in EMC: evolution problems, initial condition

- C. JACOBONI"Generalization of the Monte Carlo method for charge transport to BIASED simulations",*NASECODE VI*, Dublin, 1989.
- L. Rota, C. Jacoboni, and P. Poli, "Weighted EMC" *Solid-St. Electron.*, 12, 1989.
- M. Nedjalkov, P. Vitanov,"Iteration Approach.." *Solid St. Electron*, 10, 1989.
- F. Rossi, P. Poli, C. Jacoboni, "The Weighted..' *Semicon. Sci. Technol.*, 7, 1992.

Single Particle MC: $(\mathbf{k}, \mathbf{r})$ - stationary problem, boundary condition

- H. Kosina, M. Nedjalkov, S. Selberherr, "Variance Reduction...event biasing", *Proc. MSM 2001*
- H. Kosina, M. Nedjalkov, S. Selberherr, "The Stationary MC..- Part I and II", *J. Appl. Phys.*, 93, 2003

Event Biasing: Concepts of MC integration

Random variable ψ: takes values $\psi(Q)$ with probability $p_\psi(Q)$.

$$E_\psi = \int dQ p_\psi(Q)\psi(Q) \text{ – expectation value}$$

N realizations of $p_\psi \rightarrow Q_1, \ldots, Q_N$ sampling points

$$E_\psi \simeq \frac{1}{N}\sum_{i=1}^{N}\psi(Q_i) \text{ – sample mean; Precision}(N,\sigma_\psi)$$

Evaluation of integrals:

$$I = \int f(Q)dy = \int p(Q)\frac{f(Q)}{p(Q)}, \qquad (\psi = f/p = \psi(p))$$

Different $\psi(p)$ - all have expectation value $E_\psi = I$, but different σ_ψ

Event Biasing: Evaluation of integral equations

$$f(Q) = \int dQ' f(Q') K(Q', Q) + f_0(Q) \qquad (1)$$

If the task is not f but $\langle A \rangle = \int dQ A(Q) f(Q)$

Consider the adjoint to (1) equation:

$$g(Q') = \int dQ K(Q', Q) g(Q) + A(Q') \qquad (2)$$

(1) is multiplied by g, (2) multiplied by f, integrated, compared:

$$\langle A \rangle = \int dQ A(Q) f(Q) = \int dQ f_0(Q') g(Q')$$

$$\text{Iterative expansion:} \quad g(Q') = A(Q') + \sum_{n=1}^{\infty} \int dQ K^n(Q',Q)A(Q)$$

Replace in $\langle A \rangle = \int dQ f_0(Q')g(Q')$ - series: $\langle A \rangle = \sum_i \langle A \rangle_i$;

$$\langle A \rangle_2 = \int dQ' dQ_1 dQ_2 P_0(Q')P(Q',Q_1)P(Q_1,Q_2) \frac{f_0(Q')}{P_0(Q')} \frac{K(Q',Q_1)}{P(Q',Q_1)} \frac{K(Q_1,Q_2)}{P(Q_1,Q_2)} A(Q_2)$$

Numerical trajectory: points $Q_0 \to Q_1 \to Q_2$, selected by $P_0 \to P \to P$.

The random variable $\psi^{(2)}$ - product of weight $W = \frac{f_0}{P_0}\frac{K}{P}\frac{K}{P}$ and A

$$N \text{ trajectories } (Q' \to Q_1 \to Q_2)_i \quad \to \quad \langle A \rangle_2 \simeq \frac{1}{N}\sum_i \psi_i^{(2)}$$

One ∞ trajectory samples all terms $\langle A \rangle = \sum_i \langle A \rangle_i$;

$$(Q' \to Q_1 \to Q_2 \to \ldots)_i \quad \to \quad \langle A \rangle \simeq \frac{1}{N}\sum_i \psi_i$$

Event Biasing: Problem, initial and boundary conditions

Task: evaluate mean value of physical quantity a in domain Ω at time τ

$A(Q) = a\theta_\Omega(\mathbf{k},\mathbf{r})\delta(t-\tau)$, θ_Ω - domain indicator, $\quad Q = (\mathbf{k},\mathbf{r},t)$

$$\text{adjoint BE } \rightarrow K(Q',Q) = S(\mathbf{k}',\mathbf{k},\mathbf{r})e^{-\int_{t'}^{t}\lambda(\mathbf{K}(y),\mathbf{R}(y))dy}\theta_D(\mathbf{r})\delta(\mathbf{r}'-\mathbf{r})\theta(t-t')$$

$\mathbf{K}(t),\mathbf{R}(t)$ - classical trajectory, independent on f,g - frozen field

$e^{-\int}$ and S if normalized give the natural probabilities for drift and scattering!

$$f_0(Q) = f_i(\mathbf{k},\mathbf{r})e^{-\int_0^t\lambda(\mathbf{K}(y),\mathbf{R}(y))dy} + \int_0^t \mathbf{v}_\perp(\mathbf{k})f_b(\mathbf{k},\mathbf{r},t_b)e^{-\int_{t_b}^{t}\lambda(\mathbf{K}(y),\mathbf{R}(y))dy}dt_b$$

f_i, f_b - initial and boundary conditions; $\mathbf{v}_\perp(\mathbf{k})$ - inward normal velocity at boundary

Event Biasing: EMC and WEMC

EMC is obtained by a particular choice of P_0 and P:

•Construct P_0^B from f_i, f_b •Construct P^B from K: $P = \lambda e^{-\int \lambda dy} \cdot \frac{S}{\lambda}$

Then $W = 1$ and $\langle A \rangle = \sum_{n=1}^{N_\tau} \theta_\Omega(n) a_n$

N_τ number of trajectories which at τ belong to D;
$\theta_\Omega(n) = 1$ if the endpoint of the n-th trajectory is inside Ω and 0 otherwise;
a_n is the value of a for the n-th particle;

WEMC- all other choices of P_0 and P:

Then $\langle A \rangle = \sum_{n=1}^{N_\tau} W_n \theta_\Omega(n_{um}) a_n$

$\theta_\Omega(n_{um}) = 1$ if the n-th numerical particle is inside Ω and 0 otherwise;
Biased can be the initial f_i, boundary f_b distributions,
free flight duration $\lambda exp\{-\int \lambda dy\}$,
type of scattering and the selection of the after-scattering state direction S/λ.

Event biasing: self-consistent scheme

Interacting carriers - Nonlinear problem. The frozen field approach fails. Solution - in the coupling scheme with the Poisson equation:

$$f_0 \overset{\text{EMC}}{\underset{\Delta t}{\longrightarrow}} \overset{\text{PE}}{f_{\Delta t}} \overset{\text{EMC}}{\underset{2\Delta t}{\longrightarrow}} \overset{\text{PE}}{f_{2\Delta t}} \cdots \overset{\text{EMC}}{\underset{\tau}{\longrightarrow}} \overset{\text{PE}}{f_\tau}$$

To proof the scheme (the idea : PE must not know about the secret life of the MC)

$$f_0^{\mathrm{b}} \overset{\text{WEMC}}{\underset{\Delta t}{\longrightarrow}} f_{\Delta_t}^{\mathrm{b}} \rightarrow \overset{\text{PE}}{f_{\Delta t}} \rightarrow f_{\Delta_t}^{\mathrm{b}} \overset{\text{WEMC}}{\underset{2\Delta t}{\longrightarrow}} f_{2\Delta_t}^{\mathrm{b}} \rightarrow \overset{\text{PE}}{f_{2\Delta t}} \rightarrow f_{2\Delta_t}^{\mathrm{b}} \cdots$$

we must proof $f_\tau^{\mathrm{b}} \rightarrow f_\tau \rightarrow f_\tau^{\mathrm{b}}$

Main result: Particles weights survive the successive steps of solving the PE.

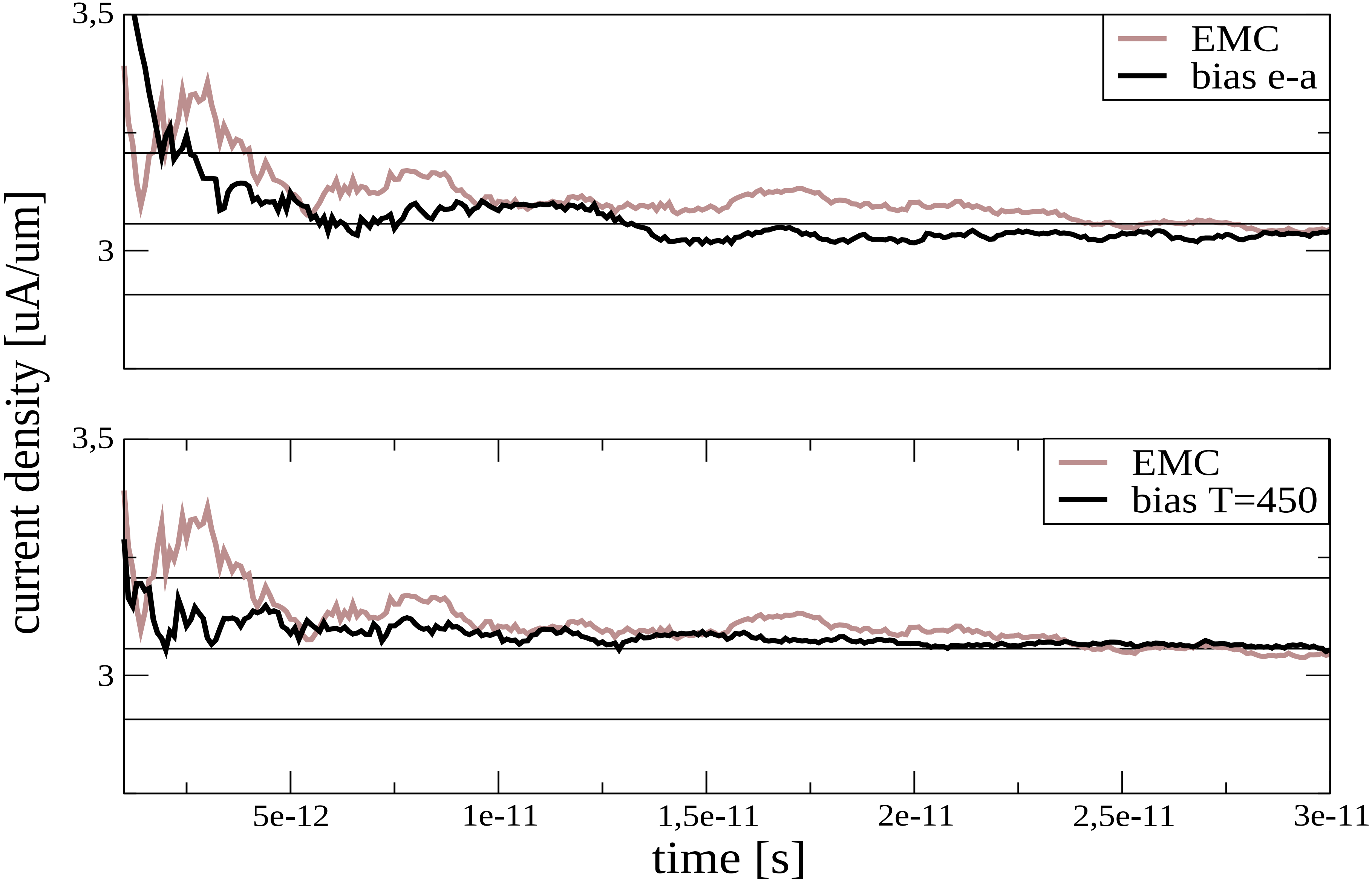
Simulation results

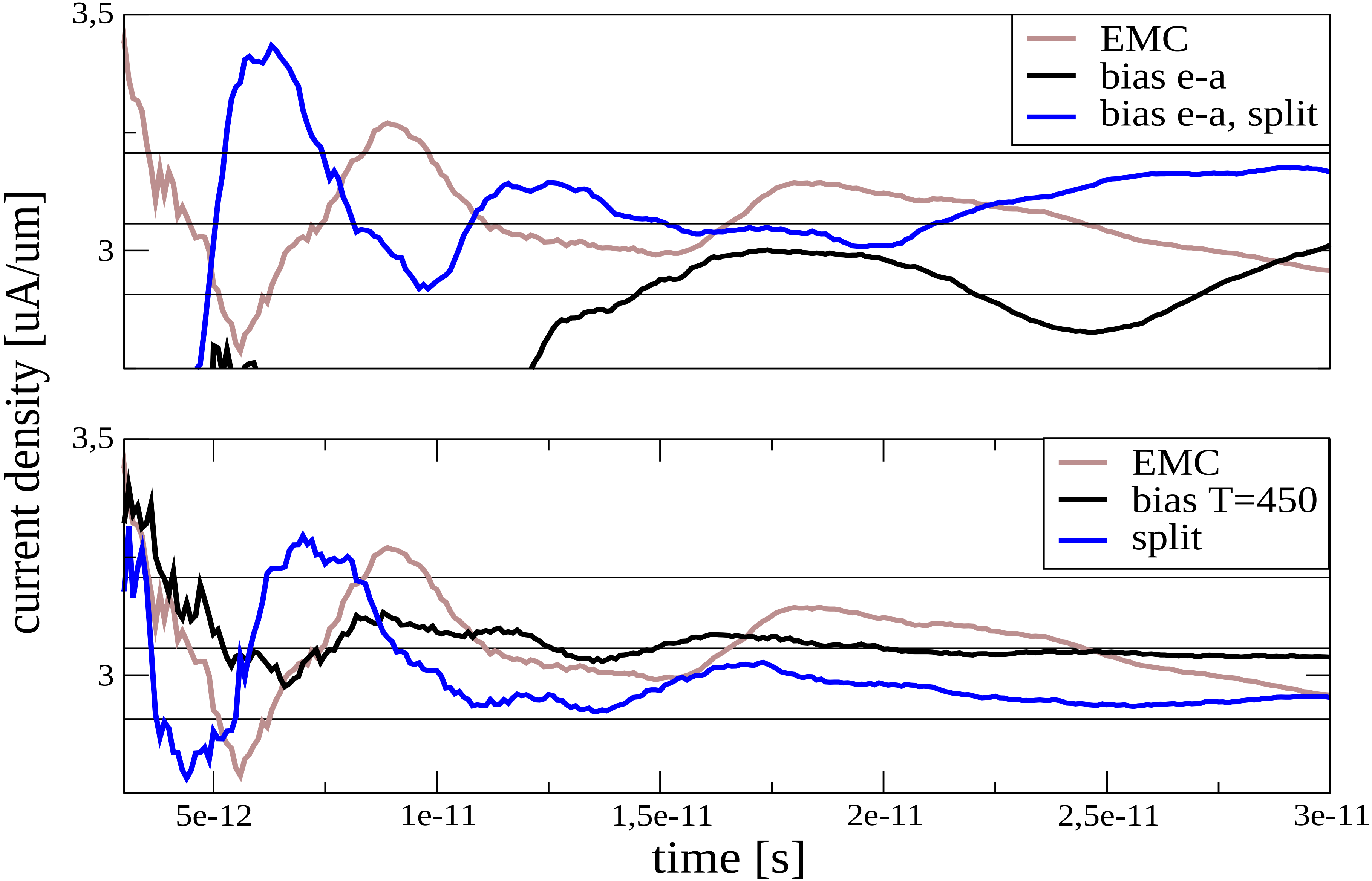
2D MC, MOSFET:
gate length $15nm$, channel doping $2.10^{19}cm^{-3}$, and oxide thickness $0.8nm$.
Subthreshold regime $V_G = 0.375V$, $V_D = 0.1V$, lattice temperature $T = 300K$.

Consistency of the biasing techniques in the thermodynamic limit:
for large N EMC and WEMC give the same distribution of the physical averages.

For smaller N we seek for bias processes with smaller variance.

Investigated is the convergence of the cumulative averages for the channel and terminal currents obtained from the velocity and particle counting respectively.


3,5
3
3,5
3
EMC
bias e-a
EMC
bias T=450
current density [uA/um]
5e-12
1e-11
1,5e-11
2e-11
2,5e-11
3e-11
time [s]



current density [uA/um]
3,5
3
EMC
bias e-a
bias e-a, split
3,5
3
EMC
bias T=450
split
5e-12
1e-11
1,5e-11
2e-11
2,5e-11
3e-11
time [s]

Conclusions

- Event biasing has been derived in presence of both, initial and boundary conditions and generalized for self-consistent simulations.

- A bias technique, particularly useful for small devices, is obtained by injection of hot carriers from the boundaries.

- The coupling with PE requires a precise statistics in the S/D regions.

- Event biasing in combination with population control is necessary

f_0^b - from f_0/P_0 - biasing of the initial/boundary distribution.

Decompose the phase space into cells $\Omega_{l,m} = \Psi_l \Phi_m$, $(\mathbf{r}_l, \mathbf{k}_m) \in \Omega_{l,m}$:
$f_\tau^{\mathrm{b}} \rightarrow f_\tau$: directly from $\langle A \rangle$ with $a = 1$:

$$f_{l,m} \simeq \frac{\sum_n \theta_{\Omega_{l,m}(n)}}{V_{\Omega_l} V_{\Phi_m}} = \frac{\sum_n W_n \theta_{\Omega_{l,m}(n_{um})}}{V_{\Omega_l} V_{\Phi_m}}$$

Introduce distribution function of the numerical particles:

$$f_{l,m}^{\mathrm{num}} \simeq \frac{\sum_n \theta_{\Omega_{l,m}(n_{um})}}{V_{\Omega_l} V_{\Phi_m}} \rightarrow \qquad f_{l,m} = W_{l,m} f_{l,m}^{\mathrm{num}} \quad \mathrm{if} \quad V_{\Omega_l}, V_{\Phi_m} \rightarrow 0$$

Hence $W_{l,m} = f_{l,m}/f_{l,m}^{\mathrm{num}}$ and $f_\tau \rightarrow f_\tau^{\mathrm{b}}$ follows with $f_\tau^{\mathrm{b}} = f^{\mathrm{num}}$.