Analysis of numerical schemes for semiconductors energy-transport models

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Semiconductor models

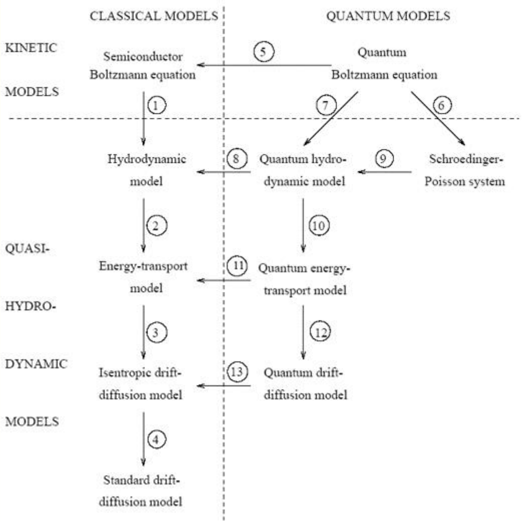


Figure: A. Jüngel, *Quasi-hydrodynamic semiconductor equations*, 2001.

Unipolar energy transport model

$$\partial_t \rho_1 + \mathsf{div} J_1 = 0,$$
$$\partial_t \rho_2 + \mathsf{div} J_2 = \nabla V \cdot J_1 + W,$$
$$-\lambda^2 \Delta V = C(x) - \rho_1,$$

$+$ initial condition and mixed Dirichlet-Neumann boundary conditions.

- ρ_1 electron density, ρ_2 internal energy density,
- V electrostatic potential,
- J_1 electron current density, J_2 energy current density,
- W energy relaxation term,
- $C(x)$ given doping profile,
- λ rescaled Debye length.

Unipolar energy transport model

$$\partial_t \rho_1 + \mathsf{div} J_1 = 0$$
$$\partial_t \rho_2 + \mathsf{div} J_2 = \nabla V \cdot J_1 + W$$
$$-\lambda^2 \Delta V = C(x) - \rho_1$$

Kreuzer, *Nonequilibrium thermodynamics and its statistical foundations*, 1981.
$J_i = J_i(X_1, X_2)$ where thermodynamics forces are

$$X_1 = \nabla \left(\frac{\mu}{T}\right) + \frac{\nabla V}{T}, \quad X_2 = -\frac{\nabla V}{T},$$

with μ the chemical potential and T the temperature.

Near thermal equilibrium ($J_i = 0$),

$$J_i = -L_{i1} X_1 - L_{i2} X_2, \quad i = 1,\, 2.$$

- Onsager's principle $\Rightarrow \mathbb{L} = (L_{ij})_{1 \le i,j \le 2}$ is symmetric.
- Second law of thermodynamics $\Rightarrow \mathbb{L}$ is positive definite.

Unipolar energy transport model

ρ_1, ρ_2 and $\mathbb{L}$ depend on $\mathbf{u} = (u_1, u_2) := (\mu/T, -1/T)$.

Boltzmann statistics and parabolic band approximation:

$$\rho_1(\mathbf{u}) = (-1/u_2)^{3/2} e^{u_1}, \quad \rho_2(\mathbf{u}) = 3/2(-1/u_2)^{5/2} e^{u_1},$$

$$\mathbb{L}(\mathbf{u}) = c_0\, \rho_1(\mathbf{u})\, T^{1/2-\beta} \begin{pmatrix} 1 & (2-\beta)T \\ (2-\beta)T & (3-\beta)(2-\beta)T^2 \end{pmatrix}.$$

Chen model: $c_0 = 1$, $\beta = 1/2$.
Lyumkis model: $c_0 = 2/\sqrt{\pi}$, $\beta = 0$.

Mathematical framework

P. Degond, S. Génieys, A. Jüngel, *J. Math. Pures Appl.*, 1997.

$$\partial_t \rho_1(\mathbf{u}) + \mathrm{div} J_1 = 0,$$
$$\partial_t \rho_2(\mathbf{u}) + \mathrm{div} J_2 = \nabla V \cdot J_1 + W(\mathbf{u}),$$
$$-\lambda^2 \Delta V = C(x) - \rho_1(\mathbf{u}),$$

where

$$J_i = -L_{i1}(\mathbf{u})(\nabla u_1 + u_2 \nabla V) - L_{i2}(\mathbf{u}) \nabla u_2, \quad i = 1,\, 2.$$

Assumptions

- $\mathbb{L}(\mathbf{u}) = (L_{ij}(\mathbf{u}))_{1 \le i,j \le 2}$ is a symmetric uniformly positive definite matrix,
- $W(\mathbf{u})(u_2 - u_2^D) \le 0$,
- $\rho = (\rho_1, \rho_2) \in W^{1,\infty}(\mathbb{R}^2)$ satisfies

$$(\rho(\mathbf{u}) - \rho(\mathbf{v})) \cdot (\mathbf{u} - \mathbf{v}) \ge C_0 |\mathbf{u} - \mathbf{v}|^2, \quad \forall \mathbf{u},\, \mathbf{v} \in \mathbb{R}^2,$$

  and there exists $\chi \in \mathcal{C}^1(\mathbb{R}^2; \mathbb{R})$ convex such that $\rho(\mathbf{u}) = \nabla_{\mathbf{u}} \chi(\mathbf{u})$,
- $u_2^D < 0$ is constant on Γ^D.

Some references

Under previous assumptions

- Degond, Génieys, Jüngel (1997), Jüngel (2000): existence, uniqueness and regularity of solutions to the transient system, long time behavior.
  - Entropy method

Under more physical assumptions, for data close to equilibrium

- Griepentrog (1999), Fang, Ito (2001): existence for the stationary model.
- Chen, Hsiao (2003), Chen, Hsiao, Li (2005): existence for the transient model.

Under more physical assumptions, for simplified cases

- Jüngel, Pinnau, Röhrig (2013): existence for a model with a simplified temperature equation.
- Zamponi, Jüngel (2015): existence for a model with vanishing electric fields.

About discretizations

Stationary model

- Fournié (2002), Romano (2007): finite difference schemes.
- Degond, Jüngel, Pietra (2000), Gadau, Jüngel (2008): finite element schemes.
- Holst, Jüngel, Pietra (2003, 2004): mixed finite element schemes.

Transient model

- Chainais-Hillairet (2009): DDFV scheme.

No convergence analysis

Aim: Design and **analyse** finite volume schemes for the ET model.

$\rightarrow$ Adapt the entropy method to the discrete setting.

System in dual entropy variables

$$\partial_t \rho_1(\mathbf{u}) + \mathsf{div} J_1 = 0,$$
$$\partial_t \rho_2(\mathbf{u}) + \mathsf{div} J_2 = \nabla V \cdot J_1 + W(\mathbf{u}),$$
$$-\lambda^2 \Delta V = C(x) - \rho_1(\mathbf{u}),$$

where

$$J_i = -L_{i1}(\mathbf{u})(\nabla u_1 + u_2 \nabla V) - L_{i2}(\mathbf{u}) \nabla u_2.$$

Dual entropy variables $\mathbf{w} = (w_1, w_2)$:

$$w_1 = u_1 + u_2 V, \quad w_2 = u_2.$$

$$\partial_t b_1(\mathbf{w}, V) + \mathsf{div} I_1 = 0,$$
$$\partial_t b_2(\mathbf{w}, V) + \mathsf{div} I_2 = \widetilde{W}(\mathbf{w}) - \partial_t V b_1(\mathbf{w}, V),$$
$$-\lambda^2 \Delta V = C - b_1(\mathbf{w}, V),$$

with

$$b_1(\mathbf{w}, V) = \rho_1(\mathbf{u}), \quad b_2(\mathbf{w}, V) = \rho_2(\mathbf{u}) - V \rho_1(\mathbf{u}),$$

and **symmetrized** currents: $I_1 = J_1$, $I_2 = J_2 - V J_1$.

System in dual entropy variables

$$\partial_t b_1(\mathbf{w}, V) + \mathrm{div} I_1 = 0,$$
$$\partial_t b_2(\mathbf{w}, V) + \mathrm{div} I_2 = \widetilde{W}(\mathbf{w}) - \partial_t V b_1(\mathbf{w}, V),$$
$$-\lambda^2 \Delta V = C - b_1(\mathbf{w}, V),$$

with **symmetrized** currents: $I_1 = J_1$, $I_2 = J_2 - V J_1$.

$$\Longrightarrow I_i(\mathbf{w}, V) = -D_{i1}(\mathbf{w}, V)\nabla w_1 - D_{i2}(\mathbf{w}, V)\nabla w_2.$$

New diffusion matrix $\mathbb{D}(\mathbf{w}, V) = (D_{ij}(\mathbf{w}, V))_{1\leq i,j\leq 2}$:

$$\mathbb{D}(\mathbf{w}, V) = \mathbb{P}(V)^T \mathbb{L}(\mathbf{u}) \mathbb{P}(V),$$

with

$$\mathbb{P}(V) = \begin{pmatrix} 1 & -V \\ 0 & 1 \end{pmatrix}.$$

$\Longrightarrow \mathbb{D}$ symmetric and positive definite.

Entropy structure

Entropy function

$$S(t) = \int_\Omega \left[\boldsymbol{\rho}(\mathbf{u}) \cdot (\mathbf{u} - \mathbf{u}^D) - (\chi(\mathbf{u}) - \chi(\mathbf{u}^D))\right] - \frac{\lambda^2}{2} u_2^D \int_\Omega |\nabla(V - V^D)|^2 \geq 0.$$

Under the previous assumptions and if $\nabla w_1^D = \nabla w_2^D = 0$,

$$\frac{d}{dt} S(t) = -\int_\Omega (\nabla \mathbf{w})^T \mathbb{D}\, \nabla \mathbf{w} + \int_\Omega W(\mathbf{u})(u_2 - u_2^D) \leq 0.$$

Keypoints:

- Reformulation of the Joule heating term:

$$\nabla V \cdot J_1 = \mathrm{div}(V J_1) - V \mathrm{div} J_1.$$

- Equivalence between the systems in primal and dual entropy variables.

Entropy structure

$$S(t) = \int_\Omega \left[\boldsymbol{\rho}(\mathbf{u}) \cdot (\mathbf{u} - \mathbf{u}^D) - (\chi(\mathbf{u}) - \chi(\mathbf{u}^D))\right] - \frac{\lambda^2}{2} u_2^D \int_\Omega |\nabla(V - V^D)|^2.$$

We have

$$\frac{d}{dt} S(t) = T_1 - u_2^D T_2,$$

with

$$T_1 = \int_\Omega \partial_t \boldsymbol{\rho}(\mathbf{u}) \cdot (\mathbf{u} - \mathbf{u}^D),$$

$$T_2 = \lambda^2 \int_\Omega \nabla(V - V^D) \cdot \partial_t \nabla V.$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 - u_2^D T_2.$$

We have

$$T_2 = \lambda^2 \int_\Omega \nabla(V - V^D) \cdot \partial_t \nabla V$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 - u_2^D T_2.$$

We have

$$\begin{aligned} T_2 &= \lambda^2 \int_\Omega \nabla(V - V^D) \cdot \partial_t \nabla V \\ &= -\lambda^2 \int_\Omega (V - V^D) \partial_t \Delta V \end{aligned}$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 - u_2^D T_2.$$

We have

$$\begin{aligned} T_2 &= \lambda^2 \int_\Omega \nabla(V - V^D) \cdot \partial_t \nabla V \\ &= -\lambda^2 \int_\Omega (V - V^D) \partial_t \Delta V \\ &= -\int_\Omega (V - V_D) \partial_t \rho_1(\mathbf{u}) \qquad {\scriptstyle -\lambda^2 \Delta V = C - \rho_1(\mathbf{u})} \end{aligned}$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 - u_2^D T_2.$$

We have

$$\begin{aligned} T_2 &= \lambda^2 \int_\Omega \nabla(V - V^D) \cdot \partial_t \nabla V \\ &= -\lambda^2 \int_\Omega (V - V^D) \partial_t \Delta V \\ &= -\int_\Omega (V - V_D) \partial_t \rho_1(\mathbf{u}) && {\scriptstyle -\lambda^2 \Delta V = C - \rho_1(\mathbf{u})} \\ &= \int_\Omega (V - V^D)\, \mathsf{div} J_1 && {\scriptstyle \partial_t \rho_1(\mathbf{u}) + \mathsf{div} J_1 = 0} \end{aligned}$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 - u_2^D T_2.$$

We have

$$\begin{aligned}
T_2 &= \lambda^2 \int_\Omega \nabla(V - V^D) \cdot \partial_t \nabla V \\
&= -\lambda^2 \int_\Omega (V - V^D) \partial_t \Delta V \\
&= -\int_\Omega (V - V_D) \partial_t \rho_1(\mathbf{u}) && {\scriptstyle -\lambda^2 \Delta V = C - \rho_1(\mathbf{u})} \\
&= \int_\Omega (V - V^D)\, \mathrm{div} J_1 && {\scriptstyle \partial_t \rho_1(\mathbf{u}) + \mathrm{div} J_1 = 0} \\
&= -\int_\Omega \nabla(V - V^D) \cdot I_1 && {\scriptstyle J_1 = I_1.}
\end{aligned}$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1.$$

$$T_1 = \int_\Omega \partial_t \rho_1 (u_1 - u_1^D) + \int_\Omega \partial_t \rho_2 (u_2 - u_2^D)$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1.$$

$$\begin{aligned} T_1 &= \int_\Omega \partial_t \rho_1 (u_1 - u_1^D) + \int_\Omega \partial_t \rho_2 (u_2 - u_2^D) \\ &= -\int_\Omega \mathrm{div} J_1 (u_1 - u_1^D) && \partial_t \rho_1 + \mathrm{div} J_1 = 0 \\ &\quad - \int_\Omega \left(\mathrm{div} J_2 - \nabla V \cdot J_1 - W\right)(u_2 - u_2^D) && \partial_t \rho_2 + \mathrm{div} J_2 = \nabla V \cdot J_1 + W \end{aligned}$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1.$$

$$T_1 = \int_\Omega \partial_t \rho_1 (u_1 - u_1^D) + \int_\Omega \partial_t \rho_2 (u_2 - u_2^D)$$

$$= -\int_\Omega \mathrm{div} J_1 (u_1 - u_1^D) \qquad \partial_t \rho_1 + \mathrm{div} J_1 = 0$$

$$-\int_\Omega \left(\mathrm{div} J_2 - \nabla V \cdot J_1 - W\right)(u_2 - u_2^D) \qquad \partial_t \rho_2 + \mathrm{div} J_2 = \nabla V \cdot J_1 + W$$

Since $\nabla V \cdot J_1 = \mathrm{div}(V J_1) - V \mathrm{div} J_1$,

$$T_1 = \int_\Omega J_1 \cdot \nabla(u_1 - u_1^D) + \int_\Omega (J_2 - V J_1) \cdot \nabla(u_2 - u_2^D)$$

$$+ \int_\Omega (-V \mathrm{div} J_1 + W)(u_2 - u_2^D).$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1,$$

with

$$T_1 = \int_\Omega J_1 \cdot \nabla(u_1 - u_1^D) + \int_\Omega (J_2 - VJ_1) \cdot \nabla(u_2 - u_2^D) + \int_\Omega (-V \mathsf{div} J_1 + W)(u_2 - u_2^D).$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D)\cdot I_1,$$

with

$$T_1 = \int_\Omega J_1 \cdot \nabla(u_1 - u_1^D) + \int_\Omega (J_2 - VJ_1)\cdot\nabla(u_2 - u_2^D)$$
$$+ \int_\Omega (-V\mathrm{div}J_1 + W)(u_2 - u_2^D).$$

$$w_1 = u_1 + u_2 V, \quad w_2 = u_2,$$
$$I_1 = J_1, \quad I_2 = J_2 - VJ_1,$$
$$\nabla w_1^D = 0 = \nabla w_2^D.$$

$$\Longrightarrow T_1 = \int_\Omega I_1 \cdot \left(\nabla w_1 - \nabla(w_2 V) + w_2^D \nabla V^D\right)$$
$$+ \int_\Omega I_2 \cdot \nabla w_2 - \int_\Omega V\mathrm{div}I_1(w_2 - w_2^D) + \int_\Omega W(u_2 - u_2^D)$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1,$$

with

$$T_1 = \int_\Omega I_1 \cdot \big(\nabla w_1 - \nabla(w_2 V) + w_2^D \nabla V^D\big) \\ + \int_\Omega I_2 \cdot \nabla w_2 + \int_\Omega I_1 \cdot (\nabla(w_2 V) - w_2^D \nabla V) + \int_\Omega W(u_2 - u_2^D)$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1,$$

with

$$\begin{aligned} T_1 &= \int_\Omega I_1 \cdot \big(\nabla w_1 - \nabla(w_2 V) + w_2^D \nabla V^D\big) \\ &\quad + \int_\Omega I_2 \cdot \nabla w_2 + \int_\Omega I_1 \cdot (\nabla(w_2 V) - w_2^D \nabla V) + \int_\Omega W(u_2 - u_2^D) \\ &= \int_\Omega I_1 \cdot \nabla w_1 + \int_\Omega I_2 \cdot \nabla w_2 + \int_\Omega W(u_2 - u_2^D) \\ &\quad - \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1. \end{aligned}$$

Entropy structure

$$\frac{d}{dt}S(t) = T_1 + \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1,$$

with

$$\begin{aligned}
T_1 &= \int_\Omega I_1 \cdot \big(\nabla w_1 - \nabla(w_2 V) + w_2^D \nabla V^D\big) \\
&\quad + \int_\Omega I_2 \cdot \nabla w_2 + \int_\Omega I_1 \cdot (\nabla(w_2 V) - w_2^D \nabla V) + \int_\Omega W(u_2 - u_2^D) \\
&= \int_\Omega I_1 \cdot \nabla w_1 + \int_\Omega I_2 \cdot \nabla w_2 + \int_\Omega W(u_2 - u_2^D) \\
&\quad - \int_\Omega w_2^D \nabla(V - V^D) \cdot I_1.
\end{aligned}$$

$$\Longrightarrow \frac{d}{dt}S(t) = -\int_\Omega (\nabla \mathbf{w})^T \mathbb{D}\, \nabla \mathbf{w} + \int_\Omega W(\mathbf{u})(u_2 - u_2^D) \leq 0.$$

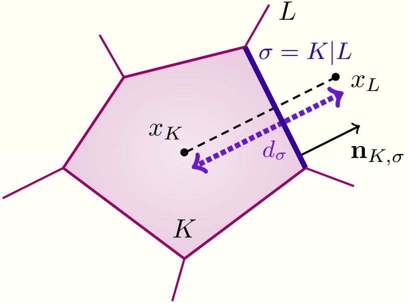
Consequences

P. Degond, S. Génieys, A. Jüngel, *J. Math. Pures Appl.*, 1997.

- *A priori* estimates: $L_t^\infty L_x^2$ on $\mathbf{u}$, $L_t^\infty H_x^1$ on V, $L_t^2 H_x^1$ on $\mathbf{w}$.
- Existence of a solution (Leray-Schauder fixed point theorem).
- Large time behavior: exponential convergence to the thermal equilibrium (discrete relative entropy with respect to equilibrium).

Aim: Transpose these results to the discrete setting.

Discretization



Admissibility: $(x_K, x_L) \perp \sigma$
Regularity: $\exists \xi > 0, d(x_K, \sigma) \geq \xi d_\sigma$

$$v_{K,\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \in \mathcal{E}_{int}, \\ v_\sigma^D & \text{if } \sigma \in \mathcal{E}^D, \\ v_K & \text{if } \sigma \in \mathcal{E}^N, \end{cases}$$

$$D_{K,\sigma} v = v_{K,\sigma} - v_K,$$
$$D_\sigma v = |D_{K,\sigma} v|.$$

Aim: design a TPFA scheme in primal variables leading to an equivalent scheme in dual entropy variables.

Main difficulty: Joule heating term $\nabla V \cdot J_1$

Discretization of $\nabla V \cdot J_1$

- **Eymard, Gallouët (SIAM J. Numer. Anal., 2003)**: two point flux ansatz, scaled with the space dimension $\rightarrow$ weakly converging gradient.

  Used in several works:
  - Bradji, Herbin (*IMA J. Numer. Anal.*, 2008): heat diffusion problem coupled with electrical diffusion problem.
  - Liero, Koprucki, Fischer, Scholz, Glitzky (*Z. Angew. Math. Phys.*, 2015): stationary thermistor model.
  - ...

  $\Longrightarrow$ not straightforward to rewrite the scheme in dual entropy variables
- **Chainais-Hillairet (Internat. J. Numer. Methods Fluids, 2009)**: complete reconstruction of gradients thanks to DDFV framework applied to the transient ET model.
- **Calgaro, Colin, Creusé (AIMS Math., 2019)**: TPFA with reformulation as $\mathrm{div}(V J_1) - V \mathrm{div} J_1$.

  $\Longrightarrow$ **Well-adapted to our objective**

Scheme in primal variables

$$\mathrm{m}(K)\frac{\rho_{1,K}^{n+1}-\rho_{1,K}^{n}}{\Delta t}+\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{1,K,\sigma}^{n+1}=0,$$

$$\mathrm{m}(K)\frac{\rho_{2,K}^{n+1}-\rho_{2,K}^{n}}{\Delta t}+\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{2,K,\sigma}^{n+1}=\mathrm{m}(K)W_K^{n+1}$$

$$+\sum_{\sigma\in\mathcal{E}_K}V_\sigma^{n+1}\mathcal{F}_{1,K,\sigma}^{n+1}-V_K^{n+1}\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{1,K,\sigma}^{n+1},$$

$$-\lambda^2\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma D_{K,\sigma}V^{n+1}=\mathrm{m}(K)(C_K-\rho_{1,K}^{n+1}),$$

with

$$\mathcal{F}_{i,K,\sigma}^{n+1}=-\tau_\sigma\left(L_{i1,\sigma}^n(D_{K,\sigma}u_1^{n+1}+u_{2,\sigma}^{n+1}D_{K,\sigma}V^{n+1})+L_{i2,\sigma}^nD_{K,\sigma}u_2^{n+1}\right),$$

where $\mathbb{L}_\sigma^n=(L_{ij,\sigma}^n)_{1\le i,j\le n}$ is defined as $\mathbb{L}_\sigma^n=\mathbb{L}((u_K^n+u_{K,\sigma}^n)/2)$.

Scheme in primal variables

$$
\mathrm{m}(K)\frac{\rho_{1,K}^{n+1}-\rho_{1,K}^{n}}{\Delta t}+\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{1,K,\sigma}^{n+1}=0,
$$

$$
\begin{aligned}
\mathrm{m}(K)\frac{\rho_{2,K}^{n+1}-\rho_{2,K}^{n}}{\Delta t}+\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{2,K,\sigma}^{n+1}&=\mathrm{m}(K)W_K^{n+1}\\
&\quad+\sum_{\sigma\in\mathcal{E}_K}\boxed{V_\sigma^{n+1}}\,\mathcal{F}_{1,K,\sigma}^{n+1}-V_K^{n+1}\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{1,K,\sigma}^{n+1},
\end{aligned}
$$

$$
-\lambda^2\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma D_{K,\sigma}V^{n+1}=\mathrm{m}(K)(C_K-\rho_{1,K}^{n+1}),
$$

with

$$
\mathcal{F}_{i,K,\sigma}^{n+1}=-\tau_\sigma\left(L_{i1,\sigma}^{n}(D_{K,\sigma}u_1^{n+1}+\boxed{u_{2,\sigma}^{n+1}}\,D_{K,\sigma}V^{n+1})+L_{i2,\sigma}^{n}D_{K,\sigma}u_2^{n+1}\right),
$$

where $\mathbb{L}_\sigma^n=(L_{ij,\sigma}^n)_{1\le i,j\le n}$ is defined as $\mathbb{L}_\sigma^n=\mathbb{L}((u_K^n+u_{K,\sigma}^n)/2)$.

Scheme in dual entropy variables

Change of variables

$$w_{1,K}^n = u_{1,K}^n + u_{2,K}^n V_K^n, \qquad w_{2,K}^n = u_{2,K}^n,$$
$$b_{1,K}^n = \rho_{1,K}^n, \qquad b_{2,K}^n = \rho_{2,K}^n - \rho_{1,K}^n V_K^n.$$

$$\Longrightarrow \quad \mathrm{m}(K)\frac{b_{1,K}^{n+1} - b_{1,K}^n}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{1,K,\sigma}^{n+1} = 0,$$

$$\mathrm{m}(K)\frac{b_{2,K}^{n+1} - b_{2,K}^n}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \left(\mathcal{F}_{2,K,\sigma}^{n+1} - V_\sigma^{n+1} \mathcal{F}_{1,K,\sigma}^{n+1} \right)$$
$$= \mathrm{m}(K)\widetilde{W}_K^{n+1} - \mathrm{m}(K)\frac{V_K^{n+1} - V_K^n}{\Delta t} b_{1,K}^n,$$

$$-\lambda^2 \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} V^{n+1} = \mathrm{m}(K)(C_K - b_{1,K}^{n+1})$$

Scheme in dual entropy variables

Change of variables

$$w_{1,K}^n = u_{1,K}^n + u_{2,K}^n V_K^n, \qquad w_{2,K}^n = u_{2,K}^n,$$
$$b_{1,K}^n = \rho_{1,K}^n, \qquad b_{2,K}^n = \rho_{2,K}^n - \rho_{1,K}^n V_K^n.$$

$$\Longrightarrow \quad \mathrm{m}(K)\frac{b_{1,K}^{n+1} - b_{1,K}^n}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \underbrace{\mathcal{F}_{1,K,\sigma}^{n+1}}_{=\mathcal{G}_{1,K,\sigma}^{n+1}} = 0,$$

$$\mathrm{m}(K)\frac{b_{2,K}^{n+1} - b_{2,K}^n}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \underbrace{\left(\mathcal{F}_{2,K,\sigma}^{n+1} - V_\sigma^{n+1}\mathcal{F}_{1,K,\sigma}^{n+1}\right)}_{=\mathcal{G}_{2,K,\sigma}^{n+1}}$$
$$= \mathrm{m}(K)\widetilde{W}_K^{n+1} - \mathrm{m}(K)\frac{V_K^{n+1} - V_K^n}{\Delta t} b_{1,K}^n,$$

$$-\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma} V^{n+1} = \mathrm{m}(K)(C_K - b_{1,K}^{n+1})$$

Equivalence of the schemes ?

$$\mathcal{G}_{i,K,\sigma}^{n+1} \stackrel{??}{=} -\tau_\sigma(\mathrm{D}_{i1,\sigma}^* D_{K,\sigma} w_1^{n+1} + \mathrm{D}_{i2,\sigma}^* D_{K,\sigma} w_2^{n+1}) \text{ with } \mathbb{D}_\sigma^* = (\mathrm{D}_{ij,\sigma}^*)_{i,j} \text{ spd}$$

Proposition [Equivalence of the schemes]

If

$$u_{2,\sigma}^{n+1} = \frac{u_{2,K}^{n+1} + u_{2,K,\sigma}^{n+1}}{2} \quad \text{and} \quad V_\sigma^{n+1} = \frac{V_K^{n+1} + V_{K,\sigma}^{n+1}}{2},$$

or

$$u_{2,\sigma}^{n+1} = \begin{cases} u_{2,K,\sigma}^{n+1} & \text{if } D_{K,\sigma} V^{n+1} > 0 \\ u_{2,K}^{n+1} & \text{if } D_{K,\sigma} V^{n+1} \leq 0 \end{cases} \text{ and } V_\sigma^{n+1} = \min(V_K^{n+1}, V_{K,\sigma}^{n+1}),$$

then both schemes are equivalent, provided that

$$\mathbb{D}_\sigma^* = (\mathbb{P}_\sigma^{n+1})^T \mathbb{L}_\sigma^n \mathbb{P}_\sigma^{n+1} \text{ with } \mathbb{P}_\sigma^{n+1} = \begin{pmatrix} 1 & -V_\sigma^{n+1} \\ 0 & 1 \end{pmatrix}.$$

Proof

$$\mathcal{G}_{1,K,\sigma}^{n+1} = \mathcal{F}_{1,K,\sigma}^{n+1}, \qquad \mathcal{G}_{2,K,\sigma}^{n+1} = \mathcal{F}_{2,K,\sigma}^{n+1} - V_\sigma^{n+1}\mathcal{F}_{1,K,\sigma}^{n+1}.$$

Aim:

$$\mathcal{G}_{i,K,\sigma}^{n+1} = -\tau_\sigma(\mathrm{D}_{i1,\sigma}^* D_{K,\sigma} w_1^{n+1} + \mathrm{D}_{i2,\sigma}^* D_{K,\sigma} w_2^{n+1}).$$

- $D_{K,\sigma} u_2^{n+1} = D_{K,\sigma} w_2^{n+1}$,

- $$D_{K,\sigma} u_1^{n+1} = \begin{cases} D_{K,\sigma} w_1^{n+1} - \boxed{V_K^{n+1}} D_{K,\sigma} w_2^{n+1} - \boxed{w_{2,K,\sigma}^{n+1}} D_{K,\sigma} V^{n+1} \\ D_{K,\sigma} w_1^{n+1} - \boxed{V_{K,\sigma}^{n+1}} D_{K,\sigma} w_2^{n+1} - \boxed{w_{2,K}^{n+1}} D_{K,\sigma} V^{n+1} \end{cases}$$
  $$= D_{K,\sigma} w_1^{n+1} - \boxed{V_\sigma^{n+1}} D_{K,\sigma} w_2^{n+1} - \boxed{w_{2,\sigma}^{n+1}} D_{K,\sigma} V^{n+1}$$

Proof

$$\mathcal{G}_{1,K,\sigma}^{n+1} = \mathcal{F}_{1,K,\sigma}^{n+1}, \qquad \mathcal{G}_{2,K,\sigma}^{n+1} = \mathcal{F}_{2,K,\sigma}^{n+1} - V_\sigma^{n+1}\mathcal{F}_{1,K,\sigma}^{n+1}.$$

Aim:

$$\mathcal{G}_{i,K,\sigma}^{n+1} = -\tau_\sigma(\mathrm{D}_{i1,\sigma}^* D_{K,\sigma} w_1^{n+1} + \mathrm{D}_{i2,\sigma}^* D_{K,\sigma} w_2^{n+1}).$$

$$\Longrightarrow \mathcal{G}_{1,K,\sigma}^{n+1} = -\tau_\sigma\left(L_{11,\sigma}^n D_{K,\sigma} w_1^{n+1} + (L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n) D_{K,\sigma} w_2^{n+1}\right)$$

$$\begin{aligned}\mathcal{G}_{2,K,\sigma}^{n+1} = -\tau_\sigma\Big((L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n) D_{K,\sigma} w_1^{n+1} \\ + (L_{22,\sigma}^n - 2V_\sigma^{n+1} L_{12,\sigma}^n + (V_\sigma^{n+1})^2 L_{11,\sigma}^n) D_{K,\sigma} w_2^{n+1}\Big).\end{aligned}$$

Proof

$$\mathcal{G}_{1,K,\sigma}^{n+1} = \mathcal{F}_{1,K,\sigma}^{n+1}, \qquad \mathcal{G}_{2,K,\sigma}^{n+1} = \mathcal{F}_{2,K,\sigma}^{n+1} - V_\sigma^{n+1}\mathcal{F}_{1,K,\sigma}^{n+1}.$$

Aim:

$$\mathcal{G}_{i,K,\sigma}^{n+1} = -\tau_\sigma(\mathrm{D}_{i1,\sigma}^* D_{K,\sigma} w_1^{n+1} + \mathrm{D}_{i2,\sigma}^* D_{K,\sigma} w_2^{n+1}).$$

$$\Longrightarrow \mathcal{G}_{1,K,\sigma}^{n+1} = -\tau_\sigma \left(L_{11,\sigma}^n D_{K,\sigma} w_1^{n+1} + (L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n) D_{K,\sigma} w_2^{n+1} \right)$$

$$\begin{aligned}\mathcal{G}_{2,K,\sigma}^{n+1} = -\tau_\sigma \Big(&(L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n) D_{K,\sigma} w_1^{n+1} \\ &+ (L_{22,\sigma}^n - 2V_\sigma^{n+1} L_{12,\sigma}^n + (V_\sigma^{n+1})^2 L_{11,\sigma}^n) D_{K,\sigma} w_2^{n+1} \Big).\end{aligned}$$

OK if

$$\begin{aligned}\mathrm{D}_{11,\sigma}^* &= L_{11,\sigma}^n, \\ \mathrm{D}_{12,\sigma}^* &= L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n, \\ \mathrm{D}_{22,\sigma}^* &= L_{22,\sigma}^n - 2V_\sigma^{n+1} L_{12,\sigma}^n + (V_\sigma^{n+1})^2 L_{11,\sigma}^n.\end{aligned}$$

Discrete entropy inequality

Discrete entropy function

$$S^n = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left[\boldsymbol{\rho}_K^n \cdot (\mathbf{u}_K^n - \mathbf{u}_K^D) - (\chi(\mathbf{u}_K^n) - \chi(\mathbf{u}_K^D))\right]$$
$$-\frac{\lambda^2}{2} u_2^D \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma(V^n - V^D))^2.$$

Proposition [Discrete entropy-dissipation inequality]

$$\frac{S^{n+1}-S^n}{\Delta t} \le -\sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_{K,\sigma}\mathbf{w}^{n+1})^T \mathbb{D}_\sigma^* D_{K,\sigma}\mathbf{w}^{n+1}$$
$$+\sum_{K\in\mathcal{T}} \mathrm{m}(K)\, W_K^{n+1}(u_{2,K}^{n+1} - u_{2,K}^D) \le 0, \quad \forall n \ge 0.$$

Keypoints:

- Discretization of the reformulated Joule heating term: $\nabla V \cdot J_1 \to \mathrm{div}(V J_1) - V\mathrm{div} J_1$.
- Equivalence of the schemes in primal and dual entropy variables.

A priori estimates

Proposition [*A priori* estimates (1/2)]

There exists a constant $C_1 > 0$, depending only on the data such that

$$\sup_{n\geq 0}\left(\|u_{1,\mathcal{T}}^n - u_{1,\mathcal{T}}^D\|_{L^2} + \|u_{2,\mathcal{T}}^n - u_{2,\mathcal{T}}^D\|_{L^2} + |V_{\mathcal{M}}^{n+1} - V_{\mathcal{M}}^D|_{1,\mathcal{M}}^2\right) \leq C_1. \quad (1)$$

- Entropy estimate $\Longrightarrow S^n \leq S^0$.
- Definition of

$$S^n = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left[\boldsymbol{\rho}_K^n \cdot (\mathbf{u}_K^n - \mathbf{u}_K^D) - (\chi(\mathbf{u}_K^n) - \chi(\mathbf{u}_K^D))\right]$$
$$-\frac{\lambda^2}{2} u_2^D \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma(V^n - V^D))^2,$$

and properties of $\boldsymbol{\rho} \Longrightarrow$ (1).

A priori estimates

Proposition [*A priori* estimates (2/2)]

There exists a constant $C_2 > 0$, depending only on the data and C_V such that:

$$\sum_{n=0}^{N_T-1} \Delta t \left(\left| w_{1,\mathcal{M}}^{n+1} \right|_{1,\mathcal{M}}^2 + \left| w_{2,\mathcal{M}}^{n+1} \right|_{1,\mathcal{M}}^2 \right) \leq C_2. \tag{2}$$

Cancès et al (2020): $(V_K)_{K\in\mathcal{T}}$ solution of

$$-\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma} V = \mathrm{m}(K)(C_K - \rho_{1,K})$$

with $C - \rho_1 \in L^\infty$

$$\Longrightarrow \max_{K\in\mathcal{T}} |V_K| \leq C_V.$$

$\Longrightarrow \mathbb{D}_\sigma^\star = (\mathbb{P}_\sigma^{n+1})^T \mathbb{L}_\sigma^n \mathbb{P}_\sigma^{n+1}$ uniformly positive definite.

Control of the dissipation term in the entropy inequality $\Longrightarrow$ (2)

Existence

Theorem [Existence of a solution]

Under the previous assumptions, for all $n \geq 0$, the dual scheme has a solution $(w_{1,\mathcal{T}}^n, w_{2,\mathcal{T}}^n, V_{\mathcal{T}}^n)$.
Then by equivalence the primal scheme has also a solution $(u_{1,\mathcal{T}}^n, u_{2,\mathcal{T}}^n, V_{\mathcal{T}}^n)$.

Outline of proof. By induction on $n \geq 0$, using the Leray-Schauder fixed point theorem. Construction of an application

$$\mathcal{L}^n : (\tilde{\mathbf{u}}_{\mathcal{T}}, \kappa) \in \mathbb{R}^{2\theta} \times [0,1] \mapsto \mathbf{u}_{\mathcal{T}} \in \mathbb{R}^{2\theta}$$

based on a linearization of the scheme and equivalence between the schemes.

- A fixed point $\mathbf{u}_{\mathcal{T}}$ of $\mathcal{L}^n(\cdot, \kappa = 1)$ is a solution to the primal scheme.
- $\exists M > 0$ such that $\forall \kappa \in [0,1]$, $\forall \mathbf{u}_{\mathcal{T}}$ satisfying $\mathcal{L}^n(\mathbf{u}_{\mathcal{T}}, \kappa) = \mathbf{u}_{\mathcal{T}}$, we have $\|\mathbf{u}_{\mathcal{T}}\|_2 \leq M$ ($\rightarrow$ thanks to *a priori* estimates).

Large time behavior

Assuming BC at equilibrium,

$$\nabla \mathbf{w}^D = 0, \quad W(\mathbf{u}^D) = 0, \quad -\lambda^2 \Delta V^D = C - \rho_1(\mathbf{u}^D),$$

thermal equilibrium $(\mathbf{w}^{eq}, V^{eq})$ is the unique solution of

$$-\lambda^2 \Delta V^{eq} = C - b_1(\mathbf{w}^{eq}, V^{eq}), \qquad \mathbf{w}^{eq} = \mathbf{w}^D.$$

Classical TPFA discretization $\Longrightarrow \exists!$ discrete equilibrium $(\mathbf{w}^{eq}_{\mathcal{T}}, V^{eq}_{\mathcal{T}})$.

Large time behavior

Discrete relative entropy

$$\widetilde{S}^n = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left[\boldsymbol{\rho}_K^n \cdot (\mathbf{u}_K^n - \mathbf{u}_K^{eq}) - (\chi(\mathbf{u}_K^n) - \chi(\mathbf{u}_K^{eq}))\right]$$
$$-\frac{\lambda^2}{2} u_2^D \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma(V_\mathcal{M}^n - V_\mathcal{M}^{eq}))^2.$$

Discrete entropy–dissipation estimate

$$\widetilde{S}^{n+1} - \widetilde{S}^n \leq -\Delta t \left(\left| w_{1,\mathcal{M}}^{n+1} \right|_{1,\mathcal{M}}^2 + \left| w_{2,\mathcal{M}}^{n+1} \right|_{1,\mathcal{M}}^2 \right) \leq -\frac{\Delta t}{C_{SI}} \widetilde{S}^{n+1}.$$

Theorem [Exponential convergence to equilibrium]

There exists $\gamma > 0$ depending only on the data and ξ such that

$$\widetilde{S}^n \leq \widetilde{S}^0 e^{-\gamma t^n},$$

from which we deduce

$$\|\mathbf{u}_\mathcal{T}^n - \mathbf{u}_\mathcal{T}^{eq}\|_{L^2}^2 + \|V_\mathcal{M}^n - V_\mathcal{M}^{eq}\|_{1,\mathcal{M}}^2 \leq c\, \widetilde{S}^0 e^{-\gamma t^n} \quad \forall n \geq 0.$$

Model

Unipolar energy transport model under Boltzmann statistics:

$$\rho_1(\mathbf{u}) = (-u_2)^{-3/2} \exp(u_1),$$
$$\rho_2(\mathbf{u}) = \frac{3}{2}(-u_2)^{-5/2} \exp(u_1).$$

Diffusion matrix:

$$\mathbb{L} = \rho_1(\mathbf{u}) T^{1/2-\beta} \begin{pmatrix} 1 & (2-\beta)T \\ (2-\beta)T & (3-\beta)(2-\beta)T^2 \end{pmatrix},$$

where $T = -1/u_2$.

- $\beta = 1/2$: Chen model
- $\beta = 0$: Lyumkis model

Implementation

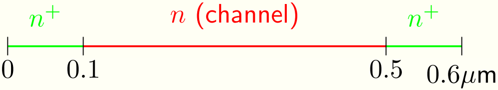
Fully implicit discretization: nonlinear system of coupled equations.

$\Longrightarrow$ **Newton's method**

- Adaptative time step needed during the first time iterations.
  Convergence criteria: tolerance (10^{-9}) is reached and $u_{2,K} < 0$ for all K.
- Best choice between primal and dual entropy variables ?

1D-n^+nn^+ ballistic diode

$\Omega = (0, l^*)$, $l^* = 6.10^{-5}$cm, $T_f = 1$ (equilibrium is reached).



Doping profile:

$$C(x) = \begin{cases} c_1 = 5.10^{17} cm^{-3} \text{ in the } n^+ \text{ region,} \\ c_0 = 2.10^{15} cm^{-3} \text{ in the } n \text{ region.} \end{cases}$$

Boundary conditions:

$$\rho_1(x=0) = \rho_1(x=l^*) = c_1,$$
$$T(0) = T(l^*) = 300K,$$
$$V(0) = 1.5V, \quad V(l^*) = 0.$$

Discretization parameters

- $\Delta x = 5.10^{-3}$,
- $\Delta t = 10^{-3}$ with adaptative time step if necessary.

1D-n^+nn^+ ballistic diode

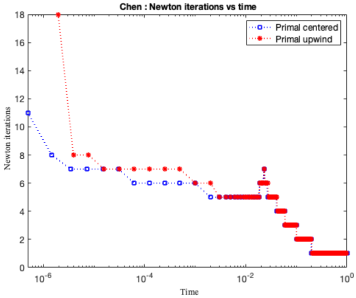
Chen model

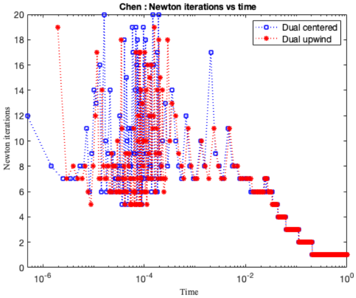
		Newton's iter	Nb time steps	Adapt time steps
Primal variables	Centered	1630	1011	21
	Upwind	1623	1009	19
Dual variables	Centered	4481	1106	214
	Upwind	5090	1132	266

Lyumkis model

		Newton's iter	Nb time steps	Adapt time steps
Primal variables	Centered	1791	1011	21
	Upwind	1868	1010	21
Dual variables	Centered	4324	1096	193
	Upwind	5256	1122	245

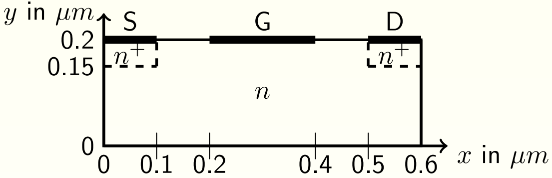
1D-n^+nn^+ ballistic diode





Distribution of the Newton iterations in time with the primal scheme (left) and dual scheme (right).

MESFET device



Doping profile:

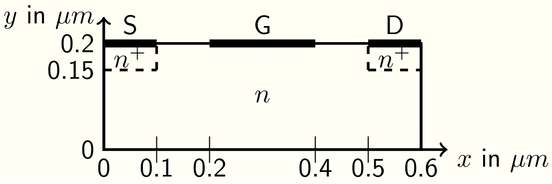
$$C = C_m = 3 \times 10^{17} cm^{-3} \quad \text{in the } n^+ \text{ region,}$$
$$C = C_n = 1 \times 10^{15} cm^{-3} \quad \text{in the } n \text{ region.}$$

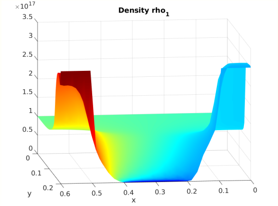
Boundary conditions:

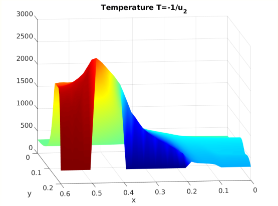
- at the source S: $\rho_1(\mathbf{u}) = C_m$, $u_2 = -1/T_0$, $V = \Phi_0$,
- at the drain D: $\rho_1(\mathbf{u}) = C_m$, $u_2 = -1/T_0$, $V = \Phi_0 + 2$V,
- at the gate G: $\rho_1(\mathbf{u}) = 3.9 \times 10^5\text{cm}^{-3}$, $u_2 = -1/T_0$, $V = \Phi_0 - 0.8$V.

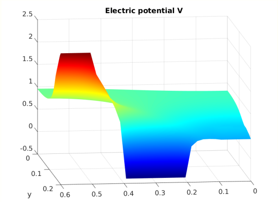
Discretization parameters: 3584 triangles, $T_{max} = 1$.

MESFET device



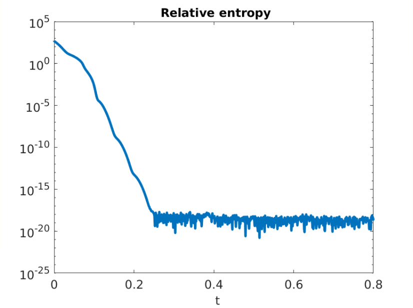


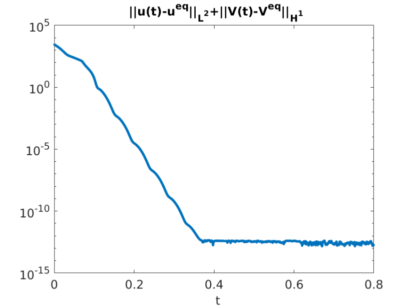




MESFET device

Approximate stationary state computed at $T = 5$.





Motivations

Difference in thickness between different parts of the domain may require local refinements.

$\Longrightarrow$ **Difficult to construct admissible meshes !**

DDFV methods:

- allow to consider very general meshes,
- reconstruct and mimic the dual properties of the continuous differential operators.

Design of the DDFV scheme

Same strategy as for the TPFA framework.
Reformulation of the Joule heating term

$$\nabla V \cdot J_1 = \mathsf{div}(V\, J_1) - V \mathsf{div} J_1.$$

Main difference: reformulate $u_2 \nabla V$ in J_i as $\mathsf{div}(u_2\, V) - V \nabla u_2$.

$\Longrightarrow$ Allow to prove equivalence between the schemes in primal and dual entropy variables with a unique definition of the diamond reconstruction operator.

Main results

M. B.-C., G. Lissoni & H. Mathis *Comp. Appl. Math.*, 2022.

- Equivalence between the DDFV schemes in primal and dual variables.
- Discrete entropy–dissipation inequality.
- $L_t^\infty L_x^2$ *a priori* estimate for approximations of $\mathbf{u} - \mathbf{u}^D$ and $\nabla(V - V^D)$.
- Existence of solutions for the schemes in primal and dual variables.

Outlook

- **Complete convergence analysis of the TPFA schemes**

  Difficulty: nonlinear densities $\rho_i(\mathbf{u})$.

  Andreianov, Cancès, Moussa, *J. Funct. Anal.*, 2017: space-time compactness from spatial *a priori* estimates.

- **Analysis of DDFV schemes**

  No $L_t^2 H_x^1$ estimate on $\mathbf{w}_{\mathcal{M}}$, since it requires L^∞ bound on $V_{\mathcal{T}}$.
  Difficulty: no maximum principle for classical DDFV discretizations even for linear elliptic problems.

  Camier, Hermeline, *Internat. J. Numer. Methods Engrg.*, 2016: nonlinear monotone DDFV scheme, but lack of coercivity...

Thank you for your attention !