Implicit-Explicit Runge-Kutta schemes for the Boltzmann-Poisson equation for semiconductors

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MOSFET modelling

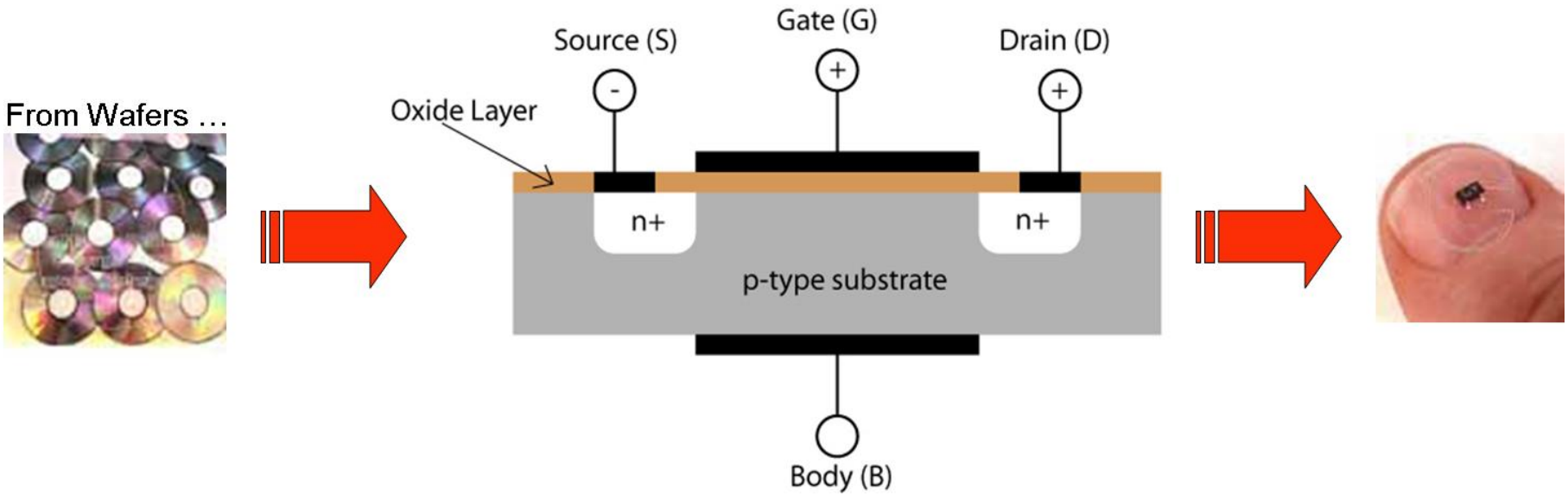

Figure: Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) device modelling from *http://nanohub.org/topics/MOSFETLabPage*

Outline

Prototype example

A prototype hyperbolic system of conservation laws with diffusive relaxation that we will use to illustrate the subsequent theory is the following:

$$\begin{aligned} u_t + v_x &= 0, \\ v_t + \frac{1}{\varepsilon^2} p(u)_x &= -\frac{1}{\varepsilon^2}(v - q(u)), \end{aligned} \tag{1}$$

where $p(u)' > 0$.

Characteristic speeds:

$$\pm \frac{\sqrt{p(u)'}}{\varepsilon}$$

Prototype example

In the small relaxation limit $\varepsilon \to 0$, the behavior of the solution is, at least formally, governed by the *convection-diffusion* equation

$$\begin{aligned} u_t + q(u)_x &= p(u)_{xx}, \\ v &= q(u) - p(u)_x. \end{aligned} \tag{2}$$

Ensure that the schemes possess the *correct zero-relaxation limit*:
the numerical scheme applied to system (1) should be a *consistent* and *stable* scheme for the limit system (2) as the parameter $\varepsilon \to 0$.

asymptotic preservation (AP)

Problems

1. Characteristic speeds of the hyperbolic part is of order $1/\varepsilon$, standard IMEX R-K schemes developed for hyperbolic systems with stiff relaxation become useless in such parabolic scaling, because the CFL condition would require $\Delta t = O(\varepsilon \Delta x)$.

2. Most previous works on asymptotic preserving schemes, in the limit of infinite stiffness become consistent explicit schemes for the diffusive limit equation: such explicit schemes clearly suffer from the usual stability restriction $\Delta t = O(\Delta x^2)$.

IMEX Runge-Kutta schemes for diffusive relaxation

The starting point is to reformulate problem (1) as the equivalent system [1]

$$u_t = \underbrace{-(v + \mu p(u)_x)_x}_{\text{Explicit}} + \underbrace{\mu p(u)_{xx}}_{\text{Implicit}},$$

$$\varepsilon^2 v_t = \underbrace{-p(u)_x - v + q(u))}_{\text{Implicit}}.$$

Here $\mu = \mu(\varepsilon) \in [0, 1]$ is a free parameter such that $\mu(0) = 1$.

[1] Boscarino, Pareschi, Russo (2011)

IMEX Runge-Kutta schemes for diffusive relaxation

This system can be written in the form

$$\begin{aligned} u_t &= \underbrace{f_1(u,v)}_{\text{Explicit}} + \underbrace{f_2(u)}_{\text{Implicit}} \\ \varepsilon^2 v_t &= \underbrace{g(u,v)}_{\text{Implicit}}, \end{aligned}$$

to which we can apply and study the properties of an IMEX-RK scheme.

IMEX Runge-Kutta schemes for diffusive relaxation

Applying an Implicit-Explicit (IMEX) Runge-Kutta scheme [2] we obtain:

$$
\begin{aligned}
U^k &= u^n + \Delta t \sum_{j=1}^{k-1} \widetilde{a}_{kj}\, f_1\left(U^j, V^j\right) + \Delta t \sum_{j=1}^{k} a_{kj}\, f_2\left(U^j\right), \\
\varepsilon^2 V^k &= \varepsilon^2 v^n + \Delta t \sum_{j=1}^{k} a_{kj}\, g\left(U^j, V^j\right)
\end{aligned}
$$

for the **internal stages** for $k = 1, \ldots, \nu$ and

$$
\begin{aligned}
u^{n+1} &= u^n + \Delta t \sum_{k=1}^{\nu} \widetilde{w}_k\, f_1\left(U^k, R^k\right) + \Delta t \sum_{k=1}^{\nu} w_k f_2\left(U^k\right) \\
\varepsilon^2 v^{n+1} &= \varepsilon^2 v^n + \Delta t \sum_{k=1}^{\nu} w_k\, g\left(U^k, V^k\right)
\end{aligned}
$$

for the **numerical solution** .

[2] Pareschi, Russo (2010); Asher, Ruuth, Spiteri (1997)

IMEX Runge-Kutta schemes for diffusive relaxation

The $\nu \times \nu$ matrices $\widetilde{A} = (\widetilde{a}_{ik})$ and $A = (a_{ik})$ and vectors $\widetilde{b}$, $b \in \mathbb{R}^\nu$ characterize the scheme and can be represented by a *double tableau* in the usual Butcher notation:

$$\begin{array}{c|c} \widetilde{c} & \widetilde{A} \\ \hline & \widetilde{w}^t \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & w^t \end{array}$$

Matrix A is lower triangular, i.e. the implicit scheme is a Diagonally Implicit Runge-Kutta (**DIRK**) scheme. This choice guarantees that implicit terms are, indeed, always explicitly evaluated.

Boltzmann-Poisson equation for semiconductors

Let $f(t, \mathbf{x}, \mathbf{v})$ be the density distribution function for particles at time $t \geq 0$, space point $\mathbf{x} \in \mathbb{R}^d$ and that travel with velocity $\mathbf{v} \in \mathbb{R}^d$, where $d = 1, 2, 3$ is the dimension.
Distribution function f solves a kinetic equation with *diffusive scaling* [3]

$$\varepsilon \, \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{q}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} f = \frac{1}{\varepsilon} \mathbf{Q}(f) \, . \tag{3}$$

In this formula:

- ε is the mean free path,
- q is the elementary charge and m the effective mass of the electron.
- $\mathbf{E}(t, \mathbf{x}) = -\nabla_{\mathbf{x}} \Phi(t, \mathbf{x})$ is the electric field.

$\mathbf{E}$ is obtained from the electric potential Φ given by the solution of a *Poisson equation*.

[3] Poupaud (1991); Klar (1998); Jin, Pareschi (2000)

Collision term

The anisotropic *collision term* $\mathbf{Q}(f)$ is defined by

$$\mathbf{Q}(f) = \int \sigma(\mathbf{v}, \mathbf{w}) \Big[M(\mathbf{v}) f(\mathbf{w}) - M(\mathbf{w}) f(\mathbf{v}) \Big] \, d\mathbf{w},$$

where σ is the *scattering kernel* and M is the normalized *Maxwellian* at the temperature θ of the semiconductor

$$M(\mathbf{v}) = \frac{1}{(2\pi\theta)^{d/2}} \exp\left(-\frac{|\mathbf{v}|^2}{2\theta} \right) .$$

The *collision frequency* λ is defined by:

$$\lambda(\mathbf{v}) = \int \sigma(\mathbf{v}, \mathbf{w}) M(\mathbf{w}) \, d\mathbf{w} \, .$$

Diffusive limit

Define the total mass $\rho = \rho(t, \mathbf{x})$ as

$$\rho = \int f(\mathbf{v})\, d\mathbf{v}\,.$$

As $\varepsilon \to 0$, one can show that f is approximated by

$$f(t, \mathbf{x}, \mathbf{v}) \approx \rho(t, \mathbf{x}) M(\mathbf{v}) \qquad (\varepsilon \to 0)$$

with ρ satisfying the drift-diffusion equation:

$$\partial_t \rho = \nabla_{\mathbf{x}} \cdot (D \nabla_{\mathbf{x}} \rho + \eta \rho \mathbf{E})\,. \tag{4}$$

In this equation, D is the *diffusion coefficient* defined implicitly in terms of the cross section and constant η is the *mobility* given by the Einstein relation $q\,D = \eta\, m\, \theta$.

Even and Odd parities formalism

Define the *even* parity r and the *odd* parity j by:

$$r(t,\mathbf{x},\mathbf{v}) = \frac{f(t,\mathbf{x},\mathbf{v}) + f(t,\mathbf{x},-\mathbf{v})}{2},$$
$$j(t,\mathbf{x},\mathbf{v}) = \frac{f(t,\mathbf{x},\mathbf{v}) - f(t,\mathbf{x},-\mathbf{v})}{2\varepsilon}.$$

Splitting eq. (3) into two equations, one for $\mathbf{v}$ and one for $-\mathbf{v}$ and adding and subtracting them we obtain:

$$\begin{aligned} &\partial_t r + \mathbf{v}\cdot\nabla_{\mathbf{x}} j - \frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} j = \frac{1}{\varepsilon^2}\mathbf{Q}(r), \\ &\partial_t j + \frac{1}{\varepsilon^2}\left(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} r\right) = -\frac{1}{\varepsilon^2}\lambda j\,, \end{aligned} \tag{5}$$

Even and Odd parities formalism

In the fluid-dynamic limit, i.e. as $\varepsilon \to 0$, we obtain:

$$\begin{aligned} \mathbf{Q}(r) &= 0\,, \\ \lambda j &= -\mathbf{v}\cdot\nabla_{\mathbf{x}} r + \frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} r\,, \end{aligned} \qquad (\varepsilon = 0)$$

from which

$$r(t,\mathbf{x},\mathbf{v}) = \rho(t,\mathbf{x})M(\mathbf{v})$$

and

$$j = \frac{1}{\lambda(\mathbf{v})}\left(-\mathbf{v}\cdot\nabla_{\mathbf{x}} r + \frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} r\right) = \frac{1}{\lambda(\mathbf{v})}\left(-M\mathbf{v}\cdot\nabla_{\mathbf{x}}\rho + \frac{q}{m}\rho\mathbf{E}\cdot\nabla_{\mathbf{v}} M\right).$$

Substituting this relations into the first equation in (5) and integrating over $\mathbf{v}$, we obtain the drift-diffusion equation (4).

Even and Odd parities formalism

Using parities formalism, our problem now reads:

$$\begin{aligned} \partial_t r + \mathbf{v}\cdot\nabla_{\mathbf{x}} j - \mathbf{E}\cdot\nabla_{\mathbf{v}} j &= \frac{1}{\varepsilon^2}\mathbf{Q}(r), \\ \partial_t j + \frac{1}{\varepsilon^2}(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r) &= -\frac{1}{\varepsilon^2}\lambda j\,, \end{aligned}$$

As was done before, we add and subtract in the first equation the term

$$\mathbf{v}\cdot\nabla_{\mathbf{x}}\left(\mu\frac{\mathbf{v}}{\lambda}\cdot\nabla_{\mathbf{x}} r\right),$$

where $\mu = \mu(\varepsilon)$ is a real positive parameter, such that $\mu(0) = 1$.

The idea behind this choice is that we want to compute such term with the *implicit* solver when the equation is in the *fluid-dynamic regime*, in order to use the appropriate solver for the diffusion term.

IMEX scheme for parity equations

The system we are going to solve now reads as follows:

$$\partial_t r + \underbrace{\mathbf{v}\cdot\nabla_{\mathbf{x}}\left(j+\mu\frac{\mathbf{v}}{\lambda}\cdot\nabla_{\mathbf{x}} r\right) - \mathbf{E}\cdot\nabla_{\mathbf{v}} j}_{\text{Explicit}} = \underbrace{\frac{1}{\varepsilon^2}\mathbf{Q}(r) + \mathbf{v}\cdot\nabla_{\mathbf{x}}\left(\mu\frac{\mathbf{v}}{\lambda}\cdot\nabla_{\mathbf{x}} r\right)}_{\text{Implicit}},$$

$$\partial_t j + \underbrace{\frac{1}{\varepsilon^2}\left(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r\right)}_{\text{Implicit}} = \underbrace{-\frac{1}{\varepsilon^2}\lambda j}_{\text{Implicit}}.$$

Remark: such scheme can be used for *easy to invert* collision terms $\mathbf{Q}$; this is true, e.g., for the *relaxed time approximation* (RTA), which is the case when $\sigma \equiv 1$, which implies:

$$Q(r) = M\rho - r.$$

Hermite approximation of the velocity space

Because of the structure of the problem, it is convenient to write unknowns r and j as follows:

$$r = \phi M \qquad \text{and} \qquad j = \psi M,$$

with $\phi = \phi(t, x, v)$ and $\psi = \psi(t, x, v)$.

Set $r = \phi M, j = \psi M$, with

$$\phi(v) = \sum_{k=0}^{N} \phi_k \widetilde{H}_k(v)\,, \qquad \psi(v) = \sum_{k=0}^{N} \psi_k \widetilde{H}_k(v)\,,$$

being the Hermite expansion.

Hermite approximation of the velocity space

The system then becomes:

$$\begin{aligned} \partial_t \phi \quad &+ \quad v\partial_x \left(\psi + \mu \frac{v}{\lambda}\partial_x \phi\right) - E\left(\partial_v \psi - 2\theta v \psi\right) = \\ &= \quad \frac{1}{\varepsilon^2}\widetilde{Q}(\phi) + \mu \frac{v^2}{\lambda}\partial_{xx}\phi\,, \end{aligned}$$

for ϕ and, similarly for ψ:

$$\partial_t \psi = -\frac{1}{\varepsilon^2}\left(\lambda\psi + v\partial_x \phi - E\partial_v \phi + 2\theta v E \phi\right).$$

Hermite approximation of the velocity space

For the collision operator, we have

$$Q(r)(v) = M(v) \sum_{j=0}^{N} \sigma(v, v_j)\phi(v_j)w_j - \lambda(v)r(v)\,,$$

and for the collision frequency

$$\lambda(v) = \sum_{j=0}^{N} \sigma(v, v_j)w_j\,,$$

where (v_j, w_j) are the points and weights of the Gauss-Hermite quadrature rule.

Hermite approximation of the velocity space

Derivatives with respect to v become easy to compute:

$$\partial_v r = M\partial_v \phi - 2vM\phi\,, \quad \partial_v j = M\partial_v \psi - 2vM\psi\,,$$

which can be evaluated using

$$\partial_v \phi = \sum_{k=1}^{N} \phi_k \sqrt{2k}\widetilde{H}_{k-1}(v) = \sum_{j=0}^{N} \phi(v_j) c_j(v), \quad \partial_v \psi = \sum_{j=0}^{N} \psi(v_j) c_j(v)\,.$$

for ϕ and for ψ.
Coefficients $c_j(v_i) = c_{ij}$ are given by

$$c_j(v) = \sum_{k=1}^{N} \sqrt{2k}\widetilde{H}_k(v_j)\widetilde{H}_{k-1}(v) w_j\,.$$

and are constant in time.

Space discretization

General requirements for the space discretization:

1. **correct diffusion limit:** for an implicit approximation in the limit $\varepsilon = 0$, require that $\mu(0) = 1$;
2. **compact stencil:** it is important to obtain a scheme which uses a compact stencil in the limit $\varepsilon \to 0$: this is guaranteed by point (1) and by a suitable discretization for the diffusion term;
3. **shock capturing:** this is necessary for large values of ε and also for convection-diffusion type limit equations with small diffusion;
4. **avoid solving nonlinear algebraic equations:** the implicit space-derivative in the second equation is, indeed, explicitly evaluated.

High-order finite volumes Weighted-Essentially Non Oscillatory (WENO) reconstructions are a good choice in order to achieve all these goals.

Space discretization

Consider again the prototype system

$$u_t + v_x = 0,$$
$$v_t + \frac{1}{\varepsilon^2} u_x = -\frac{1}{\varepsilon^2} v.$$

In a finite volume approximation, taking into account only the space-derivative discretization, this system reads:

$$\bar{u}_t = -\frac{\hat{v}_{i+1/2} - \hat{v}_{i-1/2}}{\Delta x},$$
$$\bar{v}_t = -\frac{\hat{u}_{i+1/2} - \hat{u}_{i-1/2}}{\Delta x} - \frac{1}{\varepsilon^2} \bar{v},$$

Numerical dissipation

Using, for example, Lax-Friedrichs type fluxes, we have [4]:

$$\hat{v}_{i+1/2} = \frac{1}{2}\left[\left(v_{i+1} + v_i\right) - \frac{1}{\varepsilon}\left(u_{i+1} - u_i\right)\right],$$
$$\hat{u}_{i+1/2} = \frac{1}{2}\left[\left(u_{i+1} + u_i\right) - \varepsilon\left(v_{i+1} - v_i\right)\right].$$

To be able to use our scheme also in the limit $\varepsilon \to 0$, it is necessary to consider a modified flux.
We consider modified artificial viscosity constants:

$$\hat{v}_{i+1/2} = \frac{1}{2}\left[\left(v_{i+1} + v_i\right) - \alpha_v\left(u_{i+1} - u_i\right)\right],$$
$$\hat{u}_{i+1/2} = \frac{1}{2}\left[\left(u_{i+1} + u_i\right) - \alpha_u\left(v_{i+1} - v_i\right)\right].$$

For example, we consider

$$\alpha_u = \alpha_v = \varepsilon.$$

[4] Jin, Pareschi, Toscani (2000)

Choice for μ

For large value of ε, we want to avoid adding and subtracting terms which may cause loss of stability.

A first choice is based on the simple remark that when $\varepsilon \geq \Delta x$, we want to keep the explicit scheme; this leads to:

$$\mu = \mu(\varepsilon, \Delta x) = \begin{cases} 1 & \text{if} \quad \varepsilon < \Delta x, \\ 0 & \text{if} \quad \varepsilon \geq \Delta x, \end{cases}$$

or some smoothed version of it (e.g. $\mu = \exp(-\varepsilon/\Delta x)$).

Another possibility is to relate μ to the time step, with the goal to avoid adding backward diffusion up to $\mathcal{O}(\varepsilon^2)$.
For the IMEX Euler scheme, this leads to

$$\mu = \mu(\varepsilon, \Delta t) = \frac{\Delta t}{\varepsilon^2 + \Delta t}.$$

More accurate choices can be done by taking $\mu = \mu(\varepsilon, \Delta x, \Delta t)$.

Boundary conditions

For $x \in (x_L, x_R)$ and $v \in \mathbb{R}$, problem (1) is complemented with *boundary conditions*: for $v > 0$

$$f(t, x_L, v) = F_L(v), \qquad f(t, x_R, -v) = F_R(v),$$

where F_L and F_R are assigned non-negative functions.

To get boundary conditions for r and j, it is possible to use relations [5]: for $v > 0$,

$$r + \varepsilon j \Big|_{x=x_L} = F_L\,, \qquad r - \varepsilon j \Big|_{x=x_R} = F_R\,.$$

[5] Jin, Pareschi (2000)

Boundary conditions

When $\varepsilon \ll 1$, a reasonable approximation for j is

$$\lambda j = -v\partial_x r + E\partial_v r.$$

Applying this to the boundaries:

$$r - \frac{\varepsilon}{\lambda}(v\partial_x r - E\partial_v r)\big|_{x=x_L} = F_L\,, \qquad r + \frac{\varepsilon}{\lambda}(v\partial_x r - E\partial_v r)\big|_{x=x_R} = F_R\,.$$

Remark: from $r \pm \varepsilon j = F_{L,R}$ we have $\partial_v r = \partial_v F_{L,R} + O(\varepsilon)$.
Then, up to $O(\varepsilon^2)$:

$$r - \frac{\varepsilon}{\lambda}(v\partial_x r - E\partial_v F_L)\big|_{x=x_L} = F_L\,, \qquad r + \frac{\varepsilon}{\lambda}(v\partial_x r - E\partial_v F_R)\big|_{x=x_R} = F_R\,.$$

Properties of the IMEX scheme

General requirements for the time discretization:

1. AP;
2. Globally stiffly accurate.

Examples of schemes which uniformly work for our problem are:

- **second order:** SSP2-(3,3,2) scheme and ARS-(2,2,2) scheme;
- **third order:** ARS-(4,4,3) scheme and BPR-(3,5,3) scheme [6].

[6] Boscarino, Pareschi, Russo 2011

Numerical results

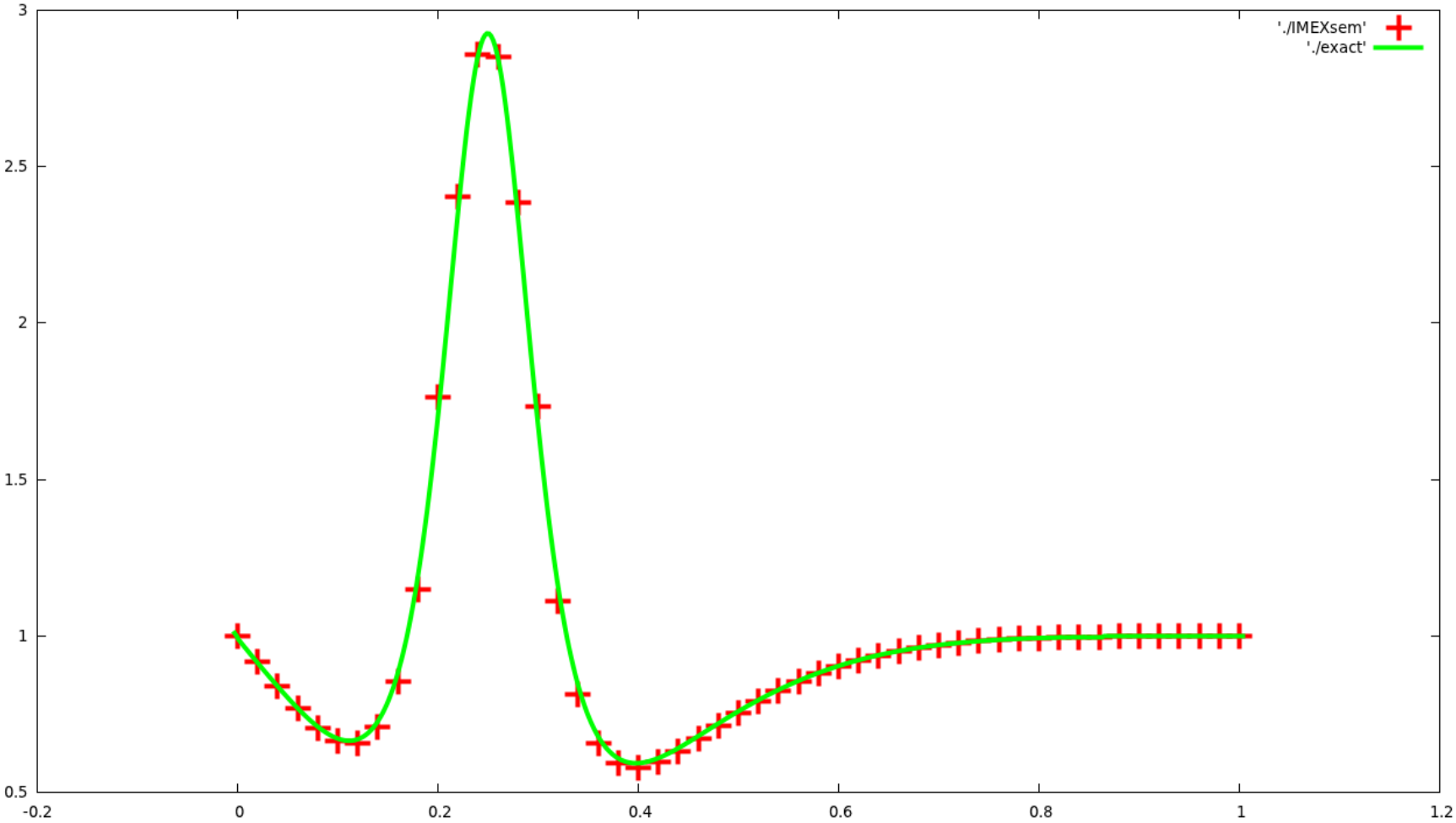

Figure: Test1 at $T_f = 0.03, \quad \varepsilon = 0.002$

$$\Delta t_{JP} = 5 * 10^{-5}, \quad \Delta t_{DPR} = 5 * 10^{-4}.$$

Numerical results

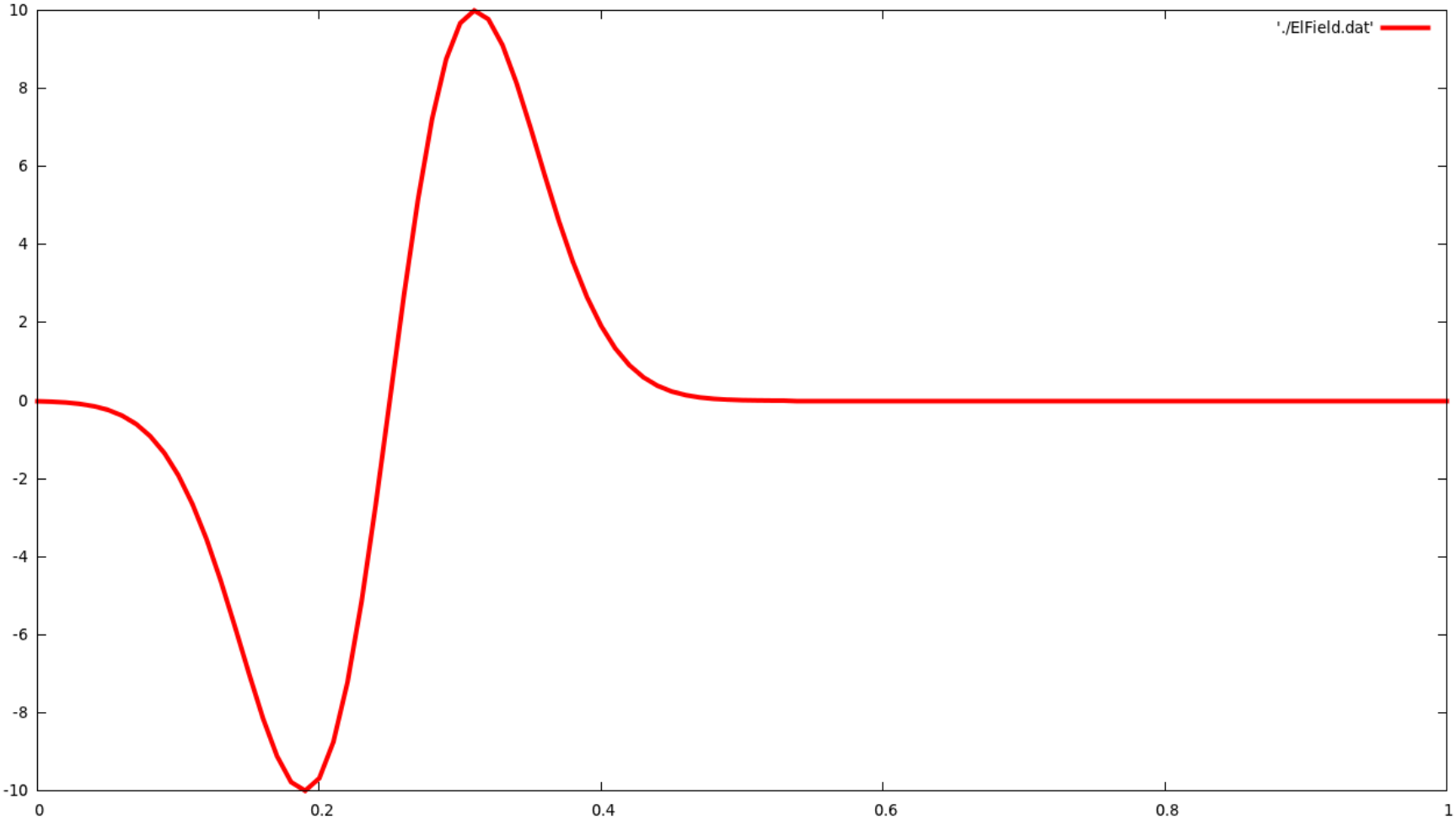

Figure: Electric field given by a potential well

Numerical results

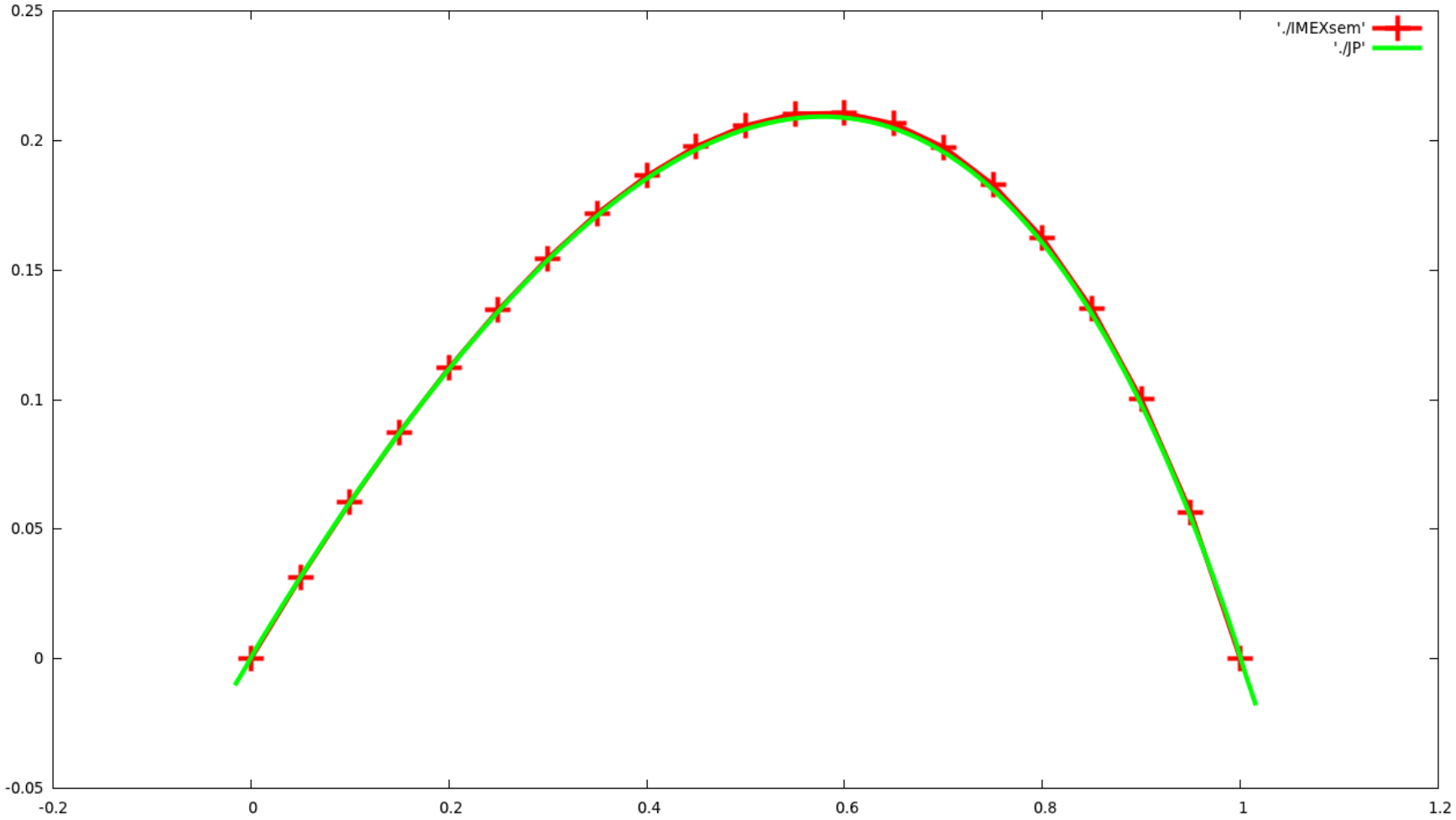

Figure: Test 2 at time $T_f = 0.4 \qquad \varepsilon = 0.001$

$$\Delta t_{JP} = 10^{-4}, \qquad \Delta t_{DPR} = 2 * 10^{-3} \qquad \Rightarrow \qquad \Delta t_{JP}/\Delta t_{DPR} = \Delta x.$$

Penalization technique for the collision term

How do we treat more realistic collision terms?

We substitute the full collision term $\mathbf{Q}$ adding and subtracting its "linearized" version [7]:

$$\underbrace{\mathbf{Q}(r)}_{\textit{Implicit}} \quad \rightarrow \quad \underbrace{\Big(\mathbf{Q}(r) - \mathbf{L}(r)\Big)}_{\textit{Explicit}} + \underbrace{\mathbf{L}(r)}_{\textit{Implicit}} .$$

For example, if

$$Q(r) = 0 \quad \Rightarrow \quad r = \rho M,$$

then such strategy can be effectively applied using the RTA approximation:

$$\mathbf{L}(r) := \rho M - r.$$

Remark: the linear part is computed implicitly to stabilize the non-linear collision operator, *without* changing the asymptotic behavior of the solution.

[7] Jin, Filbet (2010); Dimarco, Pareschi (2011)

Penalization technique for the collision term

Using such technique, the IMEX scheme for diffusive relaxation can be used also for very general collision operators:

$$\partial_t r + \underbrace{\mathbf{v}\cdot\nabla_{\mathbf{x}}\left(j+\mu\frac{\mathbf{v}}{\lambda}\cdot\nabla_{\mathbf{x}} r\right) - \mathbf{E}\cdot\nabla_{\mathbf{v}} j - \frac{1}{\varepsilon^2}\Big(\mathbf{Q}(r)-\mathbf{L}(r)\Big)}_{\text{Explicit}} =$$

$$= \underbrace{\frac{1}{\varepsilon^2}\mathbf{L}(r) + \mathbf{v}\cdot\nabla_{\mathbf{x}}\left(\mu\frac{\mathbf{v}}{\lambda}\cdot\nabla_{\mathbf{x}} r\right)}_{\text{Implicit}},$$

$$\partial_t j + \underbrace{\frac{1}{\varepsilon^2}\left(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r\right)}_{\text{Implicit}} = \underbrace{-\frac{1}{\varepsilon^2}\lambda j}_{\text{Implicit}}.$$

Remark: the asymptotic behavior is the same as in the "linear" case.

THANK YOU!