TORE SUPRA

Association EURATOM-CEA

Département de Recherches sur la Fusion Contrôlée
CEA - CADARACHE
13108 Saint-Paul-lez-Durance FRANCE

IPP AS CZECH REPUBLIC

Simulations of LH-generated fast particles in the tokamak scrape-off layer

J. P. Gunn,[a] V. Fuchs[b]

[a] Association EURATOM-CEA sur la fusion contrôlée, Saint Paul Lez Durance, France
[b] Institute of Plasma Physics, Association EURATOM-IPP.CR, Prague, Czech Republic

New simulation method : quasineutral PIC method (QPIC)

F. F. Chen : « Do not use Poisson 's equation unless it is unavoidable ! We can usually assume $n_e \cong n_i$ and div $E \neq 0$ at the same time …. »

A new PIC technique developed by G. Joyce, M. Lampe, S. P. Slinker, and W. M. Manheimer, J. Comp. Phys. **138**, 540 (1997) allows simulating quasineutral plasmas on arbitrarily large time and distance scales. **Quasineutrality can be expected if $1/\omega_{pe}$ and λ_D are much smaller than the relevant temporal and spatial scales to be resolved in the problem**

The electric field is calculated from the electron fluid momentum equation rather than from Poisson's equation.

The fluid moments are tabulated at every point on the grid at every time step and used to calculate the parallel electric field E_z felt by ***both*** ions and electrons.

QPIC method

The fluid moments are tabulated at every point on the grid at every time step and used to calculate the parallel electric field felt by *both* ions and electrons.

$$-eE = \frac{1}{n_e}\frac{\partial P_e}{\partial z} + \nu_e m_e u_e + \frac{1}{n_e}\frac{\partial}{\partial t}\left(n_e m_e u_e\right)$$

pressure gradient term
(Boltzmann equation for Maxwellian electrons)

friction or driving term
(i.e. momentum input from some external source that drives flux in phase space, e.g. collisions with ions or neutrals, or RF waves)

inertia term
(high frequency oscillations that serve only to maintain quasineutrality

The "magic ingredient" that makes QPIC work

Replace *electron density* by *ion density* and drop the inertia term:

$$-eE = \frac{1}{n_i}\frac{\partial}{\partial z}\left(n_i \left\langle v_e^2 \right\rangle\right) + \nu_e m_e u_e$$

At every time step we use the ion density and mean electron kinetic energy to calculate the self-consistent electric field.

The result is that quasineutrality is maintained. To understand why, substitute the approximate E equation in the full electron momentum equation:

$$m_e \frac{\partial u_e}{\partial t} = T_e \frac{\partial}{\partial z} \ln\left(\frac{n_i}{n_e}\right)$$

Any charge separation (due to statistical shot noise) leads to a restoring force that pulls the electrons back onto the ions in order to maintain quasineutrality.

These artificial high frequency oscillations are stable if the system is started in a quasineutral state and if the time step is small enough the resolve the oscillations.

Classical PIC simulation of the 1D SOL

PIC code: particle equations of motion $\Rightarrow n_{e,i}$ and the self-consistent field E_s is obtained from the Poisson equation, i.e. div $E_s = q(n_i-n_e)$

To guarantee numerical stability, the cell size Δz needs to resolve charge separation on the Debye scale, plus Δt needs to resolve electron plasma frequency scales:

e.g. Tore Supra : $L_{//}$~100 m, λ_D~10^{-5} m $\rightarrow$ ~ 10^7 grid points in 1-D. Equilibrium is reached after several ion transit times $\tau=L_{//}/v_{Ti}$ $\Rightarrow$ ~ 10^9 particles and ~ 10^8 time steps

Fully self consistent PIC simulations can only be attempted with greatly reduced SOL dimension (~cm) and unphysically high collisionality, and even then...

...with 100 particles per cell, the PIC code can only resolve charge densities of a few %. PIC codes work well in the non-neutral sheath where the relative charge density $(n_i-n_e)/n_o$~1, but in the quasineutral SOL the real relative charge density is ~10^{-14} (10^{-6} in the reduced SOL case). The solution of Poisson's equation is totally dominated by statistical shot noise.

$\rightarrow$For most macroscopic SOL problems, it is not necessary to resolve the Debye length; PIC stability imposes a severe constraint that motivates us to look for another numerical technique. In addition, it may be *fundamentally wrong* to apply PIC codes to quasineutral plasmas.

New QPIC (Quasineutral PIC) simulation of the 1D SOL

QPIC code: particle equations of motion $\Rightarrow n_{e,i}$ and the self-consistent field E_s is obtained from the electron fluid momentum equation.

The cell size Δz only needs to resolve the macroscopic parallel gradients. The SOL can be reasonably simulated with <100 cells (instead of 10^7 for a PIC code). The Δt should be chosen so that the particles traverse no more than 1 grid cell per time step.

e.g. Tore Supra : $L_{//}$~100 m, Δz =1 m$\rightarrow$ ~ 10^2 grid points in 1-D. Equilibrium is reached after several ion transit times $\tau = L_{//}/v_{Ti}$ $\Rightarrow$ ~ 10^3 time steps

The electric field in QPIC is derived from a derivative as opposed to an integral calculation in PIC. A large number of particles are needed in each cell (at least a few 100, but a few 1000 give nice results) in order to limit fluctuations of the electron pressure gradient. There are typically 10^5 particles in a QPIC run.

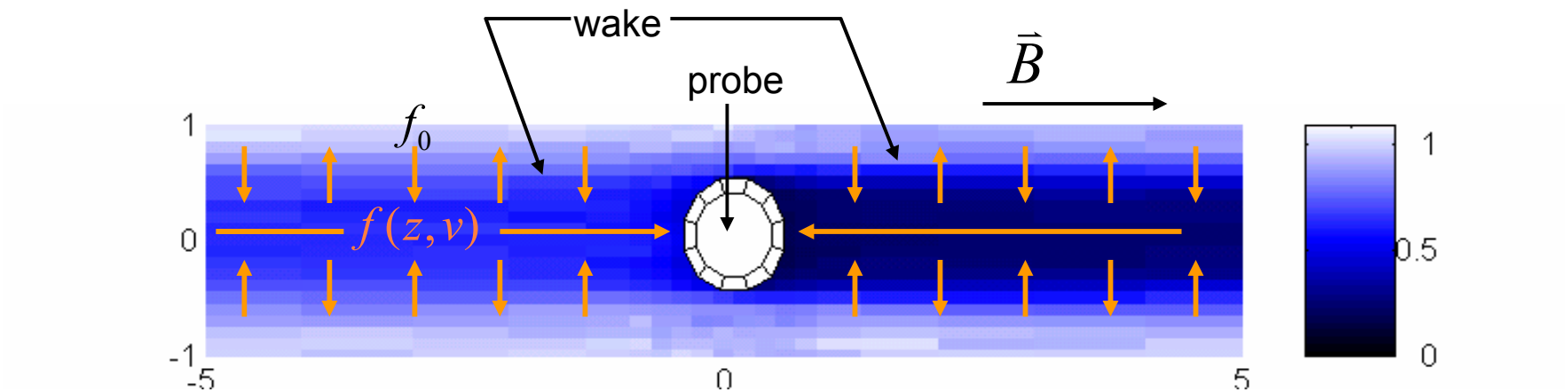
A typical test run in Fortran90 on a Linux PC takes ~1 hour. A "publication quality" high resolution run takes about half a day.

QPIC is well suited for macroscopic SOL problems because it allows the simulation of a pertinent hierarchy of spatial and temporal scales.

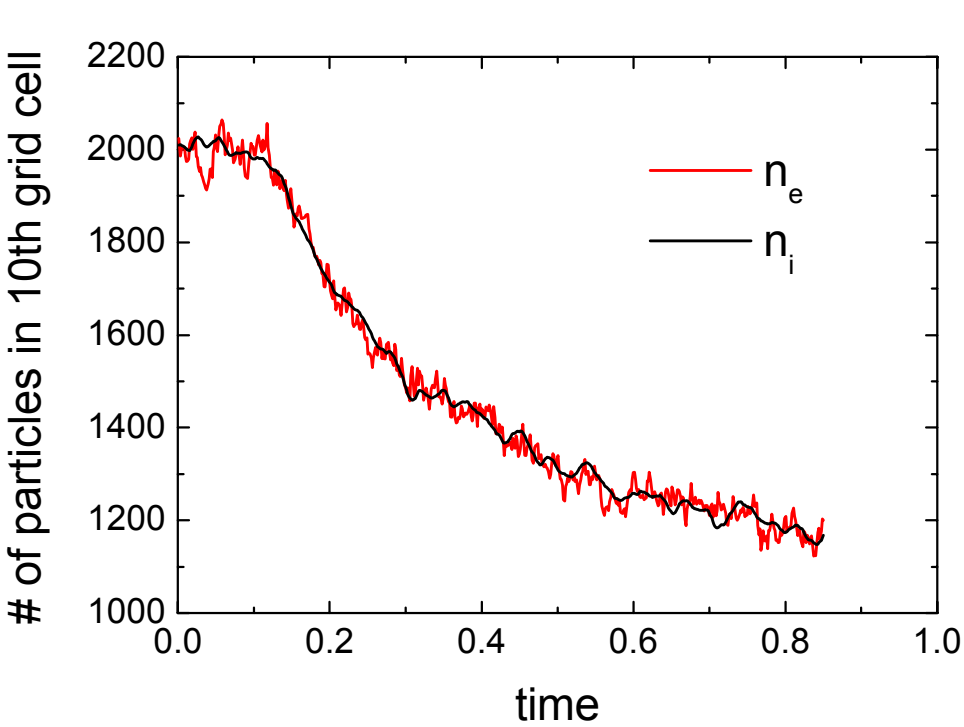
Benchmarking QPIC on a non-linear problem with a known solution: The Mach probe model of Chung and Hutchinson

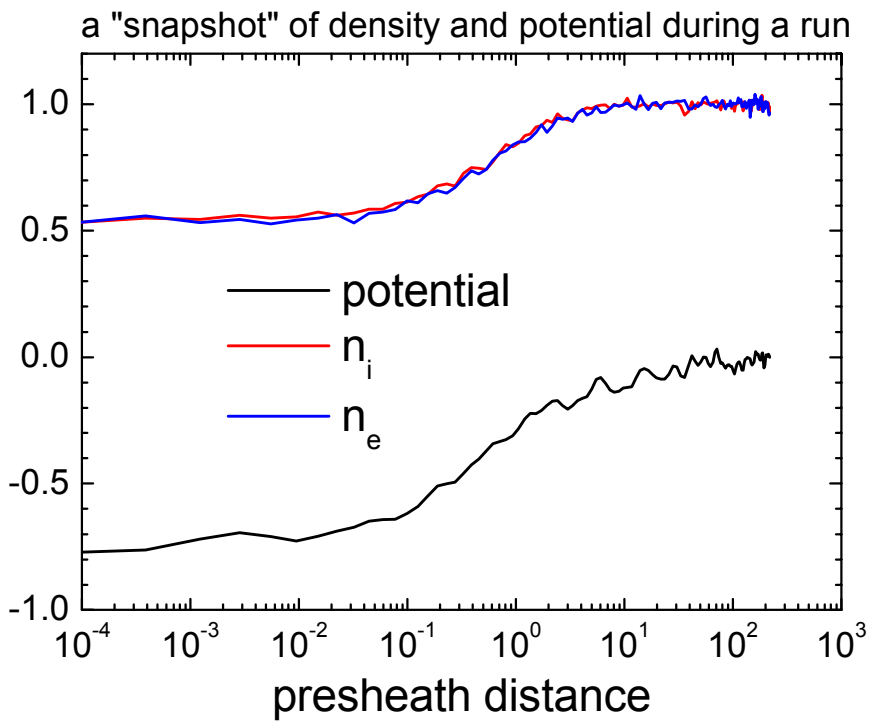
A probe collects charges from the plasma and creates a density depression in its vicinity. In a magnetized plasma, cross field transport is much weaker than parallel transport, so the density depression extends a long way along magnetic field lines. The cross-field flow of particles into the wake of the probe can be approximated by a source term.

$$v\frac{\partial f}{\partial z}+E\frac{\partial f}{\partial v}=S(z,v)=W\left[f_0(v)-f(z,v)\right];\quad W=\frac{D_\perp}{d_{probe}^2}\qquad f_0=\frac{1}{\sqrt{2\pi T_0}}\exp\left(-\frac{v^2}{2T_0}\right)$$



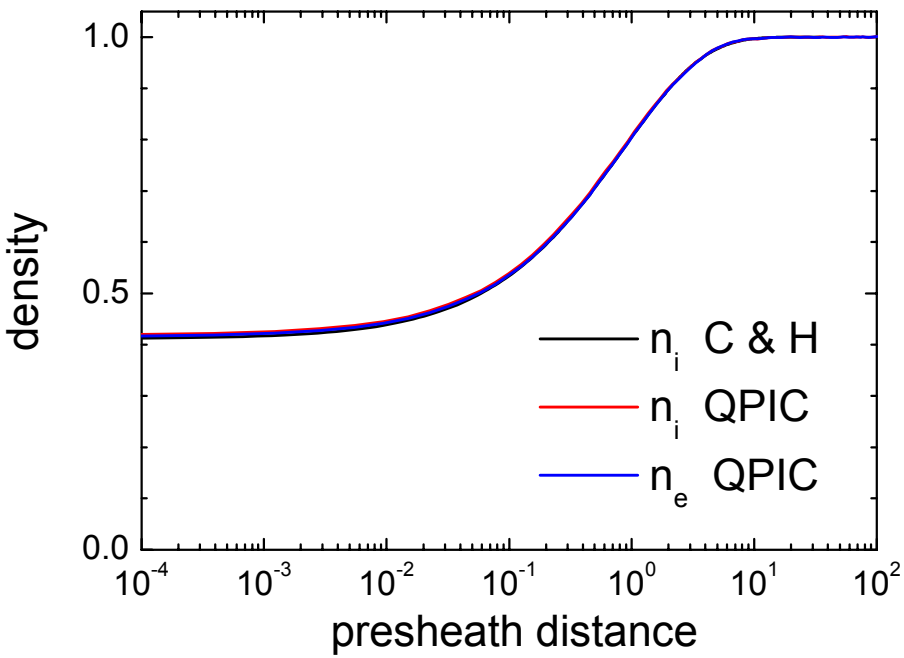
Example : sonic expansion of the density perturbation from a probe into the SOL (presheath formation). The electron density remains tied to the ion density even during violent events.

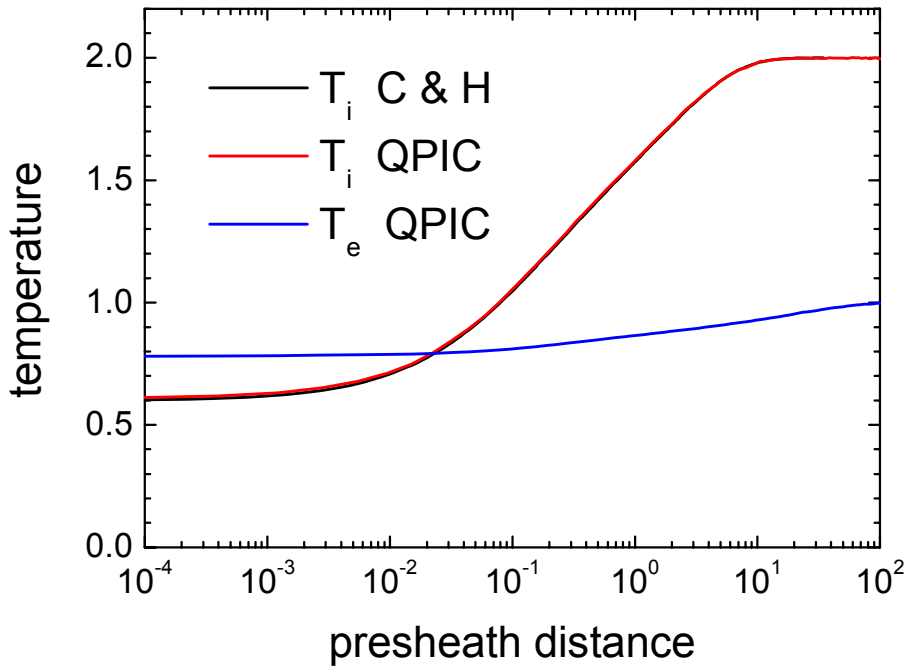




QPIC gives the right answer... and interesting new results!

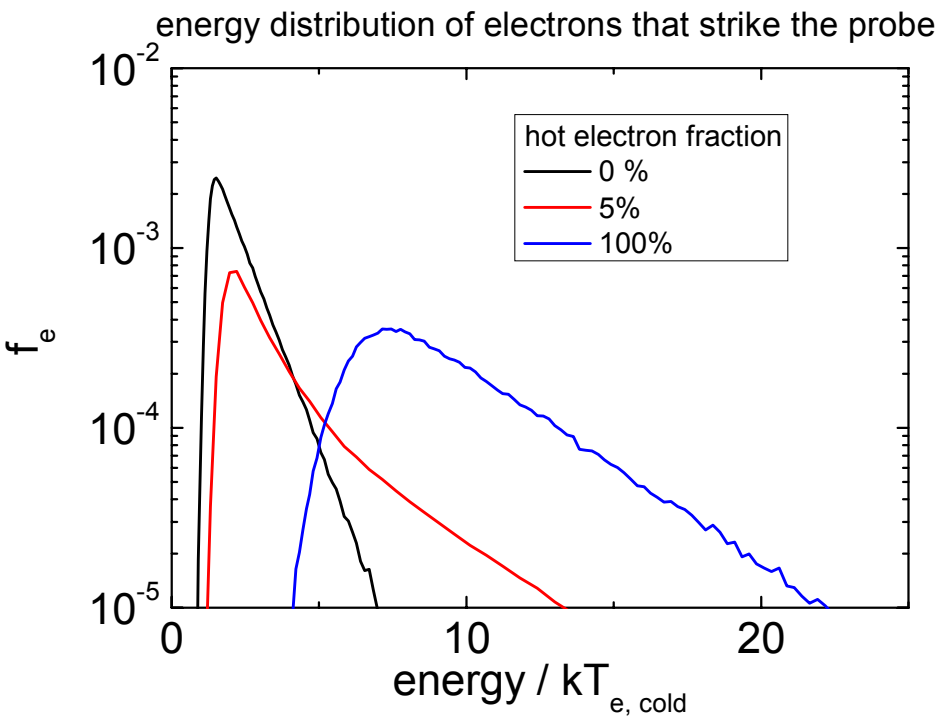
C&H modelled the ion distribution function with implicit Boltzmann electrons. QPIC should give almost the same result (except for the collection of fast electrons by the probe). With explicit electrons, we can now calculate heat flux to the probe, and the modification of the ion sound speed due to the "cooling" of the electrons near the sheath entrance.

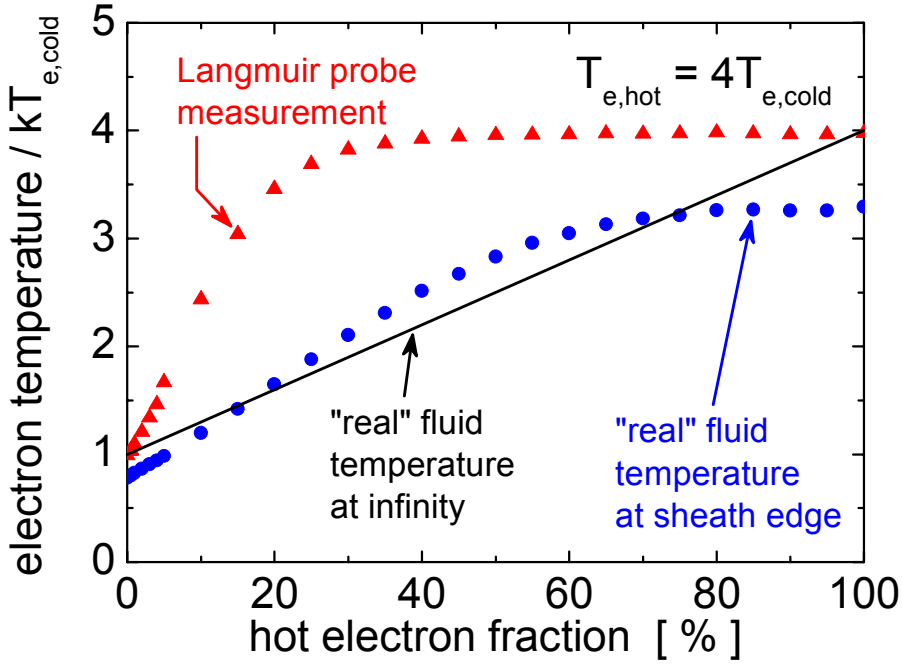




QPIC opens the door to studies of non-thermal electron dynamics

Instead of Maxwellian electrons, we can model any arbitrary distribution. For example, consider a mixture of hot and cold electrons. QPIC calculates the electron and ion fluxes to the probe surface, and allows us to predict what the current-voltage characteristic looks like.





Modeling of edge plasma response to LH grill field

Fast electron generation in front of the LH grill

Canadian, French, and Finnish groups (Fuchs, Mailloux, Goniche, Rantamaki, et al.) have studied the electron dynamics in front of the grill, ignoring the ion response.

New problem

However, another interesting question has been posed by Czech and Austrian groups (V. Petrzilka, S. Kuhn, et al.):

As the hot electrons rush out from the grill region along field lines, they leave behind the less mobile ions. This causes a positive space charge to form in front of the grill.

What happens?

Are the electrons pulled back in front of the grill?

Do the ions also rush away along field lines?

Are **ions** or **electrons** (or ***both***) responsible for hot spots?

Physical model for LH grill electric field

Good antenna - edge plasma coupling requires $\omega_{pe} \cong 1.6\omega_{LH}$, so that on the rf step QPIC does not give significant CPU time savings over PIC.

In order to restore temporal savings in QPIC we suppose that the quiver-averaged electron behaviour controls the essential physics and we look for an approximate representation that leads to equivalent behavior of the electrons in phase space.

Question: how do we average over the violent, high-frequency RF accelerations ?

Answer: we believe that a useful method is to exploit the rf - induced electron stochasticity observed in the test electron simulations. Consequently, we must find a diffusion coefficient that reproduces the main features of test particle simulations in the exact LH field and **replace the electron Newton equation in (z,t) by a Langevin equation in ($v_{//}$).** Two essential points are to have correct initial expansion rate towards higher energies, plus the stochastic boundary that leads to saturation of the wave absorption.

Transition from Newton to Langevin representation

- **Fundamental (TEM) mode:**

$E_z(z,t) = E_0 \cos[\omega t - \Phi(z)]; \qquad \Phi(z)$ is $\pi/2$ waveguide phasing

- **Electron diffusion in E_z- field:**

$$D = < \Delta v_{//}^2 > /2t = (q^2/m^2)(1/2t)\iint dt'dt'' < E(z',t')\,E(z'',t'') >$$

Integrating over unperturbed trajectories $z=v_{//}t$ gives $\mathbf{D_{ql}=|v_{//}|\, v_q^2/2d}$

- **Corresponding QL Fokker-Planck operator:**

$$(\partial/\partial v_{//})D_{ql}(\partial f/\partial v_{//}) \equiv -(\partial/\partial v_{//})F_{ql}f + (\partial/\partial v_{//})^2 D_{ql}f\,; \qquad F_{ql} = \partial D_{ql}/\partial v_{//}$$

- **Equivalent Langevin equation:**

$$\Delta v_{//} = F_{ql}\, dt + \sigma\sqrt{2D_{ql}\, dt}\,; \qquad <\sigma> = 0, \quad <\sigma^2> = 1$$

Physical model : numerical method

At every time step, we calculate the force on each particle.

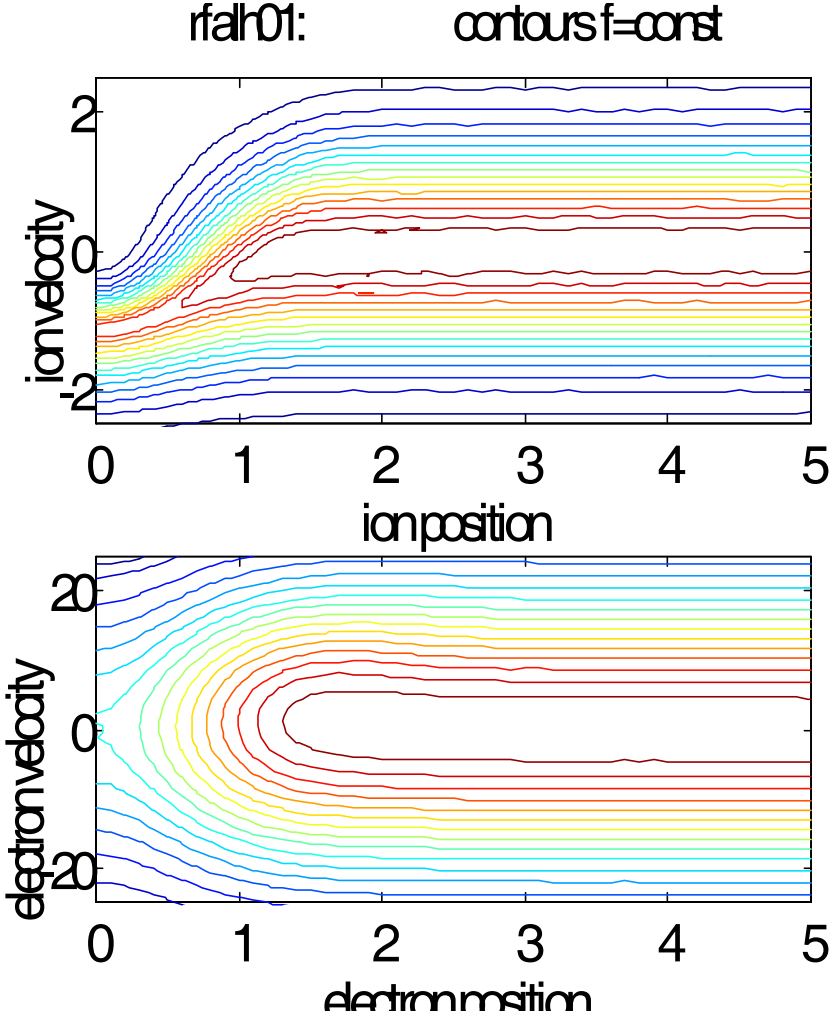
The electrons in front of the grill are given a small random kick in phase space. In addition, they feel the quasineutral electric field that arises in order to balance the pressure gradient and average RF friction force due to the *sum* of all the small RF kicks.

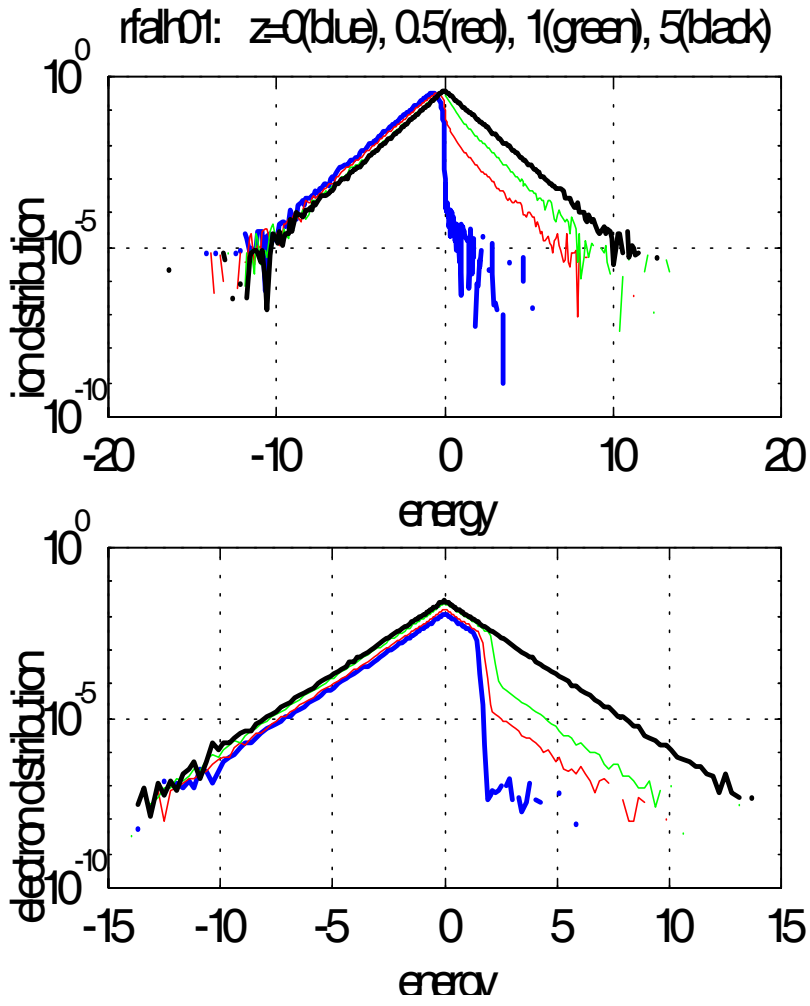
$$\frac{\partial u_e}{\partial t} = \left(\frac{\Delta u_{RF}}{\Delta t} \right) + \left(\frac{1}{m_e n_i} \frac{\partial n_i T_e}{\partial z} + \frac{\left\langle \Delta u_{e,RF} \right\rangle}{\Delta t} \right)$$

The ions only feel the quasineutral electric field. They do not receive small random kicks.

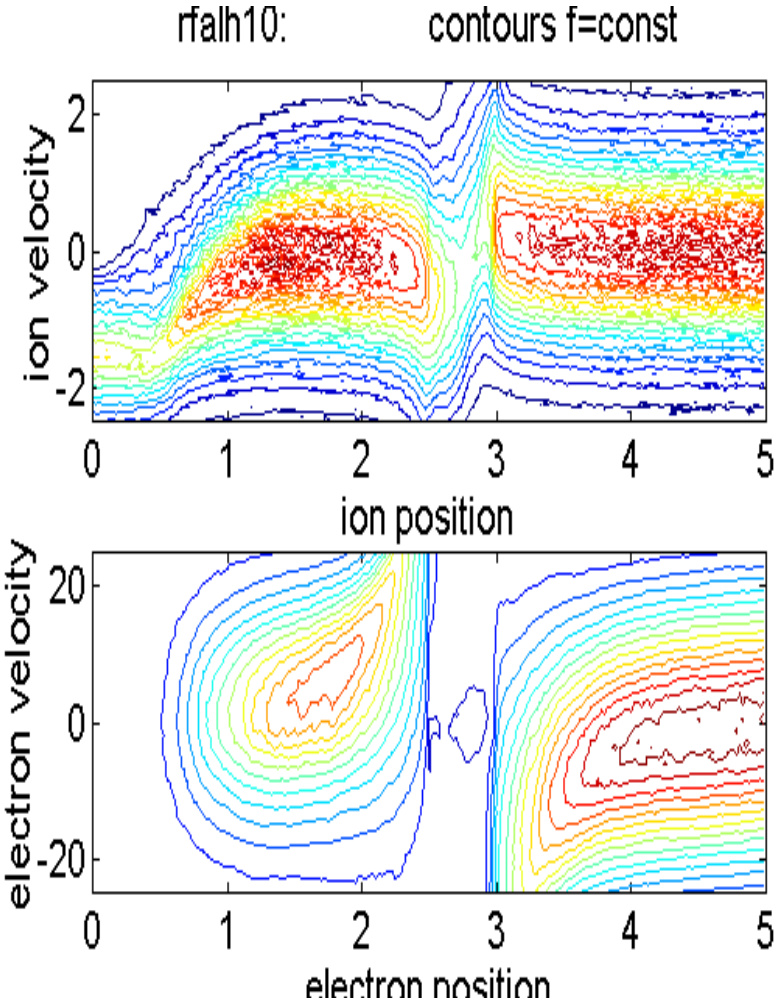
$$\frac{\partial u_i}{\partial t} = -\left(\frac{1}{m_i n_i} \frac{\partial n_i T_e}{\partial z} + \frac{\left\langle \Delta u_{e,RF} \right\rangle}{\Delta t} \right)$$

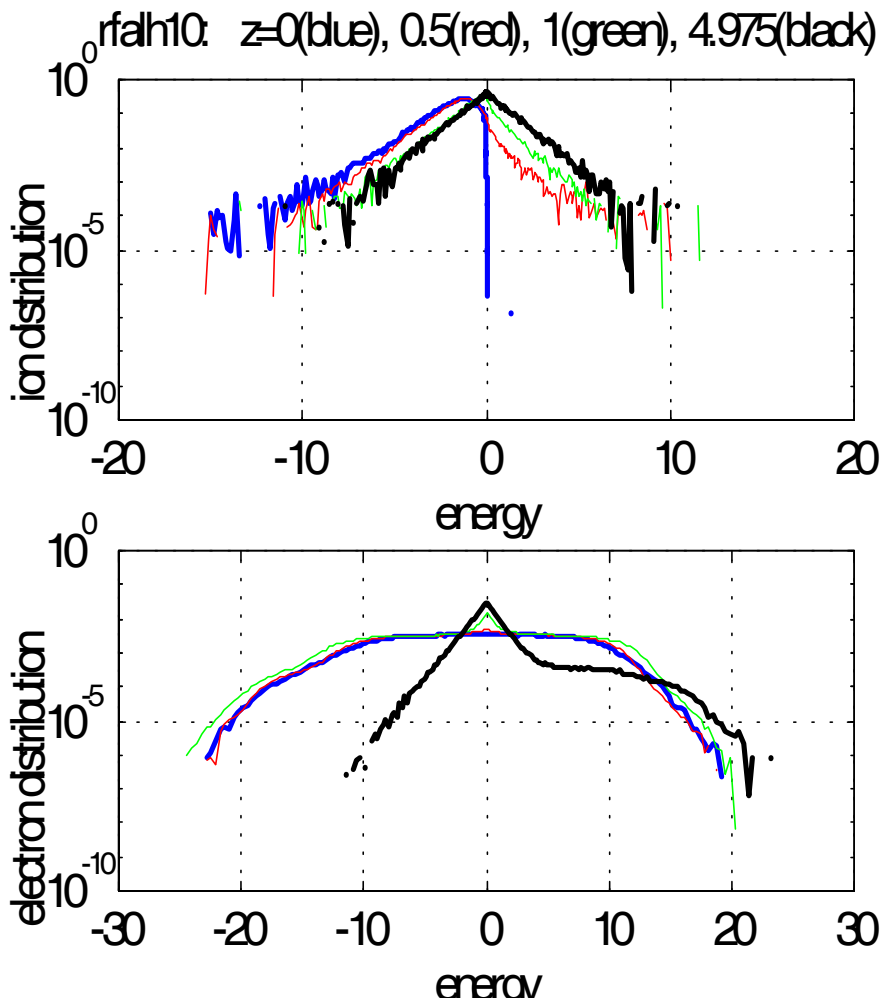
thermal case

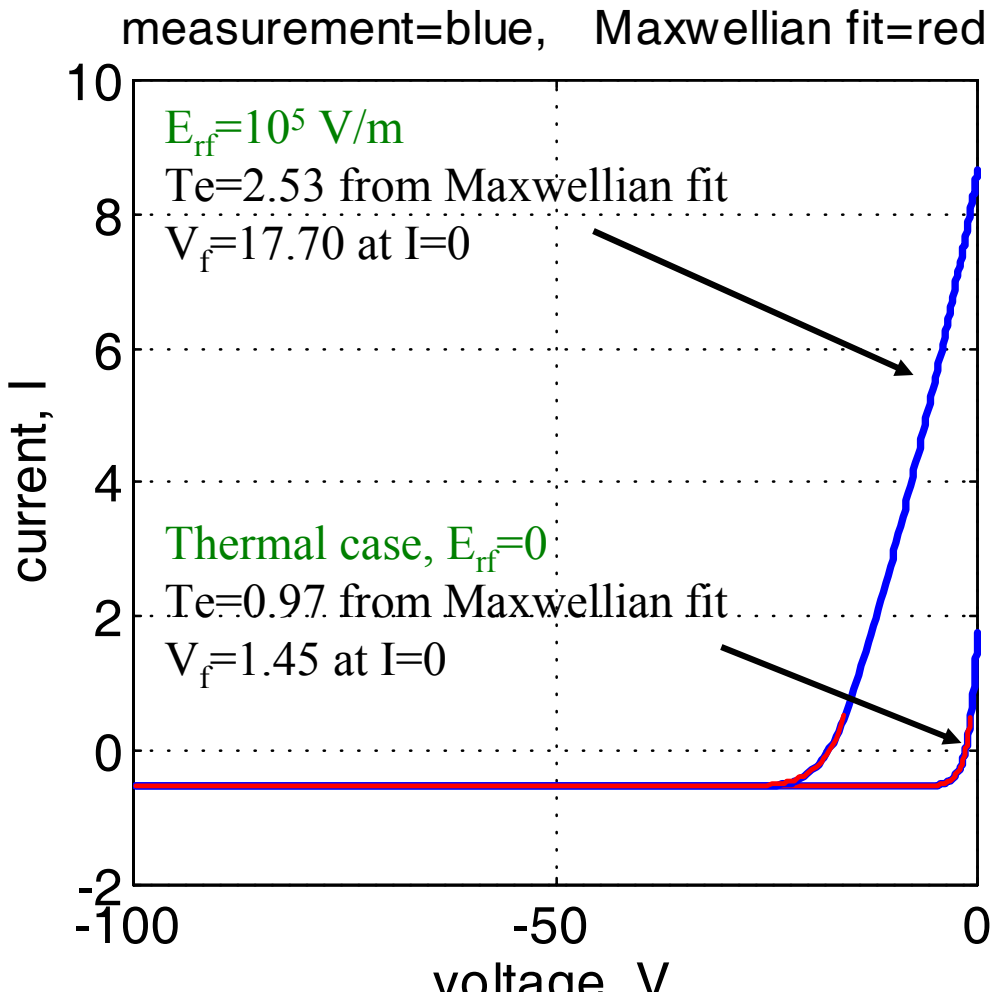


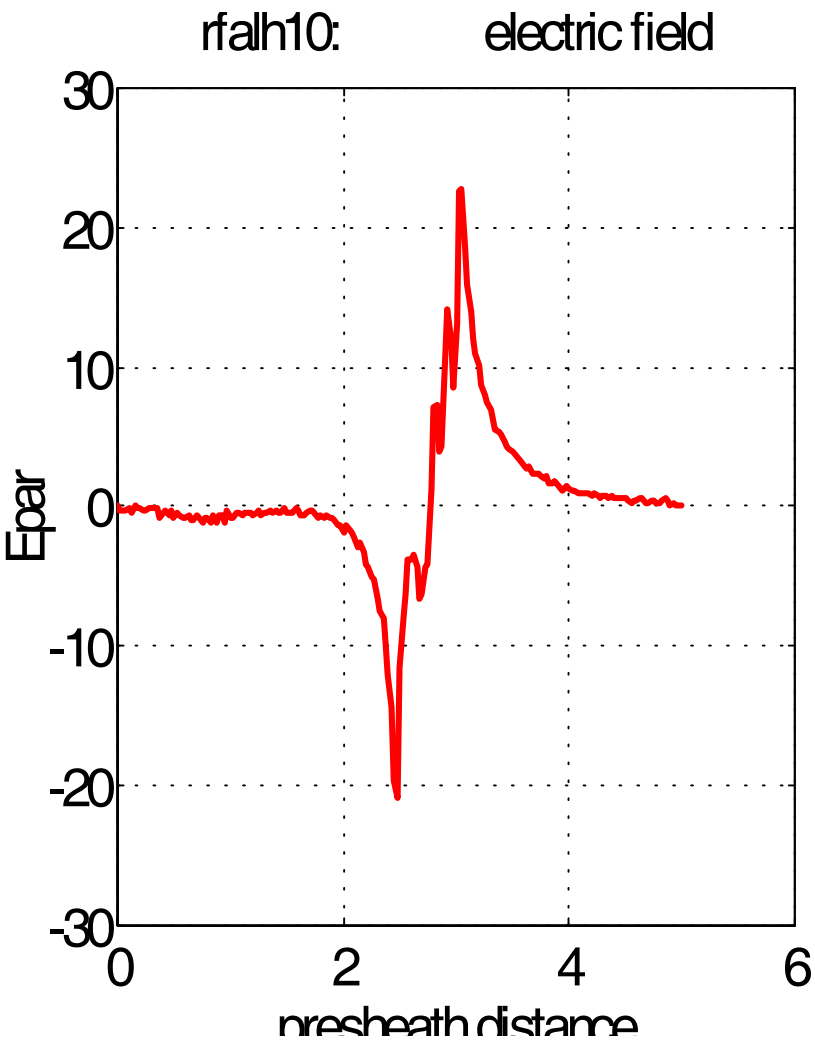


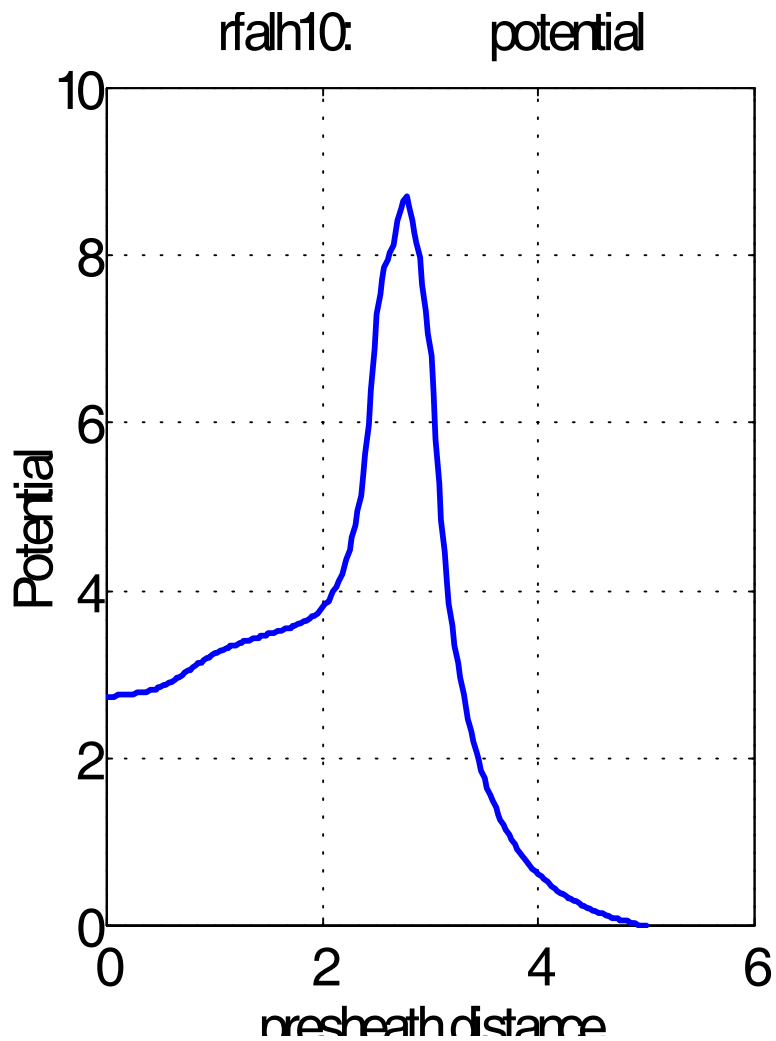
E_{RF}= 1 kV/cm

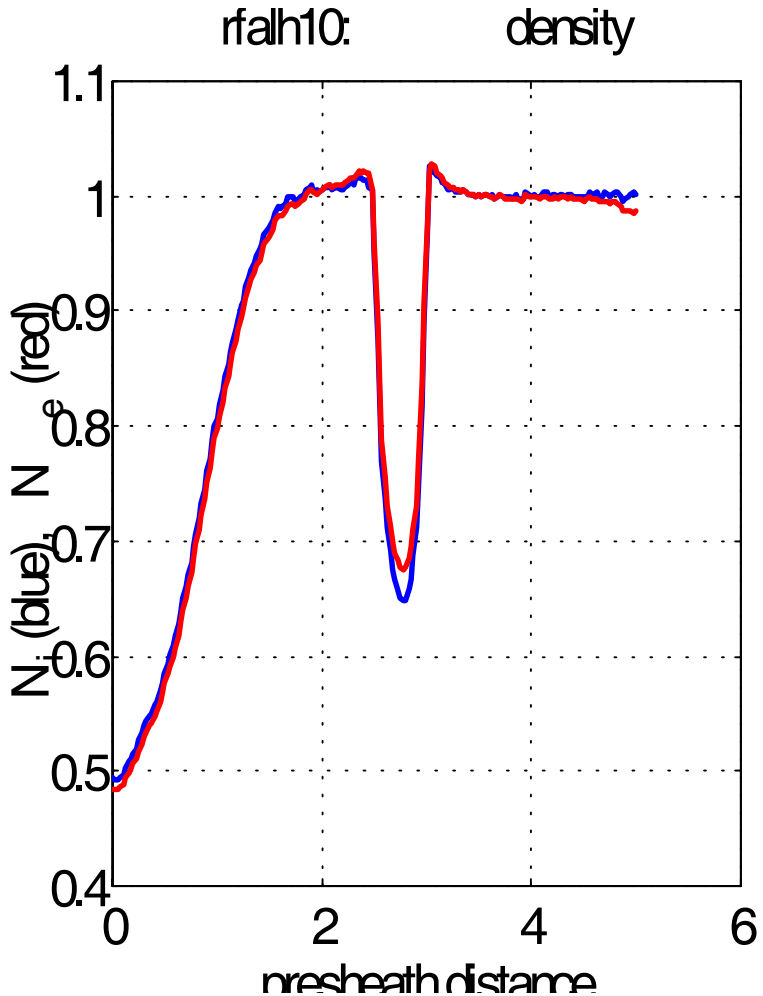

rfalh10: contours f=const
ion velocity
ion position
electron velocity
electron position

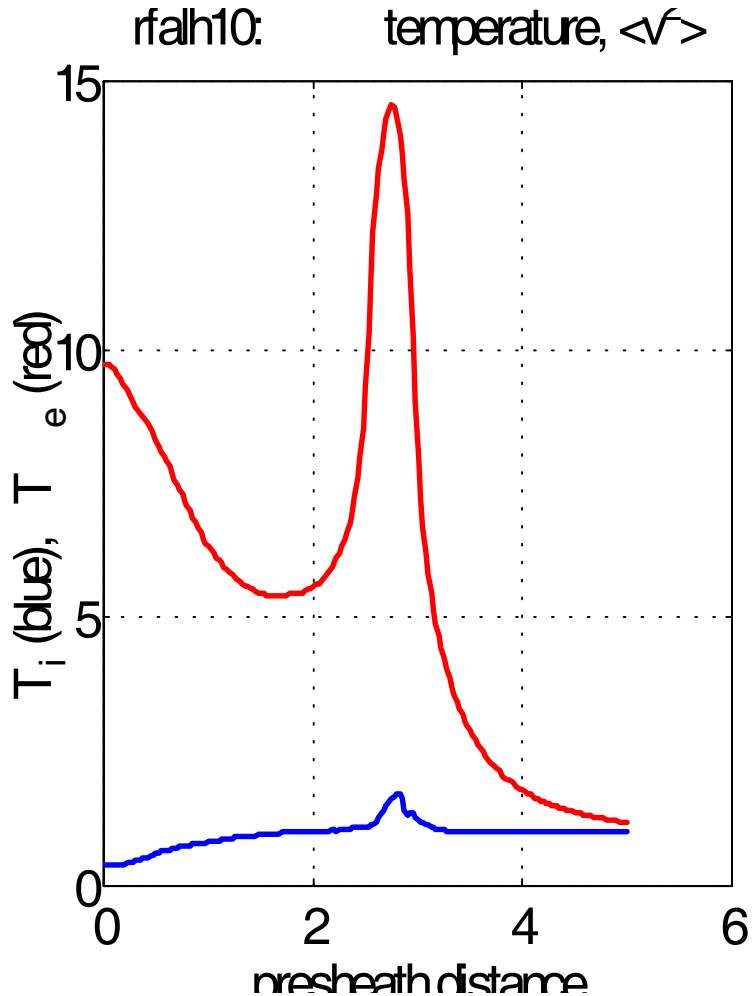

rfalh10: z=0(blue), 0.5(red), 1(green), 4.975(black)
ion distribution
energy
electron distribution
energy


measurement=blue, Maxwellian fit=red
$E_{rf}=10^5$ V/m
Te=2.53 from Maxwellian fit
V_f=17.70 at I=0
Thermal case, $E_{rf}=0$
Te=0.97 from Maxwellian fit
V_f=1.45 at I=0
current, I
voltage, V
10
8
6
4
2
0
-2
-100
-50
0

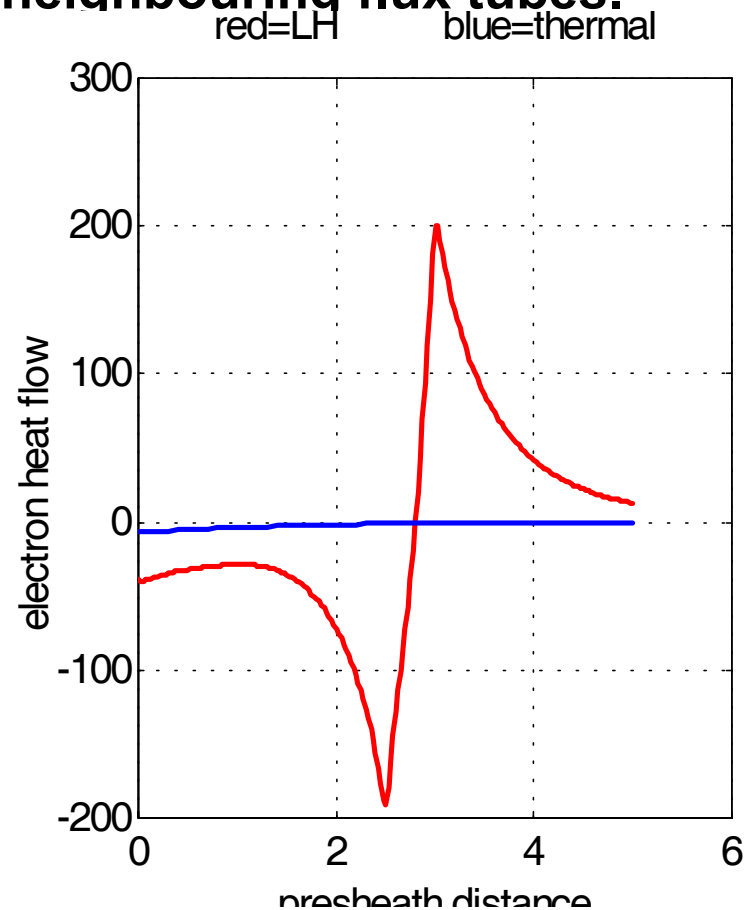

rfalh10: electric field
Epar
presheath distance
30
20
10
0
-10
-20
-30
0
2
4
6

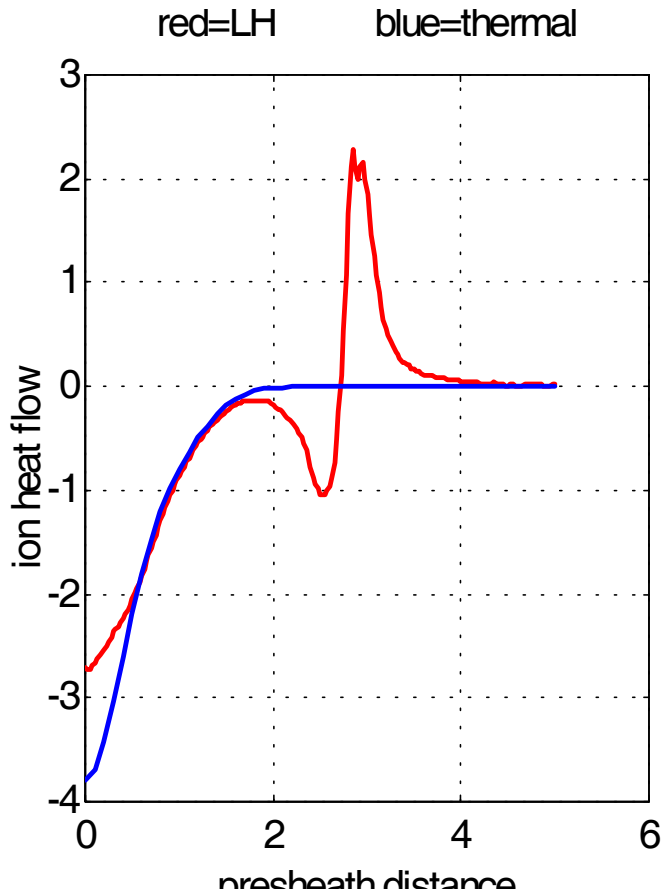

rfalh10: potential
Potential
presheath distance
10
8
6
4
2
0
0
2
4
6


rfalh10: density
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0
2
4
6
N_i (blue), N_e (red)
presheath distance


rfalh10: temperature, <v⊥>
15
10
5
0
0
2
4
6
T_i (blue), T_e (red)
presheath distance

The self-consistent LH-SOL interaction generates both ion and electron heat flows which decay due to exchange with thermal plasma on neighbouring flux tubes.





Conclusions

We have shown that the QPIC method can be applied to macroscopic SOL problems by benchmarking our code with respect to kinetic problems from the literature.

The first fully self-consistent simulations of localized electron heating in the SOL, source terms, and real target plate boundary conditions are underway.

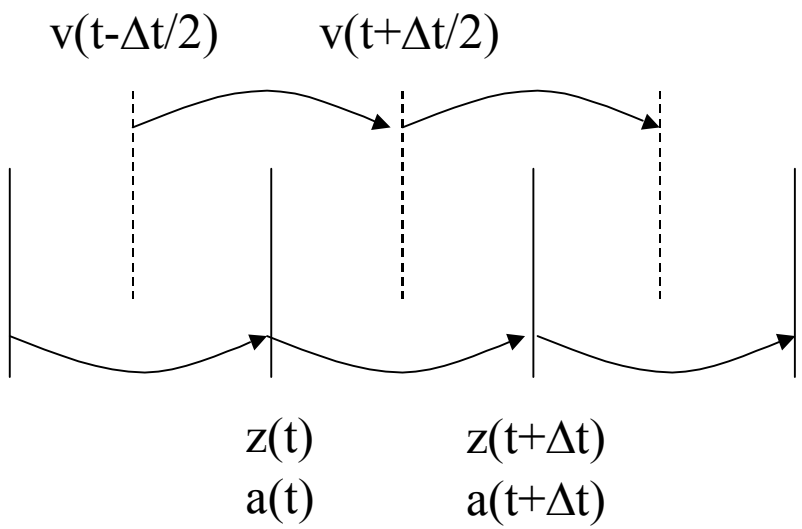
The QPIC method opens the door to a broad range of new kinetic SOL problems using realistic characteristic time and length scales.

Near term work includes the addition of weak Coulomb collisionality and neutral recycling (main ions and impurities).

Leapfrog integrator for eqs of motion $\dot{v} = a(t,z) \quad ; \quad \dot{z} = v$

$$v_{n+1/2} = v_{n-1/2} + \Delta t\, a_n \quad ; \quad z_{n+1} = z_n + \Delta t\, v_{n+1/2}$$

If the force acting on particles does not depend on velocity then exact time-centering is achieved by splitting the time level :



However, the force in QPIC has an **explicit dependence on velocity due to the electron pressure term⇒ a different method is needed ! We use the approximately time-centered 2nd order Runge-Kutta method**

Necessary condition for numerical stability

An integration scheme is numerically stable if perturbations, such as round-off errors, do not grow in the integration process. If there is no inherent damping or instability in the physical system, then phase-space area in (v,z) should be preserved. Any integration scheme takes the general form of a mapping of (v_n,z_n) on (v_{n+1},z_{n+1})

$$v_{n+1} = f(v_n, z_n; \Delta t) \quad ; \quad z_{n+1} = g(v_n, z_n; \Delta t)$$

Area is preserved during iterations if the Jacobian is unity, i.e. if

$$J = \det \begin{pmatrix} \frac{\partial f}{\partial v_n} & \frac{\partial f}{\partial z_n} \\ \frac{\partial g}{\partial v_n} & \frac{\partial g}{\partial z_n} \end{pmatrix} = 1$$

Area preservation for the LF and RK schemes

Leapfrog (LF): Recalling that a=a(z,t), we obtain $\mathbf{J_{LF} = 1}$

Runge-Kutta (RK): Let also a=a(z,t). Then $\mathbf{J_{RK} = 1+\Delta t^2(\partial a/\partial z)}$

Both the basic and midpoint RK schemes can be, however, implemented in area-preserving form so that $J_{RK} = 1$:

We exploit the particular property of equations of motion which allows without additional computation to first evaluate the new velocity v_{n+1} and then use that in the position equation instead of the first order corrected velocity $v_n + \Delta t\, a_n$, i.e. for z_{n+1} we take

$$z_{n+1} = z_n + \Delta t\left[v_n + v_{n+1}\right]/2$$

Origin of instability in finite difference schemes

A finite difference scheme does not have the same normal modes as the exact differential equation. Consider again the example of the linear oscillator $a = -z\omega_0^2$. The time-centered LF scheme leads to

$$z_{n+1} - 2z_n + z_{n-1} = -\Delta t^2\, \omega_0^2\, z_n$$

whose eigenvalues satisfy $\lambda_1\, \lambda_2 = 1$ so that the eigenfunctions have the form $\zeta_n = \exp(\pm in\omega\Delta t)$, where ω is in general complex.
The resulting dispersion relation for ω is

$$\sin\left(\tfrac{1}{2}\omega\Delta t\right) = \tfrac{1}{2}\omega_0\Delta t \qquad \text{(DR)}$$

This implies that ω is real, i.e. stable, when $\omega_0\,\Delta t < 2$.

Moreover, (DR) also gives a phase shift which can be different for various schemes which otherwise have the same stability.

Characteristic equation for the LF and RK schemes

For all the schemes discussed so far we obtain

$$\lambda^2 - 2\lambda(1+\Gamma) + J = 0 \quad ; \quad \Gamma = \tfrac{1}{2}\Delta t^2 (\partial a/\partial z)$$

where J is the Jacobian. The parameter Γ has a simple physical meaning. For example, for the linear oscillator $a = -z\omega_0^2$, so that $\Gamma = (\Delta t\, \omega_0)^2/2$

The two roots λ_1 and λ_2 obviously satisfy $\lambda_1\lambda_2 = J$. We recall that **J=1 for the LF and the area preserving RK schemes**, whereas $J=1+\Gamma^2$ for the usual RK scheme. Hence the usual RK methods are unconditionally unstable, but the LF and area-preserving RK schemes have the **stability domain $0 < -\Gamma < 2$** in which the two roots λ_1 and λ_2 are complex conjugate and **$|\lambda|=1$**.

Numerical example: electrons interacting with a nonlinear propagating wave

In this example a first integral exists in the wave reference frame plus a trapped electron should trace the orbit indefinitely

$$\ddot{z} = \omega v_q \cos(\omega t - kz) \quad \Rightarrow \quad v'^2 = v'^2_0 + U_0(\sin kz' - \sin kz'_0)$$

where $v_q = \frac{eE_0}{m\omega}$, $U_0 = \frac{2\omega v_q}{k}$ and $z' = z - \frac{\omega t}{k}$; $v' = v - \frac{\omega}{k}$

We choose initial conditions $v'_0=0$ and $z'_0= \pi/6$ inside the **separatrix**

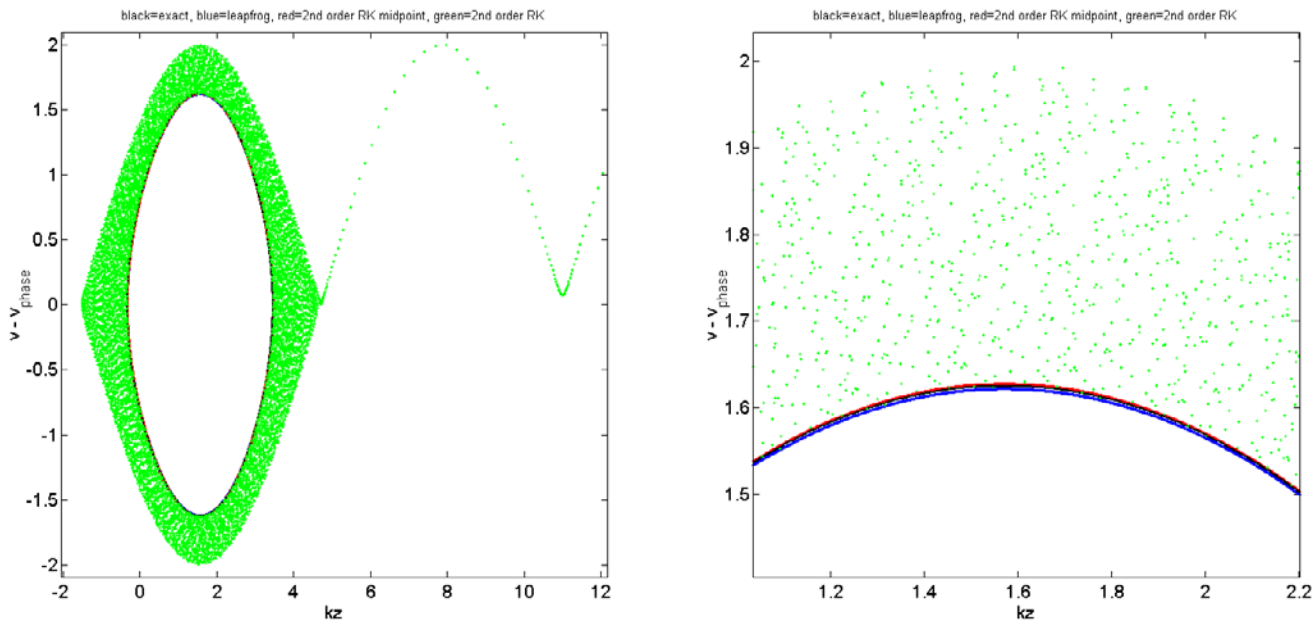
$$v'^2_S = U_0(1+\sin kz')$$

For the wave we choose E_0 = 3 kV/cm, f_{LH} = 3.7 GHz and take the first harmonic m=1 of the LH grill spectrum $k_m = \pi(1+4m)/2d$.

Results for trapped orbits: **green = 2nd order RK**, black = exact, red = 2nd order RK midpoint, blue = leapfrog

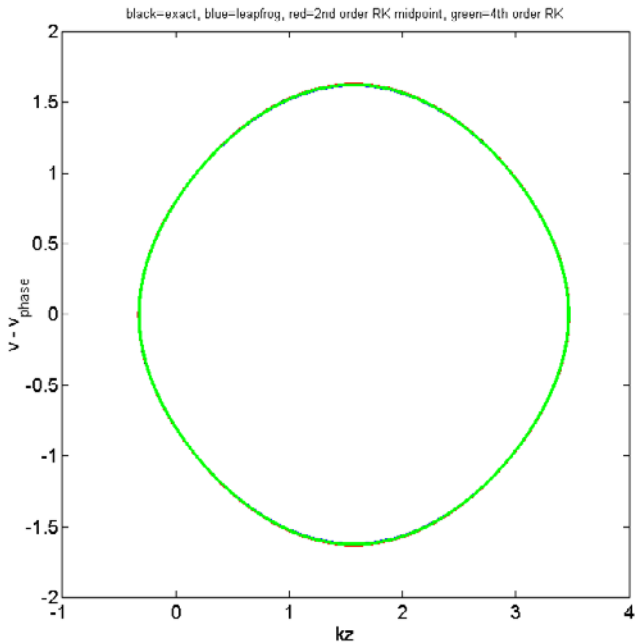
Using normalized units: $t \rightarrow \omega t$, $v \rightarrow (v - v_{phase})/v_q$, $z \rightarrow kz$,

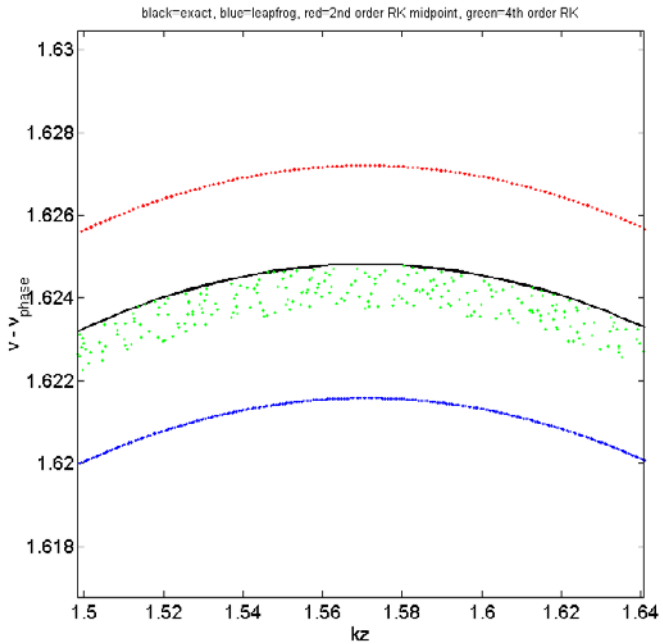
$$v_0 = 0.2, \quad |\Gamma| \approx (\Delta t^2/2) = 0.01$$



Results for trapped orbits: **green = 4th order RK**, black = exact, red = 2nd order RK midpoint, blue = leapfrog

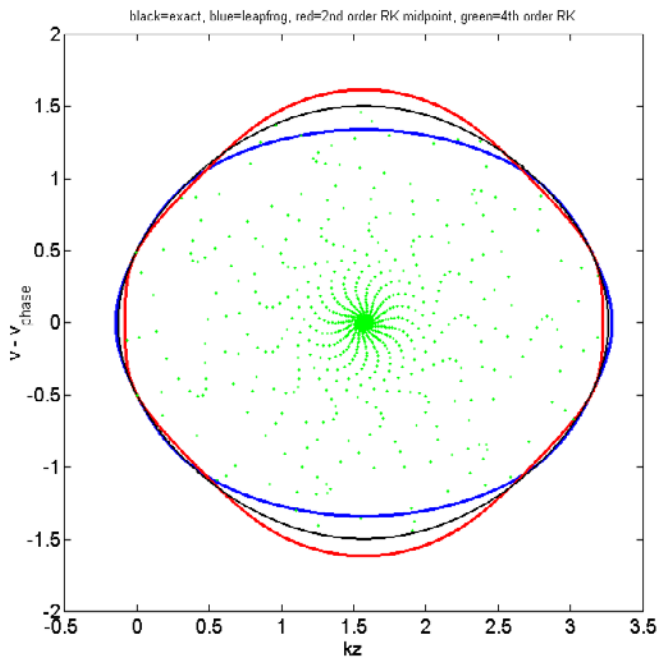
$$v_0 = 0.2, \quad |\Gamma| = 0.01$$



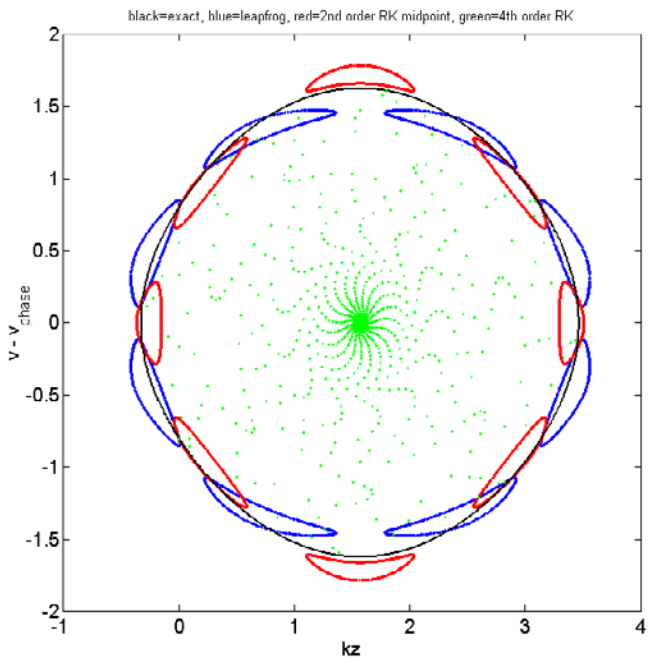


Results for trapped orbits: **green = 4th order RK**, black = exact, red = 2nd order RK midpoint, blue = leapfrog

$v_0 = 0.5$, $|\Gamma| = 0.5$



$v_0 = 0.2$, $|\Gamma| = 0.5$



Leapfrog and 2nd order RK midpoint perform equally well in terms of accuracy and stability. We use RK because it is best adapted to the QPIC force term (velocity dependence of pressure term).

$v_0 = 2.2, \ |\Gamma| = 0.4$