Modeling Electric Propulsion: Particle-in-Cell Simulations of Plasma Motion in Hall-effect and helicon double-layer thrusters

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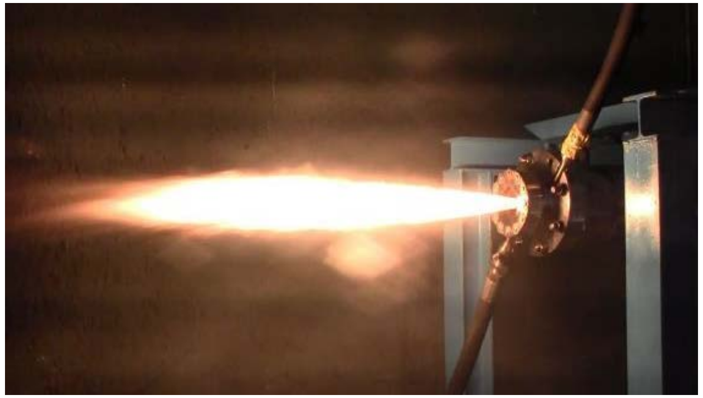
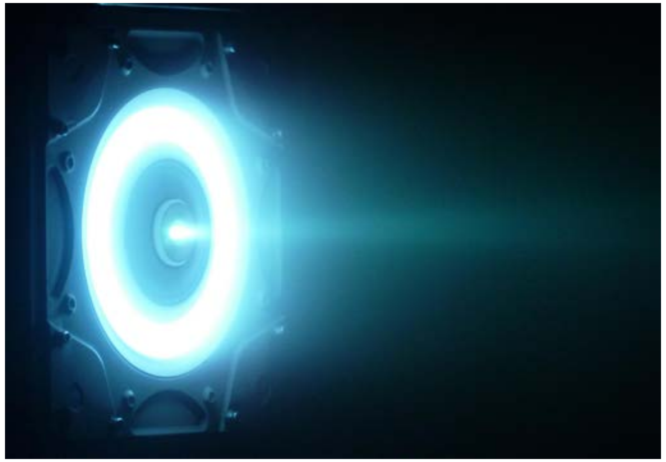
- UNINA-DII research group in Aerothermodynamics, Propulsion and Space Experimentation is coordinated by Prof Raffaele Savino
- In Space Propulsion, research activities are mainly related to chemical engines
  - **Hybrid propellant rockets**
  - **Monopropellant** rockets (H_2O_2, N_2O)
  - **CFD simulation** of rocket internal ballistics
  - Characterization of **high-temperature materials** for space propulsion
- An Aerospace propulsion **laboratory** is available inside the Military Airport in Grazzanise (CE) (http://www.dii.unina.it/index.php/it/laboratori-di-ricerca/259-laboratorio-di-propulsione-aerospaziale)



- Collaborations with AVIO, CIRA, T4i, CNR-ISSMC and several italian Universities, in ASI and ESA projects
- Currently a project is ongoing with ASI for the design of a miniature hybrid rocket for nanosatellites
- Recent interest towards electric propulsion
  - Proposal pending approval in collaboration with CIRA for the design of a low power Hall-effect thruster
  - Efforts for **modelling plasma motion in electric propulsion devices**

Introduction



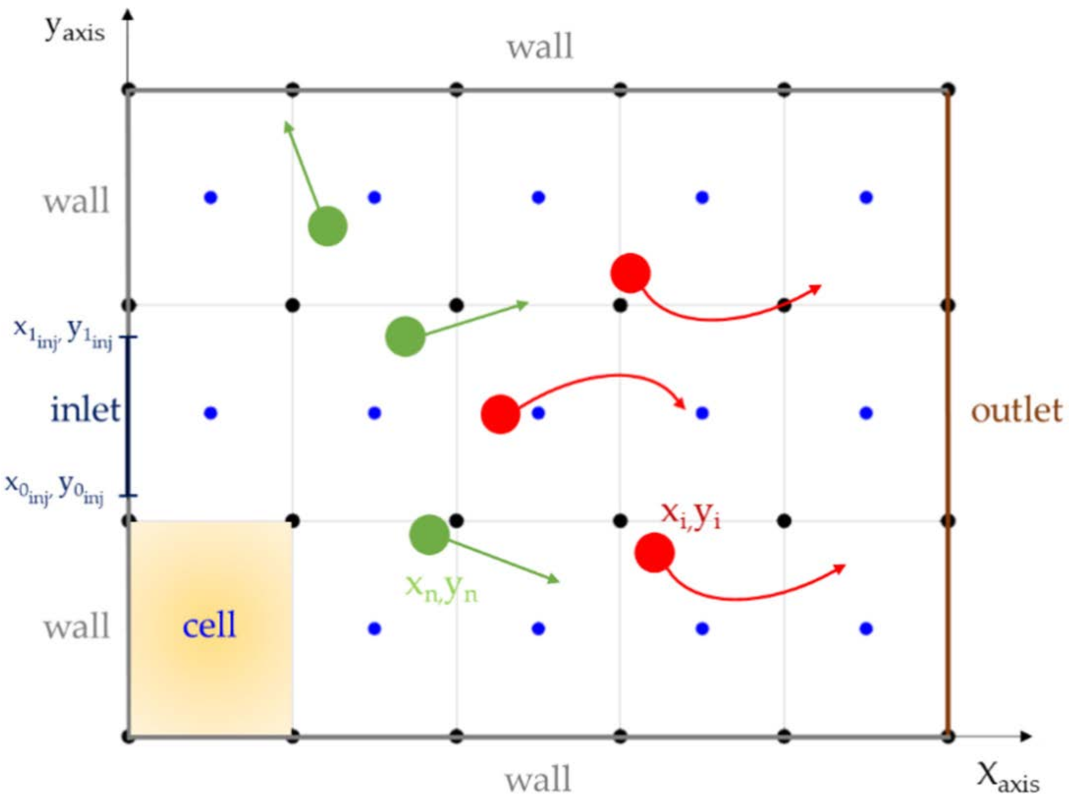
- Ever-increasing interest towards satellite electric propulsion
  - High specific impulse
  - Potentially long service life
- Need for dedicated **numerical tools** for EP simulation
  - Fluid models (electrons and ions treated as fluids)
  - Kinetic models (electrons and ions treated as macro-particles)
  - Hybrid models (electrons treated as fluids and ions as macro-particles)
- For hybrid models, **Particle-In-Cell (PIC)** treatment is used for ions, while for electrons two approaches are possible
  - Electromagnetic (full set of Maxwell equations) -> Suited for high-power thrusters (e.g. HET)
  - Electrostatic (Poisson equation) -> Suited for cathodeless thrusters (e.g. helicon double layer)
- Research is needed to
  - **Improve accuracy** of numerical schemes
  - Ensure **mass conservation** during ionization
  - Take advantage of **parallel computing** to reduce computational times

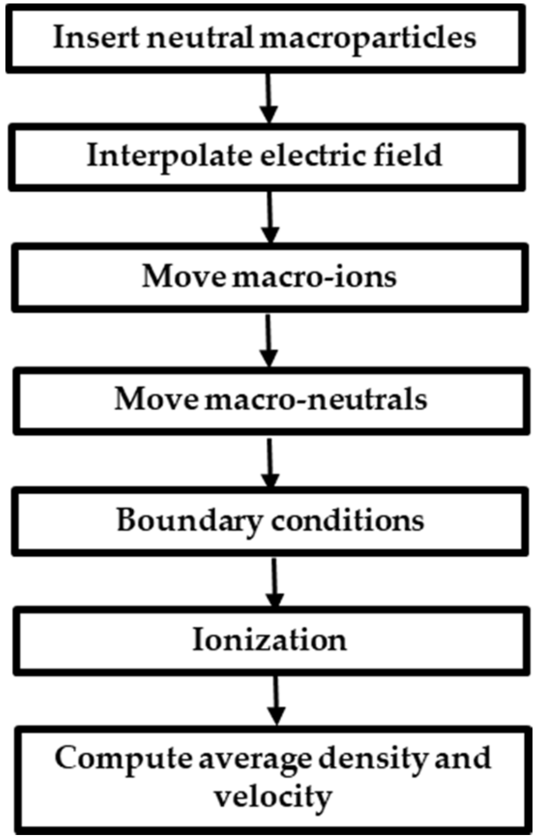
Objectives

- Development of a novel highly accurate **Particle-in-Cell (PIC**) scheme for the calculation of the macroparticle motion
  - Fourth order **Runge–Kutta** integration scheme, instead of the typically used leapfrog integration
  - **Cubic bi-spline interpolation** of the electric potential, instead of the typically used bi-linear interpolation;
  - A **new ray-tracing approach** to reflect the particles at the domain boundaries
  - A **new neutrals ionization scheme**
  - Use of **parallel programming on GPU**
- PIC implemented in Matlab
- Most demanding parts accelerated in CUDA
- Code validated and applied to:
  - Hall-effect Thrusters (2D)
  - Helicon Double-Layer Thrusters (1D)

Gallo, G.; Isoldi, A.; Del Gatto, D.; Savino, R.; Capozzoli, A.; Curcio, C.; Liseno, A. Numerical Aspects of Particle-in-Cell Simulations for Plasma-Motion Modeling of Electric Thrusters. *Aerospace* **2021**, *8*, 138. https:// doi.org/10.3390/aerospace8050138

Computational domain





- Constant electric potential (defined in nodes)
- Ions clustered in macro-particles
- Three kind of boundaries
  - Inlet
  - Wall
  - Outlet

Neutrals and Ion Macro-Particles Motion

Equations of motion for ions (i) and neutrals (n)

$$\frac{d\boldsymbol{u_i}}{dt} = \boldsymbol{a_i} = \frac{q_i}{m_i}\boldsymbol{E_i}$$
$$\frac{d\boldsymbol{x_{i,n}}}{dt} = \boldsymbol{u_{i,n}}$$

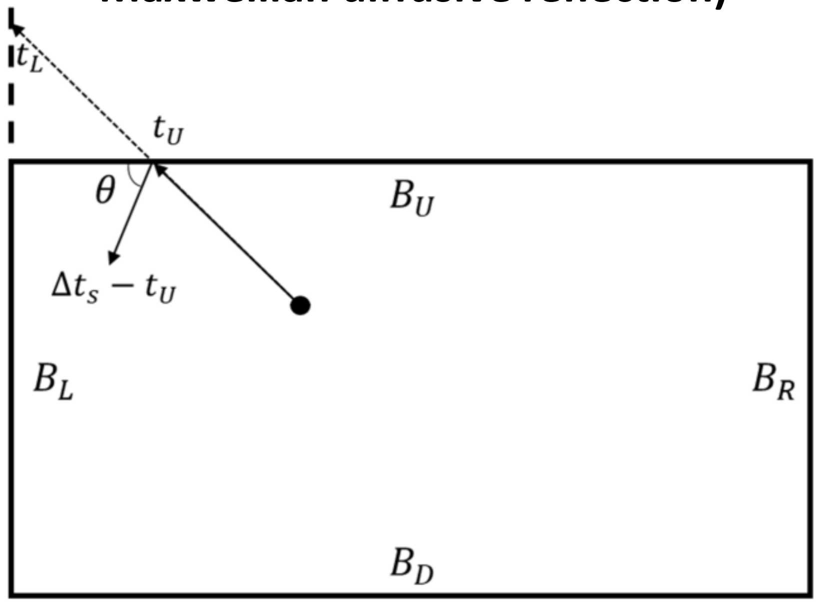
- Discretization by
  - Runge-Kutta 4th order (RK4) in time
  - Cubic bi-spline for electric field interpolation in space

$$x_{k+1} = x_k + \tfrac{1}{6}(\Delta x)_0 + \tfrac{1}{3}(\Delta x)_1 + \tfrac{1}{3}(\Delta x)_2 + \tfrac{1}{6}(\Delta x)_3$$
$$u_{k+1} = u_k + \tfrac{1}{6}(\Delta u)_0 + \tfrac{1}{3}(\Delta u)_1 + \tfrac{1}{3}(\Delta u)_2 + \tfrac{1}{6}(\Delta u)_3$$

$$\begin{aligned}
(\Delta x)_0 &= u_k \Delta t, & (\Delta u)_0 &= a_{x_k}\Delta t,\\
(\Delta x)_1 &= \left(u_k + \frac{(\Delta u)_0}{2}\right)\Delta t, & (\Delta u)_1 &= (a_{x_k} + a_{x_1})\Delta t,\\
(\Delta x)_2 &= \left(u_k + \frac{(\Delta u)_1}{2}\right)\Delta t, & (\Delta u)_2 &= (a_{x_k} + a_{x_2})\Delta t,\\
(\Delta x)_3 &= (u_k + (\Delta u)_2)\Delta t, & (\Delta u)_3 &= (a_{x_k} + a_{x_3})\Delta t,
\end{aligned}$$

$$\begin{aligned}
a_{x_k} &= \frac{q_i}{m_i}E_x(x_k),\\
a_{x1} &= \frac{q_i}{m_i}E_x(x_k + (\Delta x)_1),\\
a_{x2} &= \frac{q_i}{m_i}E_x(x_k + (\Delta x)_2),\\
a_{x3} &= \frac{q_i}{m_i}E_x(x_k + (\Delta x)_3),
\end{aligned}$$

Ray-tracing for outlet and walls (with Maxwellian diffusive reflection)



$$u = v_{mp}\sqrt{-\ln(R_1)}\cos\theta$$
$$v = v_{mp}\sqrt{-\ln(R_1)}\sin\theta$$
$$\theta = -\pi R_2$$

$$v_{mp} = \sqrt{2k_b T_w / m_i}$$

Injection

$$x_p = x_{0_{inj}} + R_3\left(x_{1_{inj}} - x_{0_{inj}}\right)$$
$$y_p = y_{0_{inj}} + R_3\left(y_{1_{inj}} - y_{0_{inj}}\right)$$

R_3 is a random number between 0 and 1
x_{0inj}, y_{0inj}, x_{1inj}, y_{1inj} are the endpoints of the injection inlet

Velocity computed as for reflection, with most probable speed at injection temperature

A total of 20 macroparticles per timestep is injected, balancing solution accuracy and computational effort

Ionization

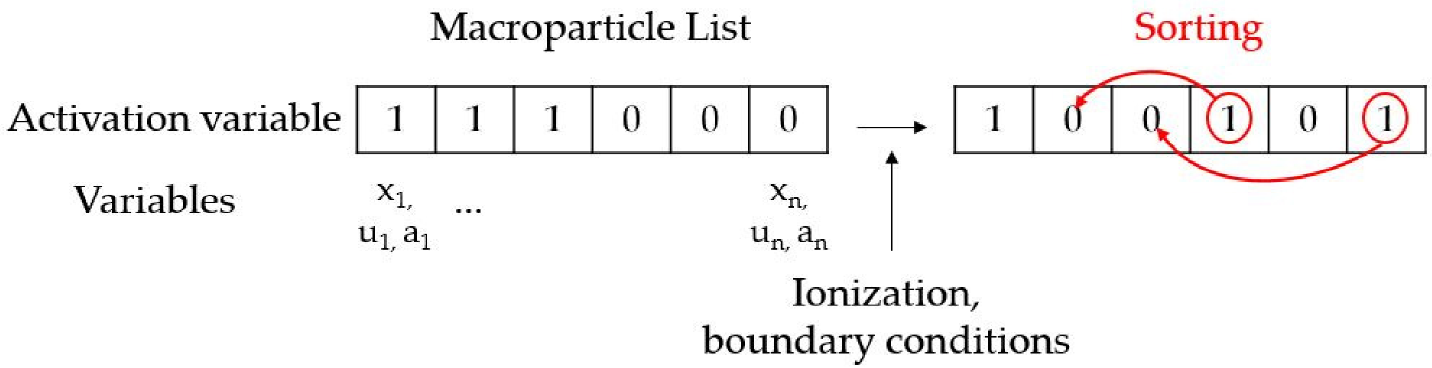
$$\dot{n}_i = \zeta(T_e)n_n n_i$$

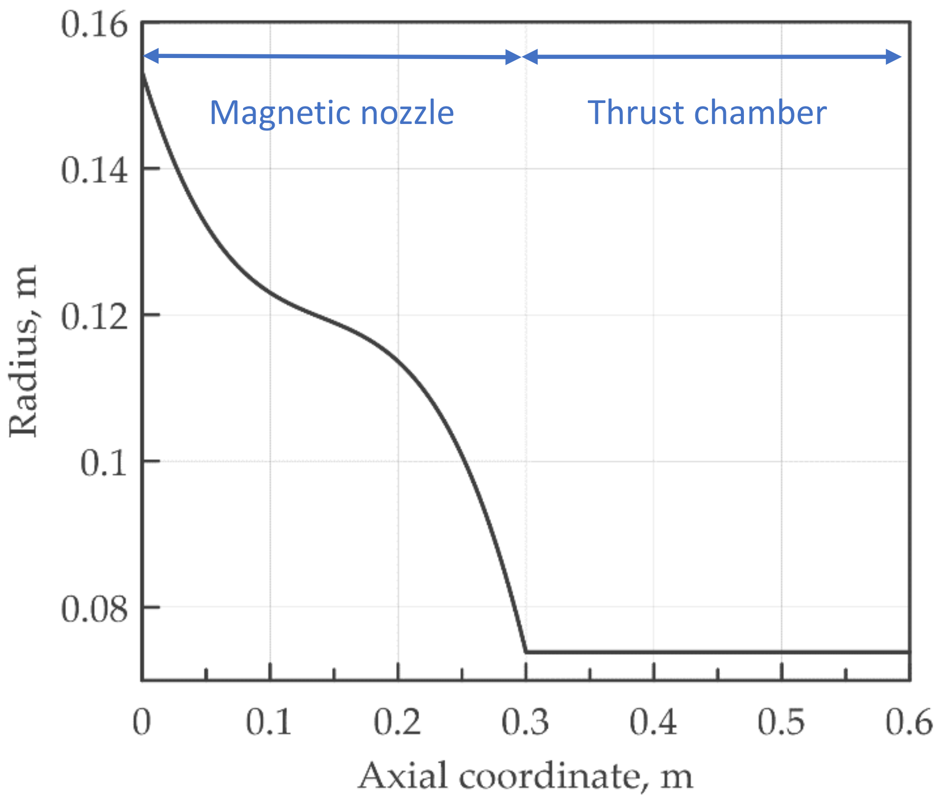
Ionization rate affected by electron temperature
Assumption of quasi-neutrality
Conservation of mass guaranteed by ad-hoc procedure

Computational strategy

- Approach implemented in Matlab for debugging and reference performance evaluation
  - Most time-consuming operations related to interpolation
- Most of parallelization carried out at high-level programming
- Only electric field interpolation implemented in CUDA

- Two independent lists of neutrals and ions generated at beginning of simulation and updated
  - 1 when injected, 0 when expelled
- Lists are sorted to cluster active particle at top
- CUDA kernels operate only on active particles, guaranteeing massive parallelism





Ionization rate (*SR*) and electron temperatures are inputs

Assumption of quasi neutrality no longer valid

$$\frac{\mathrm{d}\phi}{\mathrm{dx}}^2 = -\frac{\rho}{\varepsilon_0} \qquad \rho = q(n_i - n_e)$$

With Boltzmann approximation for electron density:

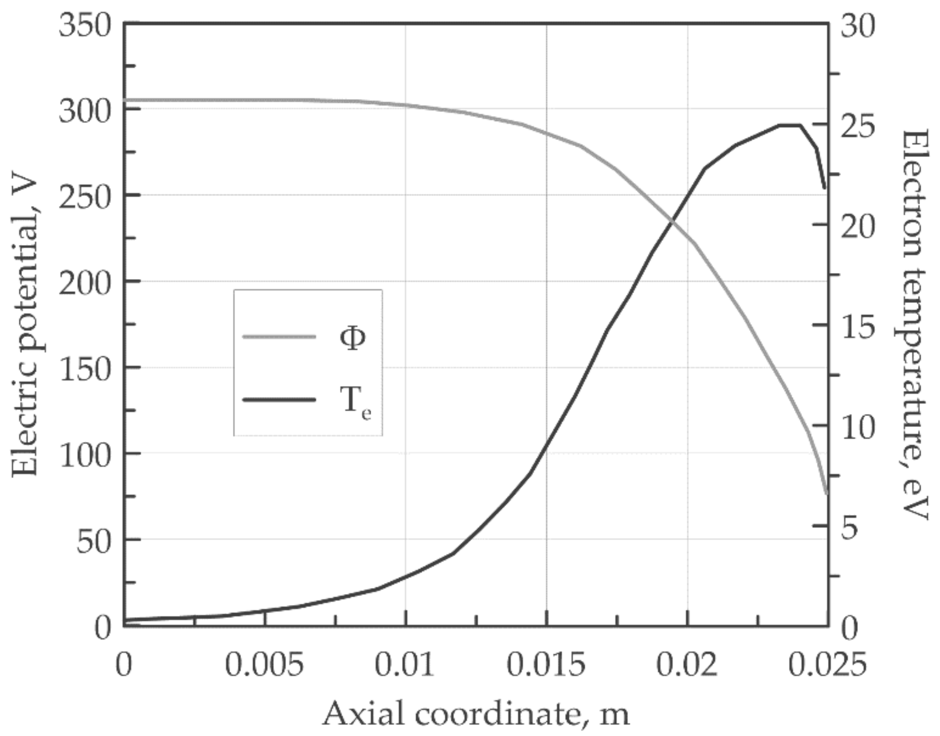
$$\frac{d^2\phi}{dx^2} = \frac{q}{\varepsilon_0}\left[n_0 e^{\frac{q\phi(x)}{k_b T_e}} \frac{r_{ch}^2}{r^2(x)} - n_i\right]$$

$$\phi(x=0) = 0, \ \ \phi(x=L) = 0$$

$$n_0 = \frac{\dot{n}_i}{v_e A_{exit}}$$ from the electron particle number balance equation

Ions are generated and moved by a 1D version of the PIC model
Solution is stopped when steady state is achieved

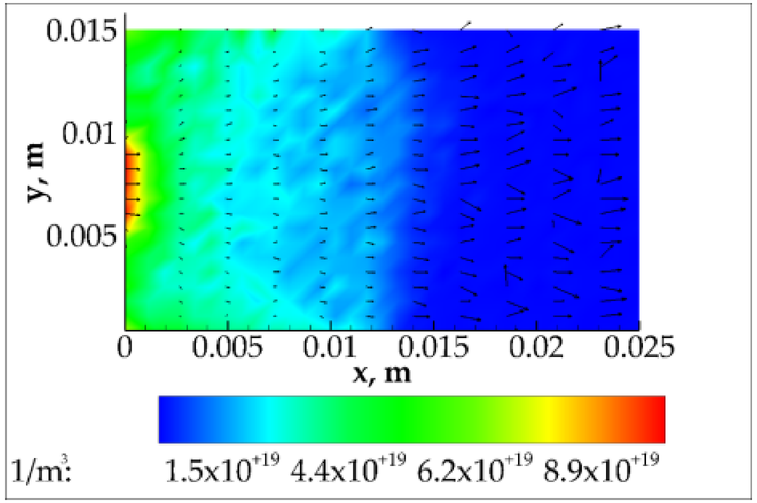
Domain: 0.025 x 0.015 m
Discretized by 34 x 22 nodes
Simulation time: 5×10^{-4} s
Time step: 5×10^{-8} s
Neutral injected mass flow rate: 5×10^{-6} kg/s
Wall temperature: 850 K
Inlet temperature: 750 K



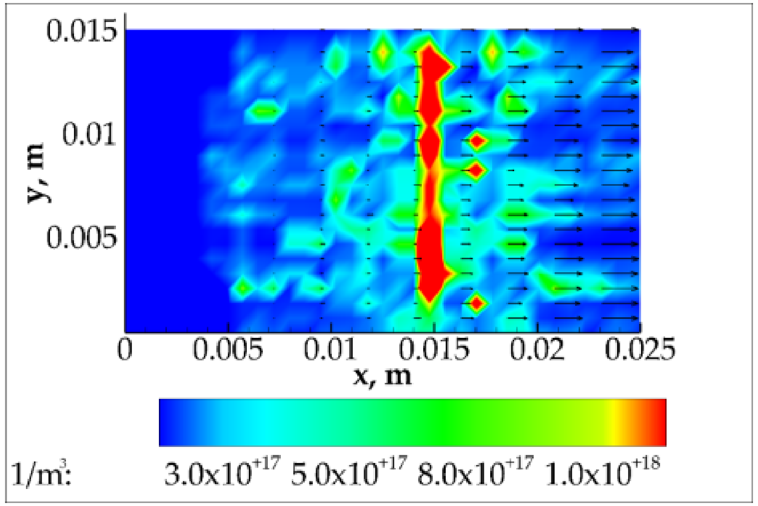
Assumed potential and electron temperature distributions

Hofer, R.R.; Mikellides, I.G.; Katz, I.; Goebel, D.M. Wall Sheath and Electron Mobility Modeling in Hybrid-PIC Hall Thruster Simulations. In Proceedings of the 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhhibit 8, Cincinnati, OH, USA, 8–11 July 2007

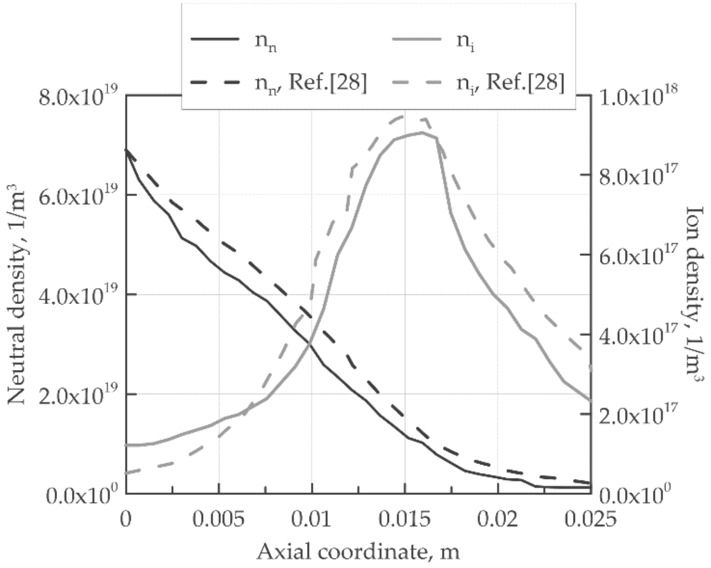
Particle density and velocity vectors



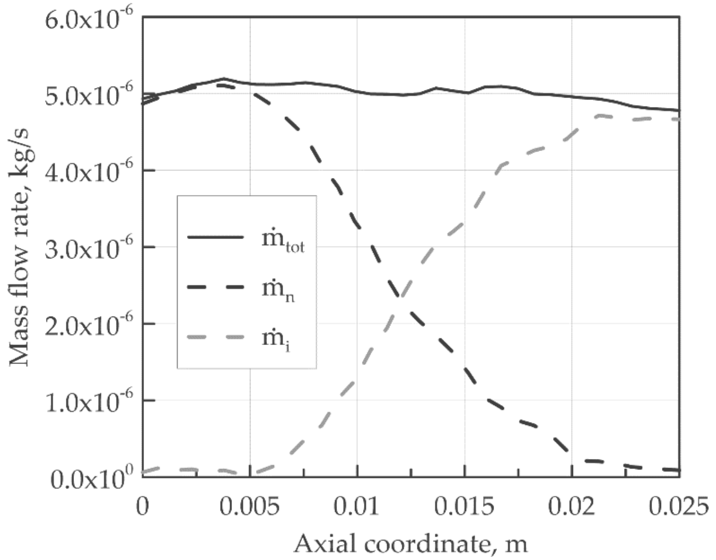
(a) Neutrals.



(b) Ions.

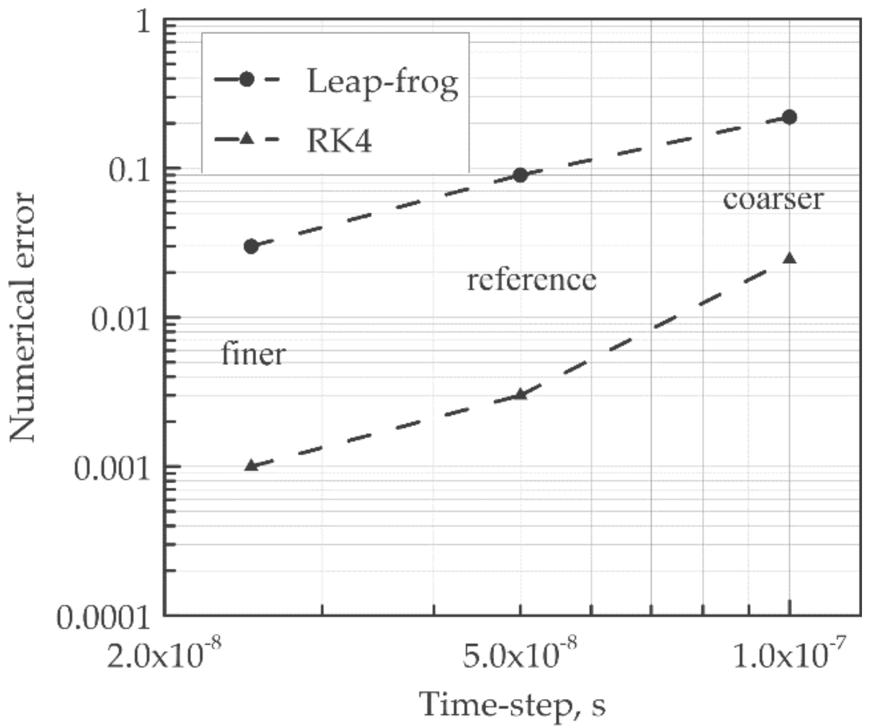


Good agreement with literature



Conservation of mass ensured

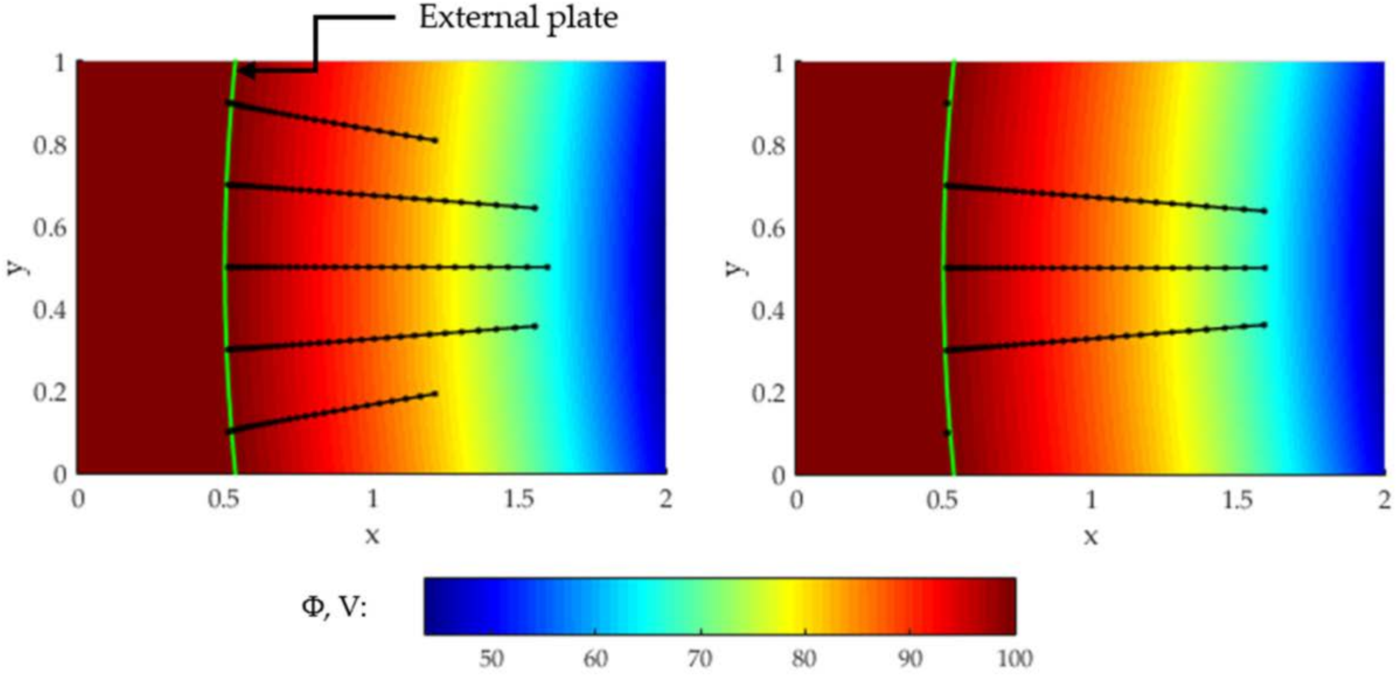
Effect of time integration scheme



Significant reduction of numerical error by RK4 time integration wrt conventional leap-frog

Effect of space interpolation of electric field

Example: capacitor with two circular concentric thin plates



(a) Linear interpolation. (b) Cubic bi-spline interpolation.

Cubic bi-spline interpolation overperforms bi-linear one in presence of highly non-linear and discontinuous electric field

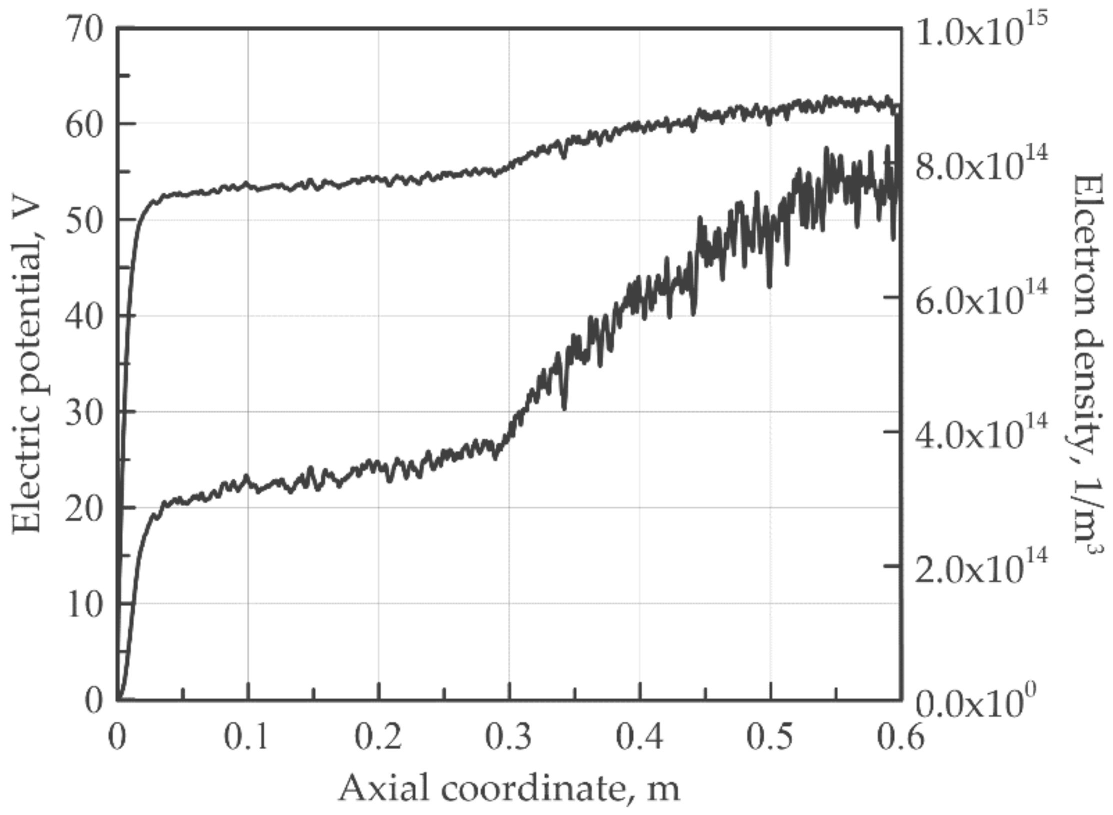
Results - Computational performance

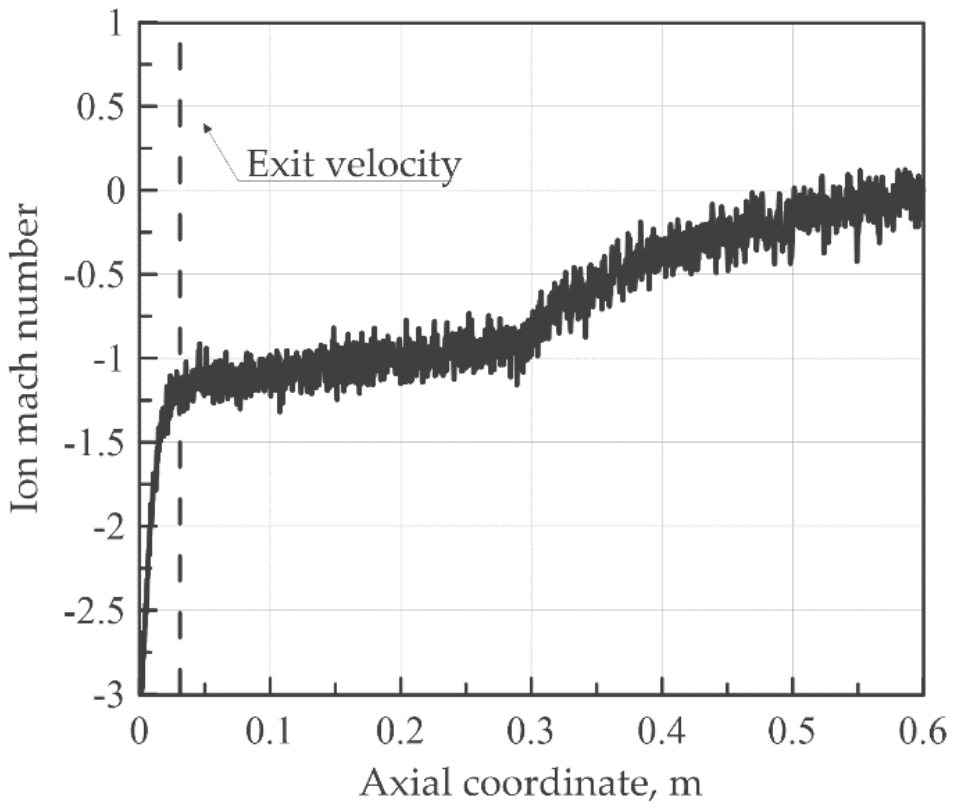
- Three versions of the new PIC model
  - **completely executed sequentially**, with all the macro-particle operations handled by using *for* loop
  - **CPU multi-core accelerated**, performing the operations for all the macroparticles in multi-core aware commands
  - **Accelerated on GPU**
- The sequential version took 1.5h to run a single timestep
- Most computational time is spent for time integration, electric field interpolation and neutral motion

	CPU Parallel, Min	GPU Parallel, Min	Computational Gain, %
Execution time	101.2	55.75	44.91
RK4	43.65	23.18	46.89
Cubic bi-spline interpolation	40.22	19.80	50.77
Neutrals motion	7.31	3.45	52.80

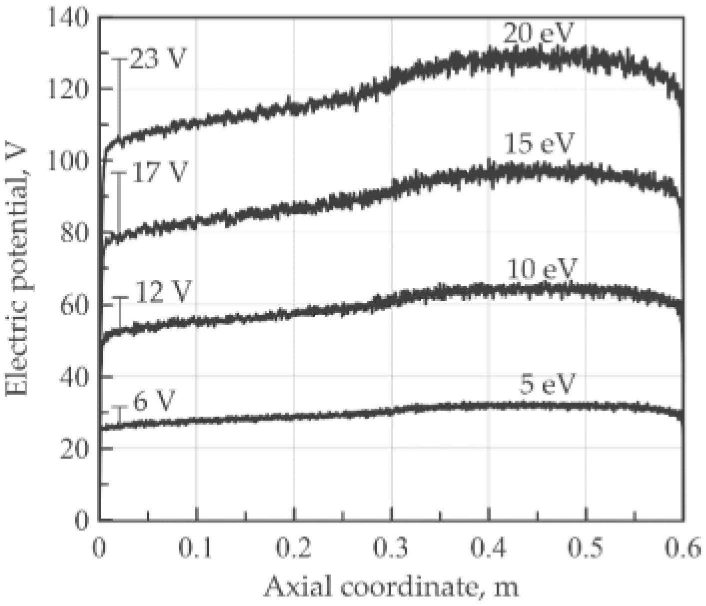
Domain discretized by 2000 nodes
150000 macro-particles
Computational time: 10 min

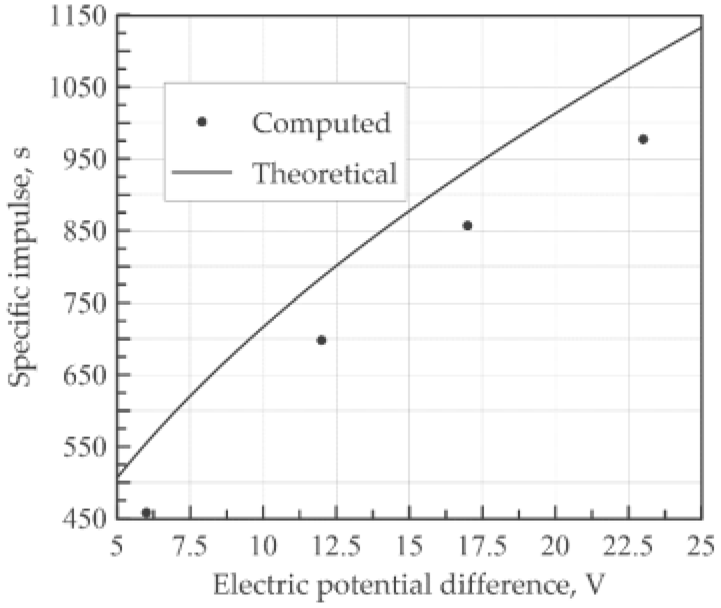
Test case with
Te = 10 eV
SR = 3 x 10^{16} ionized argon particles per second





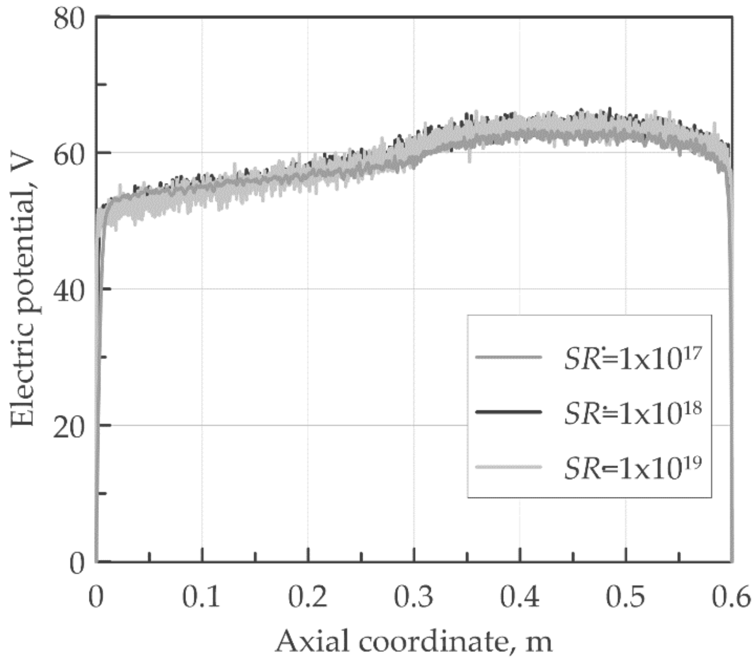
Effect of electron temperature





Te affects space averaged potential and voltage drop
Voltage drop affects specific impulse

Effect of ionization rate



No major effects on potential
Thrust increases linearly with ionization

Effect of gas composition

Gas	Molecolar Weight, g/mol	Ionization Rate, Part/s	Potential Drop, V	Specific Impulse, s	Thrust, mN
Argon	39.95	1×10^{18}	12.5	698	0.45
Iodine	126.90	3×10^{17}	12.5	352	0.22

Summary and conclusions

- Fast and accurate in-house particle-in-cell code developed for HET and Helicon thrusters simulation
- High-accuracy numerical schemes for time integration and electric field interpolation were introduced
- 2D full PIC model for Hall-effect thrusters validated versus literature
  - RK4 scheme substantially improves solution accuracy
  - Cubic bi-spline interpolation can fix unphysical accelerations in presence of electric field discontinuities
- Computational strategy introduced by GPU acceleration
  - Gain by 44.91% wrt multi-core CPU options
- Parametric studies on 1D helicon double-layer thrusters modelling
  - Electron temperature affects potential drop and therefore specific impulse
  - Ionization rate has no major effects
  - Heavier propellants degrade performance
- Future developments may include extension to non-cartesian or 3D geometries, or improvement in plasma modelling

Thanks for your attention!

Questions?