Modelling of low-temperature plasmas:
electron and chemical kinetics

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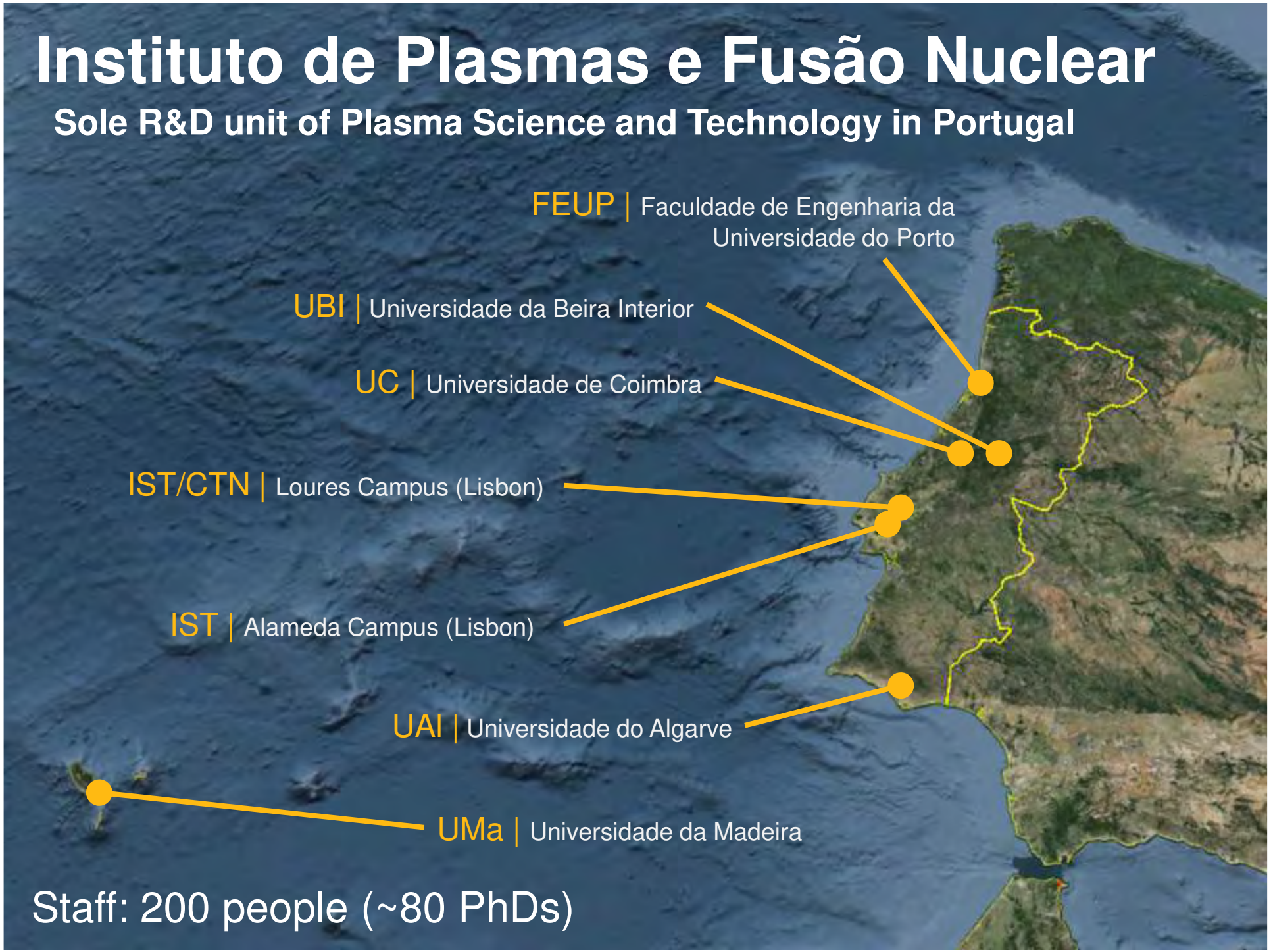
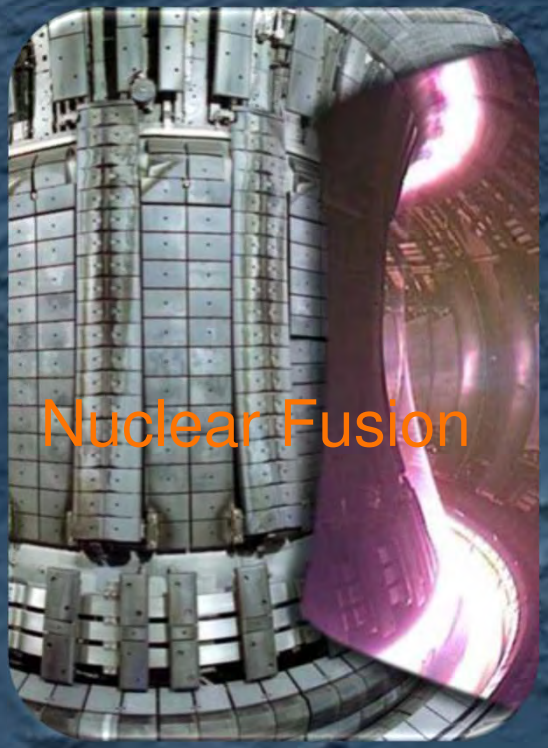
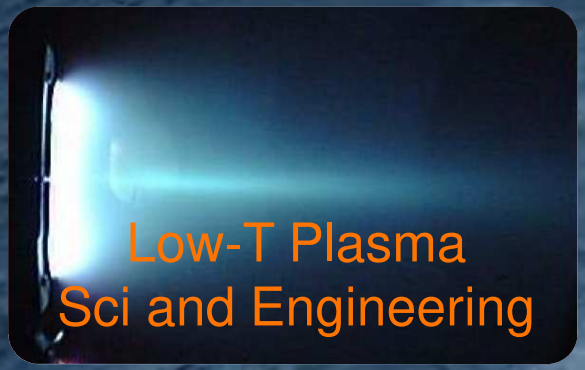

Instituto de Plasmas e Fusão Nuclear
Sole R&D unit of Plasma Science and Technology in Portugal
FEUP | Faculdade de Engenharia da Universidade do Porto
UBI | Universidade da Beira Interior
UC | Universidade de Coimbra
IST/CTN | Loures Campus (Lisbon)
IST | Alameda Campus (Lisbon)
UAl | Universidade do Algarve
UMa | Universidade da Madeira
Staff: 200 people (~80 PhDs)

Instituto de Plasmas e Fusão Nuclear

Key research activities



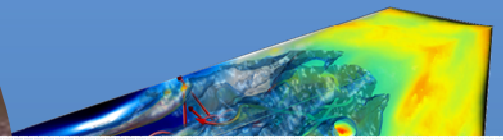


Instituto de Plasmas e Fusão Nuclear

Key research activities

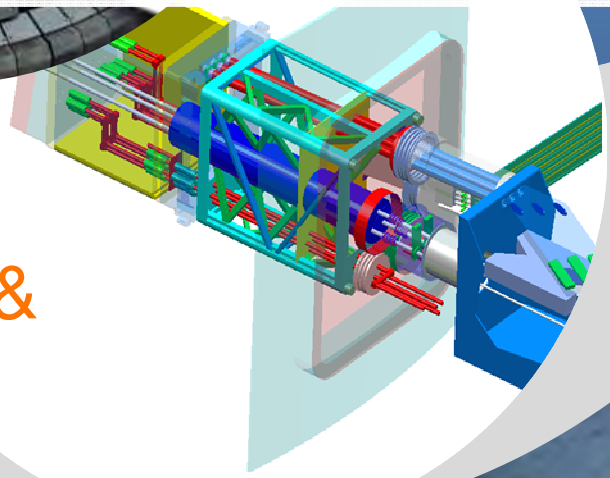
Experimental Physics

Theory & Modeling



Awarded “Outstanding”

(11/300 R&D units - 2014 evaluation procedure managed by ESF)

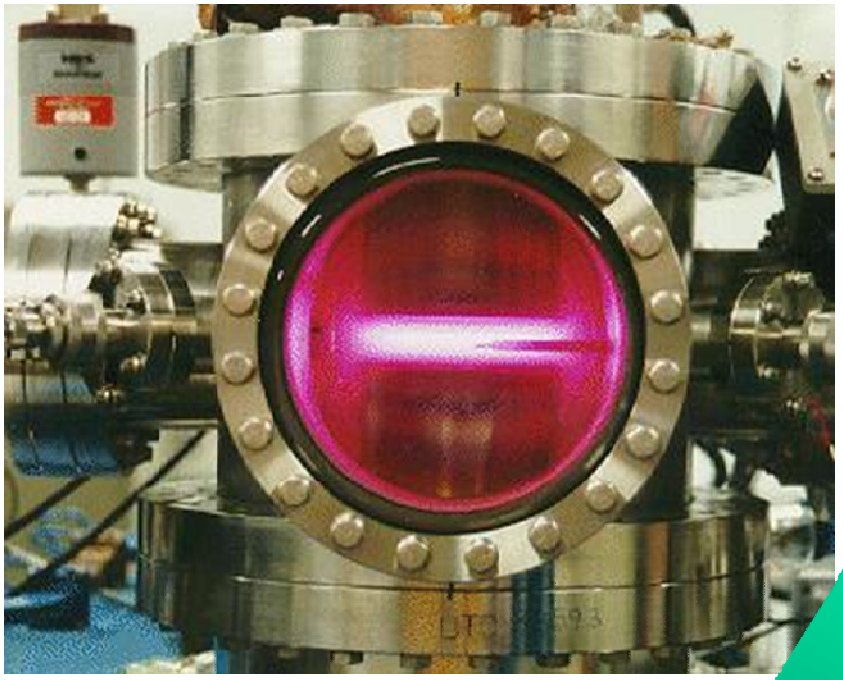


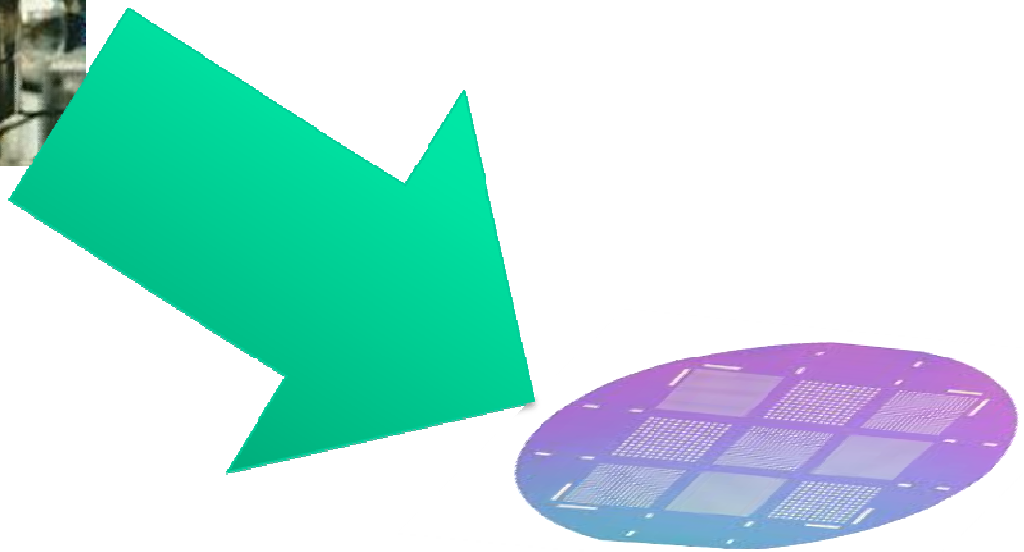
Society

Plasma Engineering & Systems Integration

Modelling of low-temperature plasmas

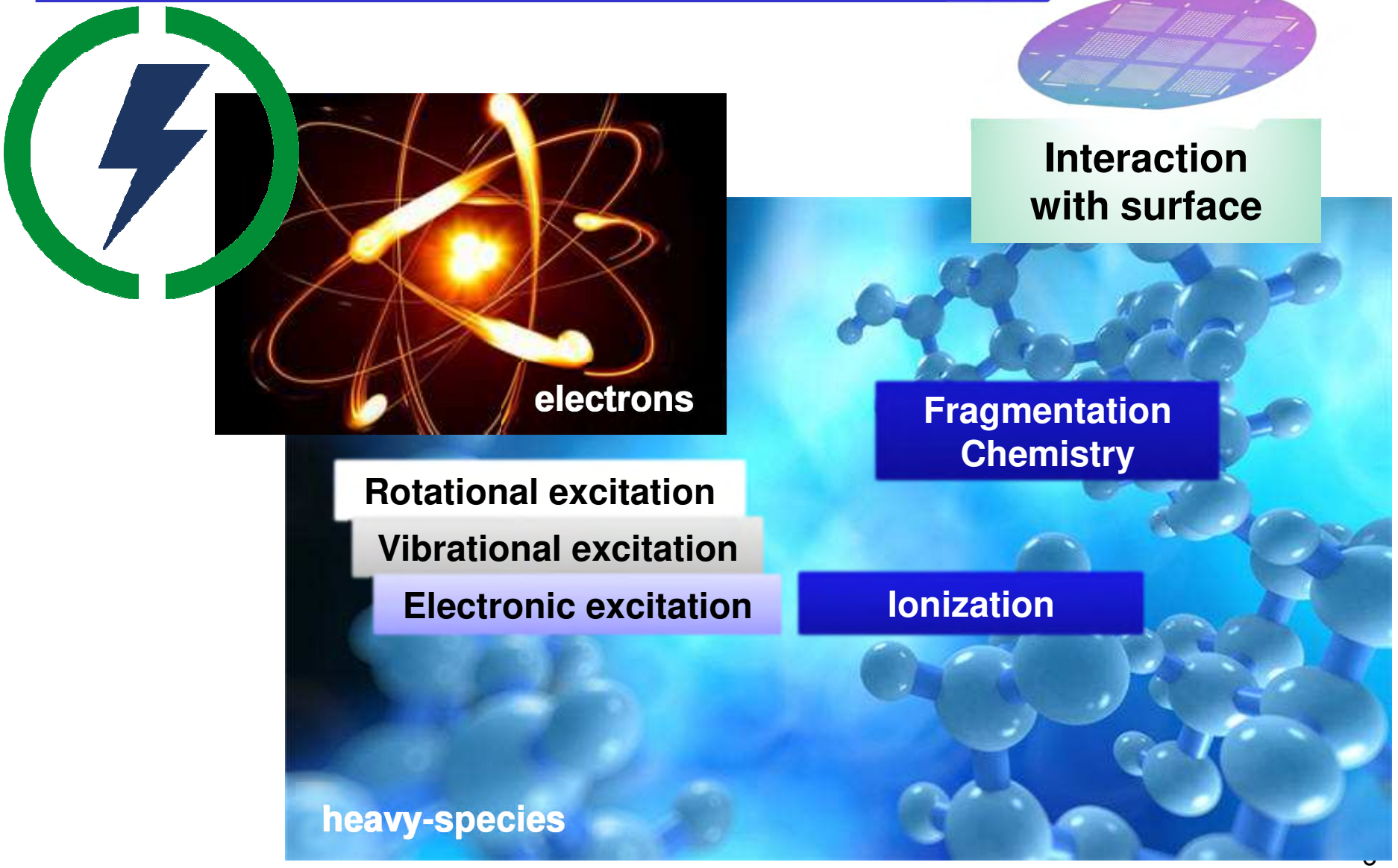
Goal: understand and predict





Modelling of low-temperature plasmas

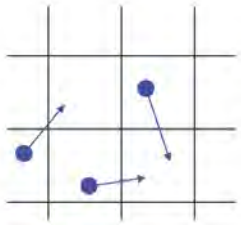
Interaction between species (in volume and at the wall)



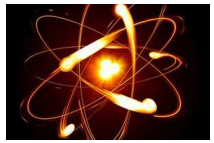
Modelling of low-temperature plasmas

Modelling approaches

- **Statistical models**



- **Kinetic models**



(electron kinetics)

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \vec{\nabla} F + \frac{\vec{X}}{m} \cdot \frac{\partial F}{\partial \vec{v}} = \left(\frac{\partial F}{\partial t} \right)_c$$

- **Fluid models**

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma} = n\nu_I$$

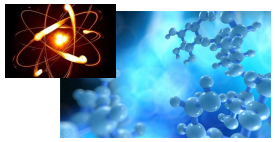
$$\vec{\Gamma} \equiv n\vec{v}_d = \pm \mu n \vec{E} - D\vec{\nabla} n$$

$$\frac{\partial (n\varepsilon)}{\partial t} + \vec{\nabla} \cdot \vec{Q} = n\vec{v}_d \cdot \vec{X} + \frac{\delta (n\varepsilon)}{\delta t}$$

Andrew Gibson's lecture

- **Hybrid models**

(combination of the above)



(electron and chemical kinetics)

Modelling LTPs – electron and chemical kinetics

Outline

- **Electron kinetic modelling**
  The electron Boltzmann equation
- **Chemical kinetic (hybrid) modelling**
  Collisional-radiative models
- **Example results**
- **Final remarks and questions**

Modelling LTPs – electron and chemical kinetics

Key references

- **Kinetics and Spectroscopy of Low Temperature Plasmas**
  J. Loureiro and J. Amorim, 2016, Springer International Publishing

- **Principles of Plasma Discharges and Materials Processing**
  M. A. Lieberman and A. J. Lichtenberg, 1994, John Wiley

- **Lecture Notes on Principles of Plasma Processing**
  F. F. Chen and J.P. Chang, 2003, Kluwer Academic / Plenum Publishers

- **Plasma Physics, Volumes 1 and 2**
  Jean-Loup Delcroix, 1965 / 1968, J. Wiley

- **Motions of Ions and Electrons**
  W. P. Allis, Handbuch der Physik, vol. 21, 1956, S. Flugge, Springer-Verlag – Berlin

- **Electron kinetics in atomic and molecular plasmas**
  C. M. Ferreira and J. Loureiro, Plasma Sources Sci. Technol. 9 (2000) 528–540

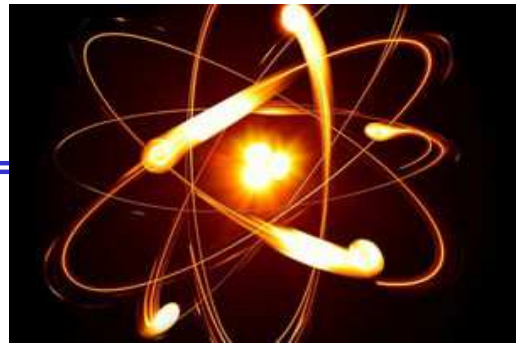
- **Fluid modelling of the positive column of direct-current glow discharges**
  L. L. Alves, Plasma Sources Sci. Technol. 16 (2007) 557–569

Electron kinetic modelling

The electron Boltzmann equation

Electron kinetic modelling

The "master" kinetic equation



- Inclusion of an energy description
- Definition of boundary conditions
- Complete problem : 6D $\Rightarrow$ long run times

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \vec{\nabla} F + \frac{\vec{X}}{m} \cdot \frac{\partial F}{\partial \vec{v}} = \left(\frac{\partial F}{\partial t} \right)_c$$

F(**r**,**v**,***t***) is the **distribution function,** representing the number of particles per unit volume in phase space (**r**,**v**), at time ***t***.

Electron kinetic modelling

The electron Boltzmann equation

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \vec{\nabla} F + \frac{\vec{X}}{m} \cdot \frac{\partial F}{\partial \vec{v}} = \left(\frac{\partial F}{\partial t} \right)_c$$

Rate of *F*

in time

in configuration space

in velocity space

due to collisions

Force acting upon particles

- The total electric field acting on electrons

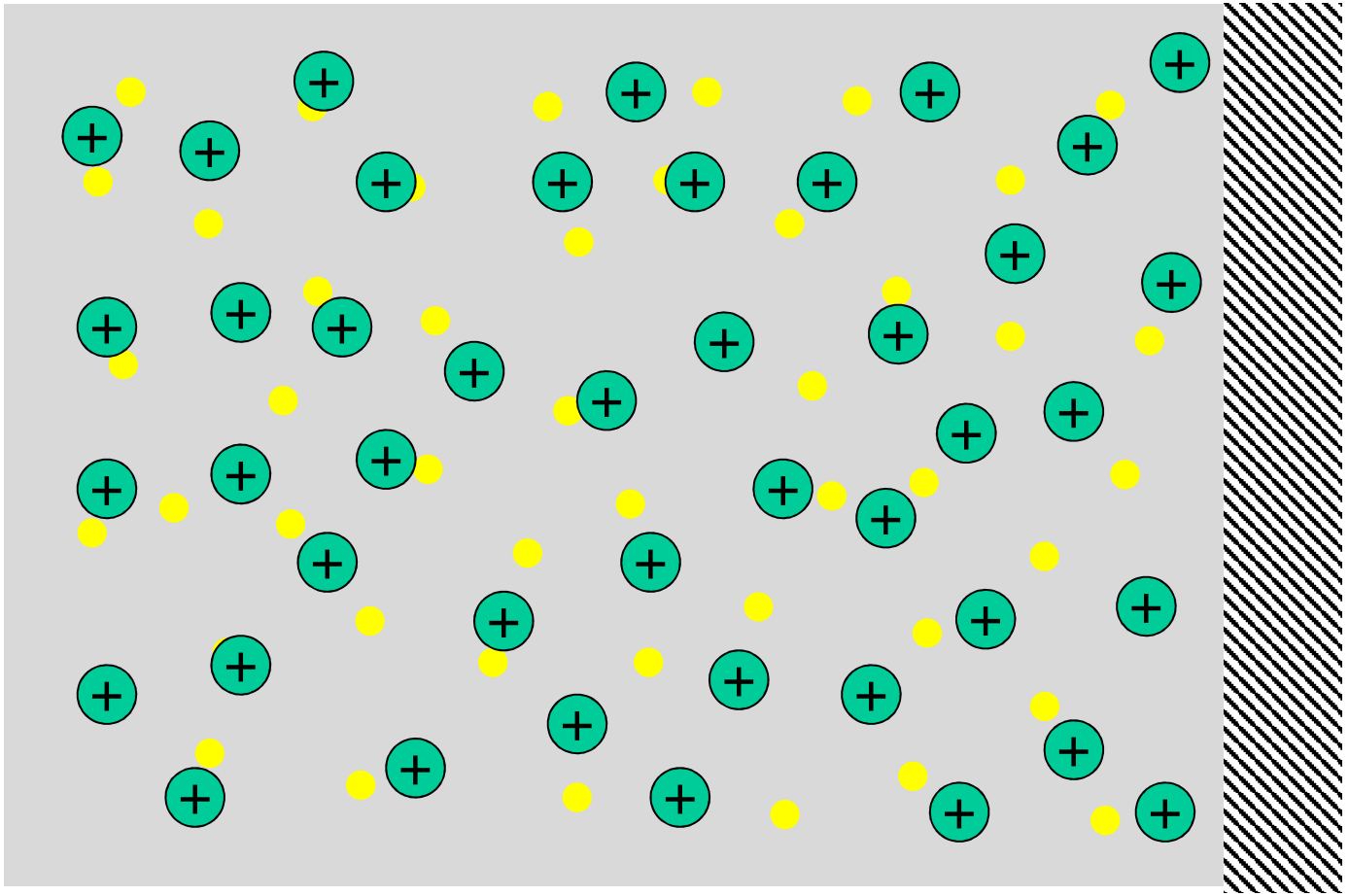
$$\vec{E} = \vec{E}_s(\vec{r}) + \vec{E}_p \exp(j\omega t)$$

dc space-charge field

hf field at frequency ω

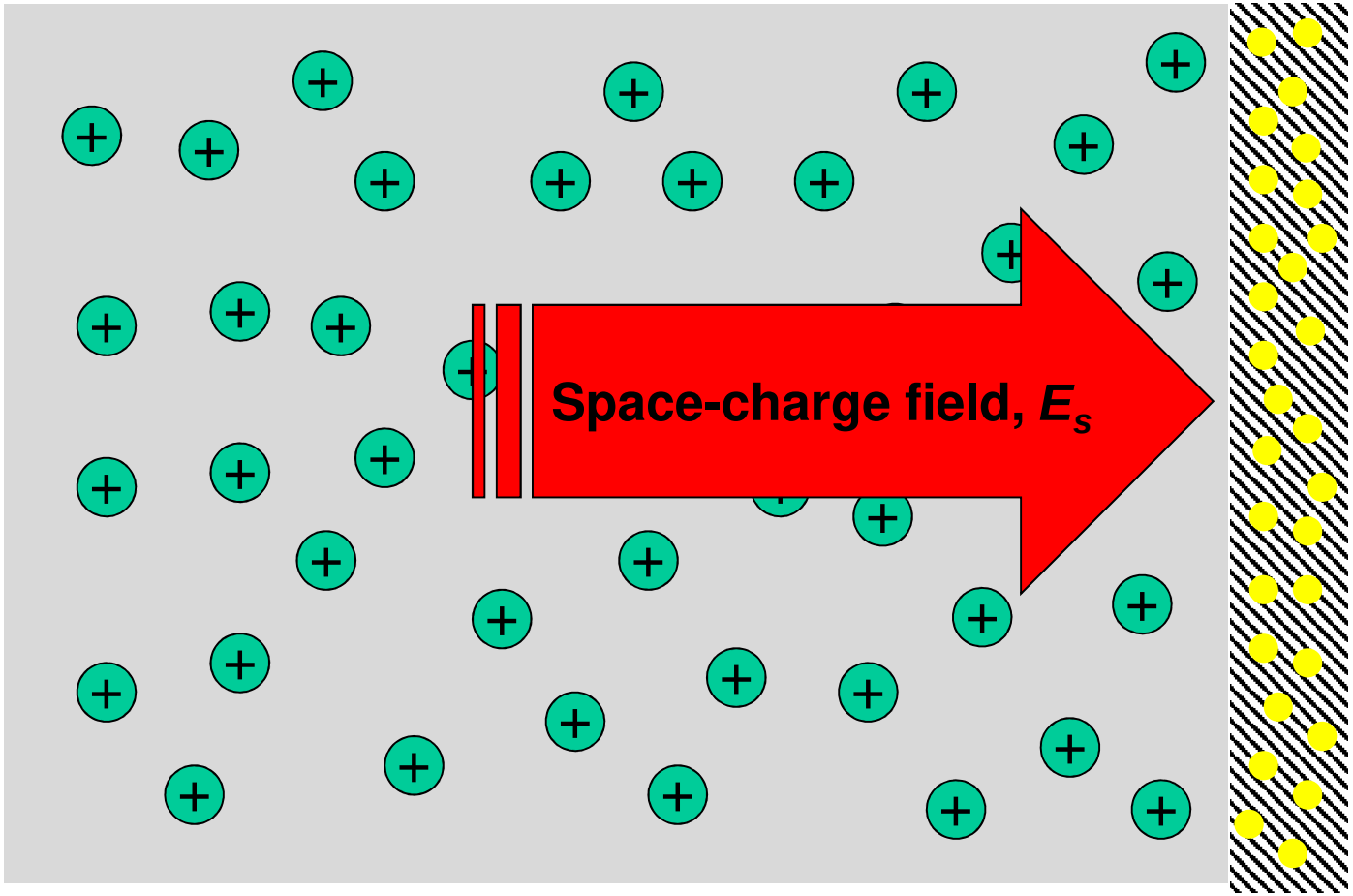
Charge separation at the boundaries

The space-charge sheath



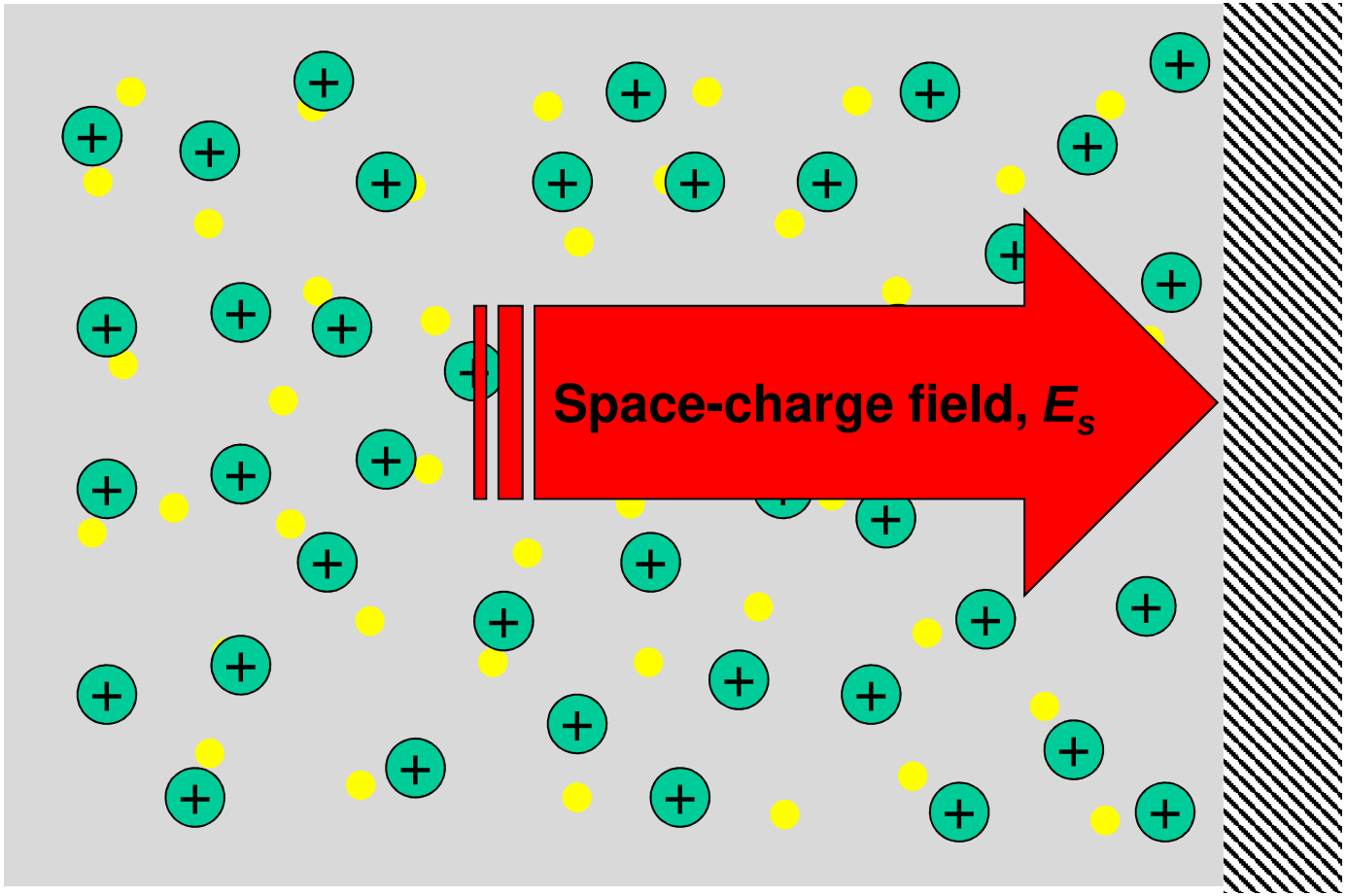
Charge separation at the boundaries

The space-charge sheath



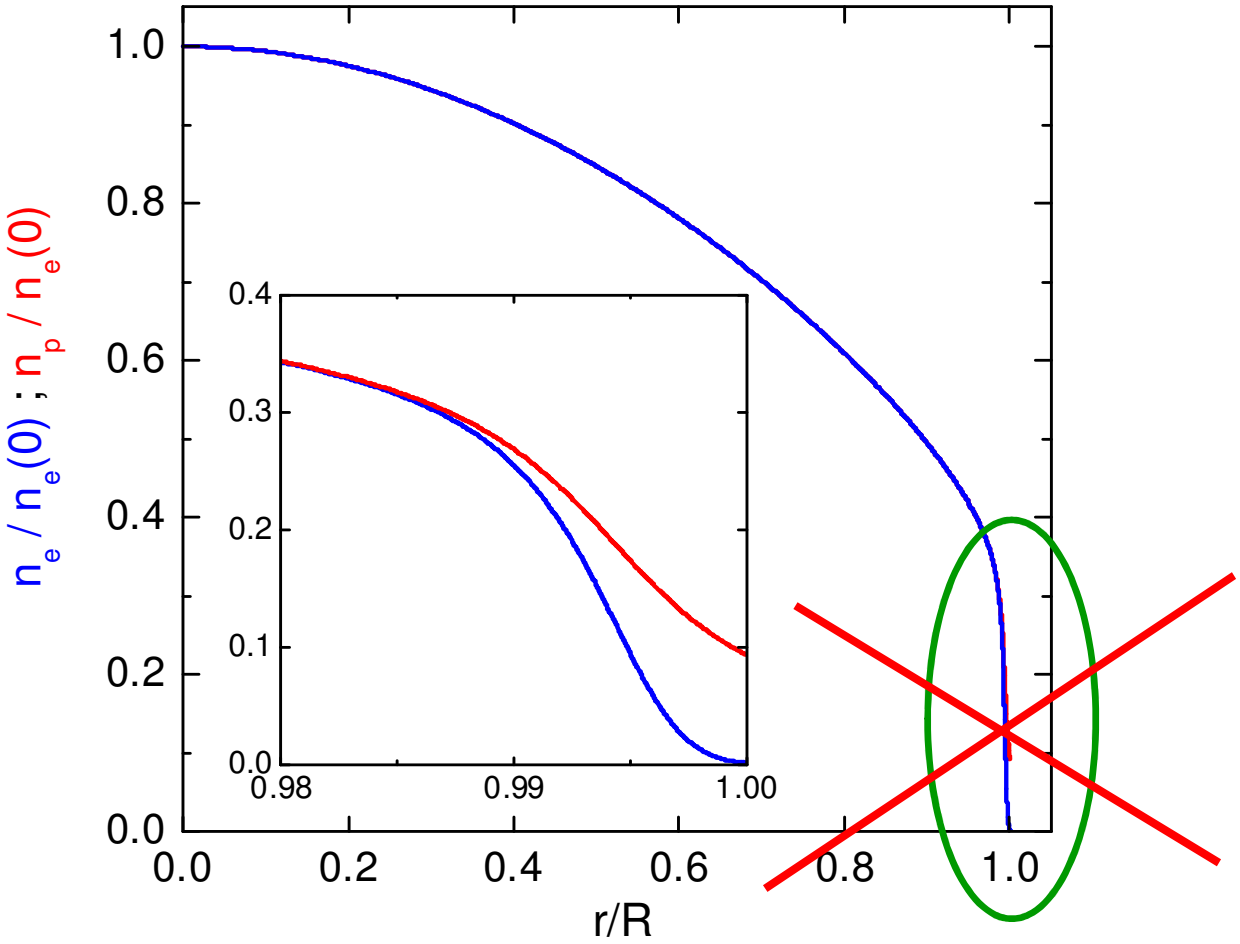
Charge separation at the boundaries

The space-charge sheath



Charge separation at the boundaries

The space-charge sheath



Source: LL Alves, PSST 16 557 (2007)

The electron Boltzmann equation

Working conditions

- **Disregard** the space-charge electric field acting on electrons

$$\vec{E} = \cancel{\vec{E}_s(\vec{r})} + \vec{E}_p \exp(j\omega t)$$

dc space-charge field — hf field at frequency ω

- No external magnetic field
- The electron distribution function F is expanded

  in spherical harmonics in velocity space

  in Fourier series in time

$$F = \sum_l \sum_p F_p^l P_l(\cos\theta) \exp(jp\omega t)$$

The electron Boltzmann equation

The small anisotropy / two-term approximation

Conditions…

- the electron mean free path is much smaller than any relevant dimension of the container, $\lambda_e \ll L$
- the energy gained from the electric field per collision by a representative electron is much smaller than the thermal energy of the electrons
- the oscillation amplitude of the electron motion under the action of the hf field is small as compared to L
- the characteristic frequency for the electron energy relaxation by collisions is much smaller than the oscillation frequency of the hf field, $\tau_e^{-1} \ll \omega$

$$F(\vec{r},v) \simeq F_0^0(\vec{r},v) + (\vec{v}/v)\cdot\left[\vec{F}_0^1(\vec{r},v) + \vec{F}_1^1(\vec{r},v)\exp(j\omega t)\right]$$

Isotropic component (energy relaxation)

Anisotropic components (transport)

The homogeneous electron Boltzmann equation

Collision operators

- The isotropic equation

$$-\frac{1}{v^2}\frac{\partial}{\partial v}\left\{\left(\frac{ev^2}{6m}\right) Re\left(\vec{E}_p \cdot \vec{F}_1^1\right) + \frac{m}{M}\nu_c v^3 F_0^0\right\} = \left(q - \nu_x - \nu_i\right) F_0^0$$

elastic collision operator

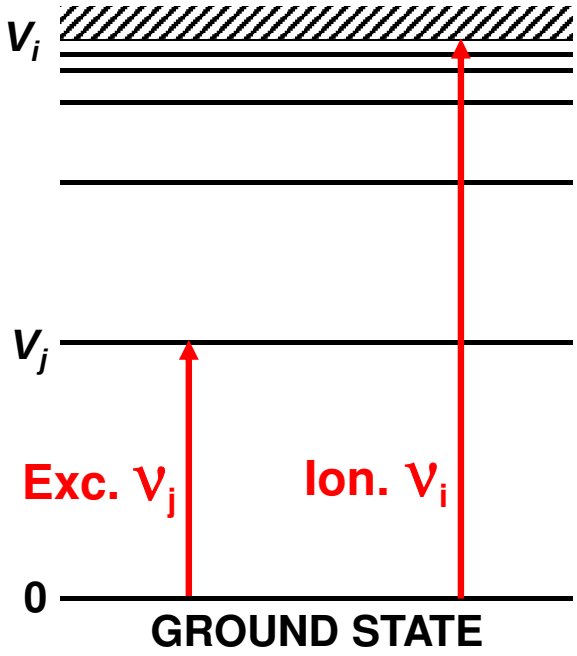
inelastic collision operator

- The anisotropic equation

$$\left(\nu_c + j\omega\right)\vec{F}_1^1 = \frac{e\vec{E}_p}{m}\frac{\partial F_0^0}{\partial v}$$

The homogeneous electron Boltzmann equation

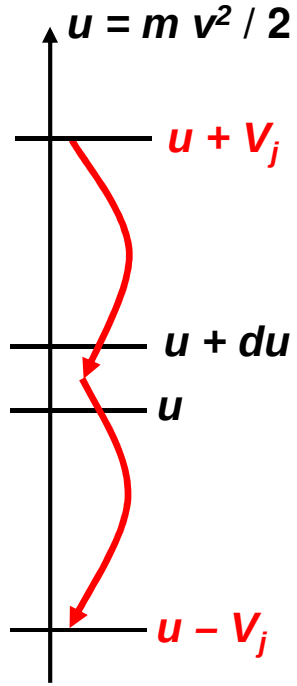
The inelastic collision operator



$$qF_0^0 - (\nu_x + \nu_i) F_0^0$$

Entrance Exit

$$\nu_x = \sum_j \nu_j$$



The homogeneous electron Boltzmann equation

Input data: working parameters

$$-\frac{1}{v^2}\frac{\partial}{\partial v}\left\{\left(\frac{ev^2}{6m}\right) Re\left(\vec{E}_p \cdot \vec{F}_1^1\right) + \frac{m}{M}\nu_c v^3 F_0^0\right\} = \left(q - \nu_x - \nu_i\right) F_0^0$$

$$\left(\nu_c + j\omega\right)\vec{F}_1^1 = \frac{e\vec{E}_p}{m}\frac{\partial F_0^0}{\partial v}$$

$$\frac{E_p}{N}, \frac{\omega}{N} \Rightarrow \textbf{Independent parameters}$$

The homogeneous electron Boltzmann equation

Input data: collisional data

$$-\frac{1}{v^2}\frac{\partial}{\partial v}\left\{\left(\frac{ev^2}{6m}\right) Re\left(\vec{E}_p \cdot \vec{F}_1^1\right) + \frac{m}{M}\nu_c v^3 F_0^0\right\} = (q - \nu_x - \nu_i) F_0^0$$

$$(\nu_c + j\omega)\vec{F}_1^1 = \frac{e\vec{E}_p}{m}\frac{\partial F_0^0}{\partial v}$$

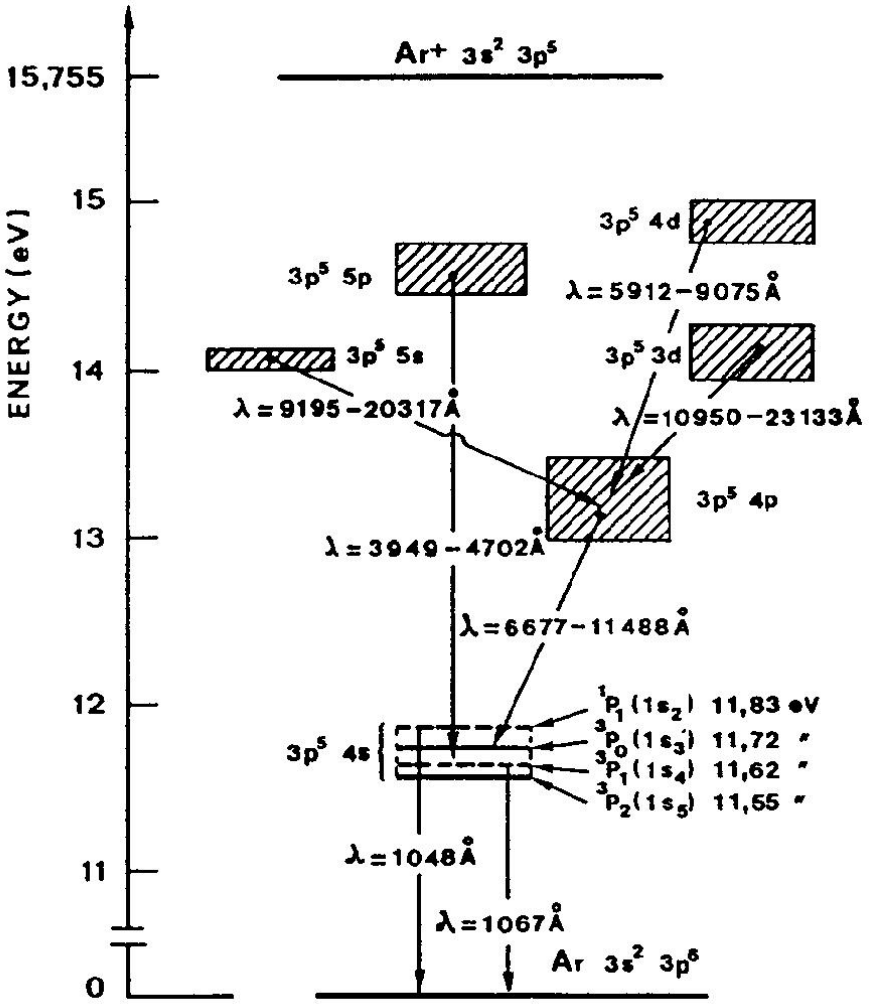
$$\nu_c = N\sigma_c\left(2eu/m\right)^{1/2} \qquad q,\nu = N_i\sigma_{ij}\left(2eu/m\right)^{1/2}$$

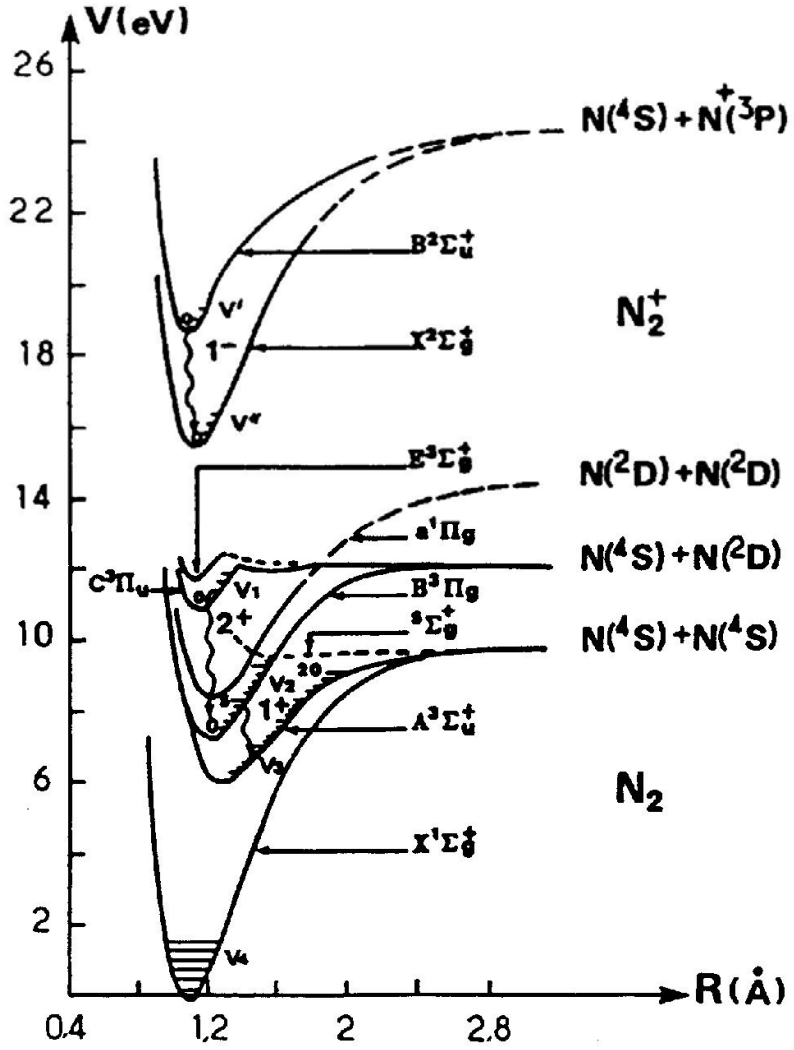
$N_{i=0} = N$ ⇒ **Gas density**

$N_{i\neq 0}$ ⇒ **Chemistry model (heavy-species kinetics)**

Input data

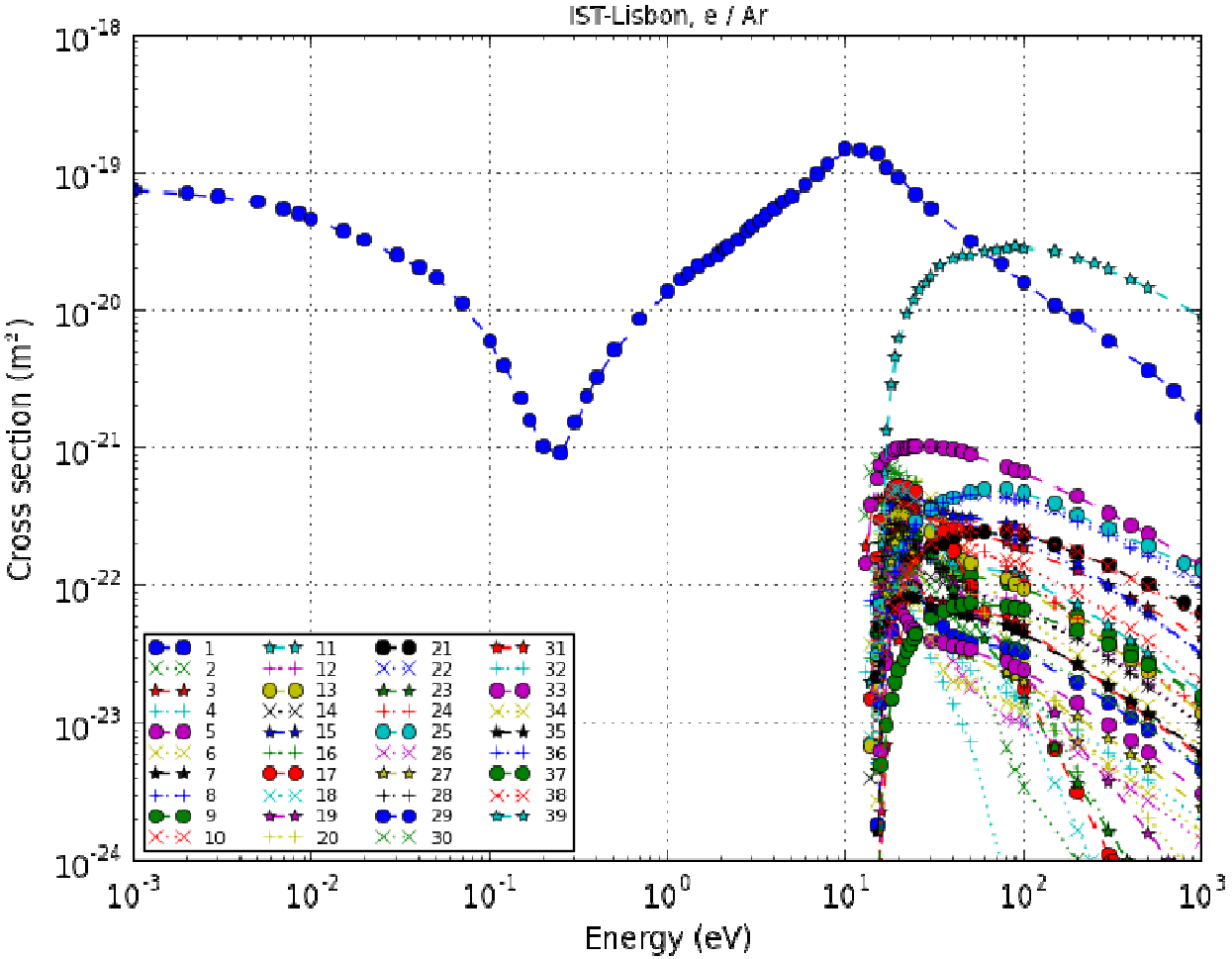
Excitation / ionization mechanisms





Input data

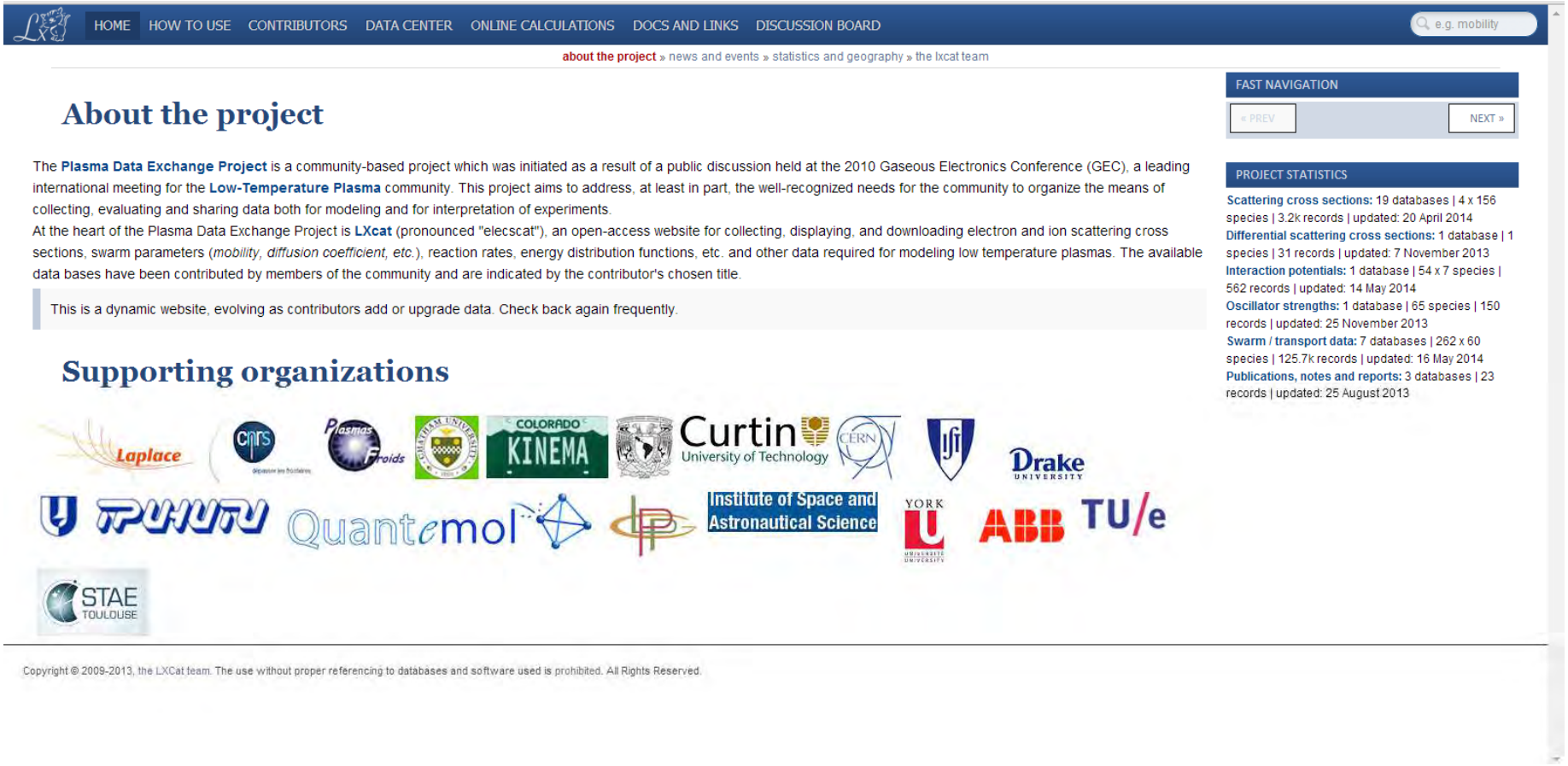
Cross sections



Data from…

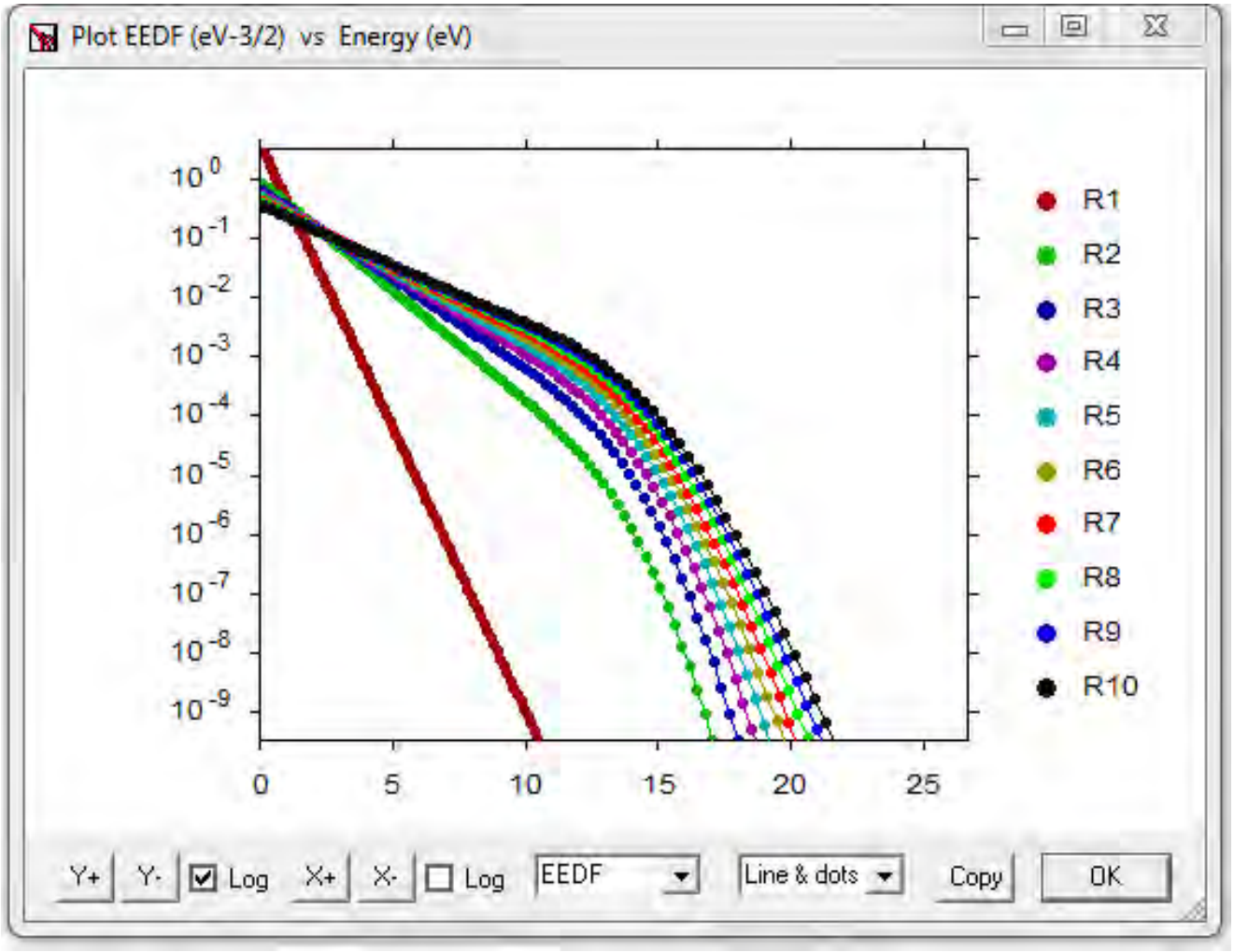
- Bibliography
- Databases (e.g. LXCat: www.lxcat.net)

Input data
The LXCat database



The homogeneous electron Boltzmann equation

The electron energy distribution function (EEDF)



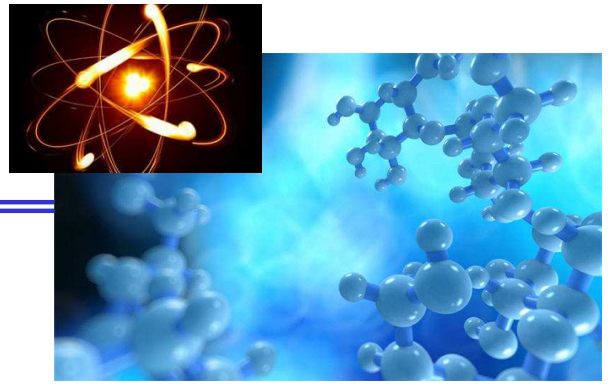
Courtesy of Bolsig+ (https://www.bolsig.laplace.univ-tlse.fr/)

Chemical kinetic (hybrid) modelling

Collisional-radiative models

Chemical kinetic (hybrid) modelling

Collisional – Radiative Models (CRM)



- Energy description for electrons only

- Spatially-averaged description

  Algebraic forms for

  - the particle balance equations
  - the particle flux equations

- Short run times

$$\begin{cases} \dfrac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma} = n\nu_I \\ \vec{\Gamma} = -D\vec{\nabla} n \end{cases} \Rightarrow \frac{\partial n}{\partial t} = -D\nabla^2 n + n\nu_I$$

System of coupled rate balance equations for the various plasma species

transport **kinetics**

Chemical kinetic (hybrid) modelling

Collisional – Radiative Models (CRM)

Transport rates

$$D\nabla^2 n \approx -\frac{D}{\Lambda^2} n$$

For electrons, the transport parameters can be related with the EEDF

Electron free diffusion coefficient

$$D_e = \int_0^\infty \frac{v^2}{3\nu_c} \frac{F_0^0}{n_e} 4\pi v^2 dv = \text{function}(E/N)$$

Electron mobility

$$\mu_e = -\int_0^\infty \frac{ev}{3m\nu_c} \frac{1}{n_e} \frac{\partial F_0^0}{\partial v} 4\pi v^2 dv = \text{function}(E/N)$$

Chemical kinetic (hybrid) modelling

Collisional – Radiative Models (CRM)

Reaction rates (for collisional-radiative kinetic mechanisms) : the source term

$$n\nu_I = \sum_j n_j \nu_j - n\sum_k \nu^k$$

For electrons, the collision frequencies can be related with the EEDF

Electron rate coefficients

$$C_j \equiv \frac{\langle \nu_j / N \rangle}{n_e} = \int_0^\infty \sigma_j v \frac{F_0^0}{n_e} 4\pi v^2 dv = \text{function}(E/N)$$

Recall …

$$-\frac{1}{v^2}\frac{\partial}{\partial v}\left\{\left(\frac{ev^2}{6m}\right) Re\left(\vec{E}_p \cdot \vec{F}_1^1\right) + \frac{m}{M}\nu_c v^3 F_0^0\right\} = (q - \nu_x - \nu_i) F_0^0$$

$$(\nu_c + j\omega)\vec{F}_1^1 = \frac{e\vec{E}_p}{m}\frac{\partial F_0^0}{\partial v}$$

$$\nu_c = N\sigma_c\left(2eu/m\right)^{1/2} \qquad q,\nu = N_i\sigma_{ij}\left(2eu/m\right)^{1/2}$$

$N_{i=0} = N$ ⇒ **Gas density**

$N_{i\neq 0}$ ⇒ **Chemistry model (heavy-species kinetics)**

Chemical kinetic (hybrid) modelling

Rate balance equations for the vibrational levels of nitrogen

$$n_e \sum_{w=0,w\neq v}^{45} N_w C_{w,v} - n_e N_v \sum_{w=0,w\neq v}^{45} C_{v,w}$$

$$+ \quad N_{v-1} N P_{v-1,v} + N_{v+1} N P_{v+1,v} - N_v (P_{v,v-1} + P_{v,v+1})$$

$$+ \quad N_{v-1} \sum_{w=0}^{44} N_{w+1} Q_{v-1,v}^{w+1,w} + N_{v+1} \sum_{w=0}^{45} N_w Q_{v+1,v}^{w,w+1}$$

$$- \quad N_v \left(\sum_{w=0}^{44} N_{w+1} Q_{v,v+1}^{w+1,w} + \sum_{w=0}^{45} N_w Q_{v,v-1}^{w,w+1} \right) + R(v) = 0$$

- electron-vibration

$$\mathrm{e} + \mathrm{N}_2(v) \underset{C_{v,w}}{\overset{C_{w,v}}{\rightleftharpoons}} \mathrm{e} + \mathrm{N}_2(w)$$

Chemical kinetic (hybrid) modelling

Rate balance equations for the vibrational levels of nitrogen

$$n_e \sum_{w=0,w\neq v}^{45} N_w C_{w,v} - n_e N_v \sum_{w=0,w\neq v}^{45} C_{v,w}$$

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$$+ \quad N_{v-1} \sum_{w=0}^{44} N_{w+1} Q_{v-1,v}^{w+1,w} + N_{v+1} \sum_{w=0}^{45} N_w Q_{v+1,v}^{w,w+1}$$

$$- \quad N_v \left(\sum_{w=0}^{44} N_{w+1} Q_{v,v+1}^{w+1,w} + \sum_{w=0}^{45} N_w Q_{v,v-1}^{w,w+1} \right) + R(v) = 0$$

- vibration-translation

$$\begin{cases} \mathrm{N_2} + \mathrm{N_2}(v) \underset{P_{v,v-1}}{\overset{P_{v-1,v}}{\rightleftharpoons}} \mathrm{N_2} + \mathrm{N_2}(v-1) \\ \mathrm{N_2} + \mathrm{N_2}(v+1) \underset{P_{v+1,v}}{\overset{P_{v,v+1}}{\rightleftharpoons}} \mathrm{N_2} + \mathrm{N_2}(v) \end{cases}$$

Chemical kinetic (hybrid) modelling

Rate balance equations for the vibrational levels of nitrogen

$$n_e \sum_{w=0,w\neq v}^{45} N_w C_{w,v} - n_e N_v \sum_{w=0,w\neq v}^{45} C_{v,w}$$

$$+ \quad N_{v-1} N P_{v-1,v} + N_{v+1} N P_{v+1,v} - N_v (P_{v,v-1} + P_{v,v+1})$$

$$+ \quad N_{v-1} \sum_{w=0}^{44} N_{w+1} Q_{v-1,v}^{w+1,w} + N_{v+1} \sum_{w=0}^{45} N_w Q_{v+1,v}^{w,w+1}$$

$$- \quad N_v \left(\sum_{w=0}^{44} N_{w+1} Q_{v,v+1}^{w+1,w} + \sum_{w=0}^{45} N_w Q_{v,v-1}^{w,w+1} \right) + R(v) = 0$$

Atom kinetics
Wall kinetics

- vibration-vibration

$$\begin{cases} \mathrm{N_2}(v) + \mathrm{N_2}(w) \underset{Q_{v,v-1}^{w,w+1}}{\overset{Q_{v-1,v}^{w+1,w}}{\rightleftharpoons}} \mathrm{N_2}(v-1) + \mathrm{N_2}(w+1) \\ \mathrm{N_2}(v+1) + \mathrm{N_2}(w) \underset{Q_{v+1,v}^{w,w+1}}{\overset{Q_{v,v+1}^{w+1,w}}{\rightleftharpoons}} \mathrm{N_2}(v) + \mathrm{N_2}(w+1) \end{cases}$$

Chemical kinetic (hybrid) modelling

Kinetic data: example for nitrogen

Nb.	Coll. type	Reaction	Rate coefficient
	Electron collisions		$C_{\alpha l,k}$
(1)[a]	Elastic	$e + N_2(X) \longrightarrow e + N_2(X)$	eedf
(2)[a]	Rot. excitation	$e + N_2(X, J) \longrightarrow e + N_2(X, J')$	eedf
(3)[a]	Vib. exc./deexc.	$e + N_2(X, v = 0\text{–}9) \longleftrightarrow e + N_2(X, w = (v+1) - 10)$	eedf
(4a)[a]	Elect. exc./deexc.	$e + N_2(X) \longrightarrow e + N_2(A, B, C, a', a, w, a'')$	eedf
(4b)[a]		$e + N_2(X) \longrightarrow e + N_2(B')$	
		$N_2(B') \longrightarrow N_2(B) + h\nu$	eedf
(4c)[b]		$e + N_2(X) \longrightarrow e + N_2(W, E,$ higher levels$)$	eedf
(5a)		$e + N_2(A) \longleftrightarrow e + N_2(B, C)$	eedf
(5b)		$e + N_2(A) \longrightarrow e + N_2(X)$	eedf
(6)[a]	Ionization	$e + N_2(X) \longrightarrow 2e + N_2^+(X, B)$	eedf
(7)		$e + N_2(A, B, a', a, w) \longrightarrow 2e + N_2^+$	eedf
(8)	Ion reaction	$e + N_2^+(X) \longrightarrow e + N_2^+(B)$	eedf
(9)	Dissociation	$e + N_2(X) \longrightarrow e + N(S) + N(S, D)$	eedf
(10)	Recombination	$e + N_2^+ \longrightarrow 2N(S)$	$4.8 \times 10^{-7}[300/T_e(\mathrm{K})]^{0.5}$
(11)		$e + N_4^+ \longrightarrow 2N_2(X)$	$2.0 \times 10^{-6}[300/T_e(\mathrm{K})]^{0.5}$

Source: LL Alves et al, PSST 21 045008 (2012)

Chemical kinetic (hybrid) modelling

Kinetic data: example for nitrogen

	Heavy-particle collisions		$K_{lm,k}$
(12)	V–T processes	$N_2 + N_2(X, v = 0\text{–}45) \longleftrightarrow N_2 + N_2(X, v \pm 1)$	$P_{v,v\pm1}$
(13)	V–V processes	$N_2(X, v = 0\text{–}45) + N_2(X, w = 0\text{–}45) \longleftrightarrow$ $N_2(X, v \pm 1) + N_2(X, w \mp 1)$	$Q_{v,v\pm1}^{w,w\mp1}$
(14)	Vib. deexc.	$N_2(A) + N_2(X, v = 5\text{–}14) \longrightarrow N_2(B) + N_2(X)$	2.0×10^{-11}
(15a)	Elect. exc./deexc.	$N_2(A) + N_2(A) \longrightarrow N_2(B) + N_2(X)$	7.7×10^{-11}
(15b)		$N_2(A) + N_2(A) \longrightarrow N_2(C) + N_2(X)$	1.5×10^{-10}
(16a)		$N_2(B) + N_2 \longrightarrow N_2(A) + N_2$	2.85×10^{-11}
(16b)		$N_2(B) + N_2 \longrightarrow N_2(X) + N_2$	1.5×10^{-12}
(17)		$N_2(a') + N_2 \longrightarrow N_2(B) + N_2$	1.9×10^{-13}
(18)		$N_2(a) + N_2 \longrightarrow N_2(a') + N_2$	2.0×10^{-11}
(19)		$N_2(w) + N_2 \longrightarrow N_2(a) + N_2$	1.0×10^{-11}
(20)		$N_2(a'') + N_2 \longrightarrow$ products	2.3×10^{-10}
(21)	Dissociation	$N_2(A) + N_2(X, v = 14\text{–}19) \longrightarrow N_2(X) + 2N(S)$	1.5×10^{-12}
(22)		$2N_2(X, v = 11\text{–}24) \longrightarrow N_2(X) + 2N(S)$	3.5×10^{-15}
(23)	Ionization	$N_2(A) + N_2(a')$	1.0×10^{-11}
		$\xrightarrow{b_{ion}} N_4^+ + e$	
		$\xrightarrow{1-b_{ion}} N_2^+ + N_2(X) + e$	
(24)		$N_2(a') + N_2(a')$	5.0×10^{-11}
		$\xrightarrow{b_{ion}} N_4^+ + e$	
		$\xrightarrow{1-b_{ion}} N_2^+ + N_2(X) + e$	
(25)	Ion reactions	$N_4^+ + N_2 \longrightarrow N_2^+ + N_2(X) + N_2$	$2.1 \times 10^{-16} \exp[T_g(\mathrm{K})/121]$
(26)		$N_2^+ + N_2(X) + N_2 \longrightarrow N_4^+ + N_2$	$6.8 \times 10^{-29}[300/T_g(\mathrm{K})]^{1.64}\ \mathrm{cm^6\ s^{-1}}$
(27)		$N_2^+(X) + N_2(X, v \geqslant 12) \longrightarrow N_2^+(B) + N_2(X, v - 12)$	1.0×10^{-11}
(28)	Radiative trans.	$N_2(B) \longrightarrow N_2(A) + h\nu$	$A_{N_2(B),N_2(A)} = 2.0 \times 10^5\ \mathrm{s^{-1}}$
(29)		$N_2(C) \longrightarrow N_2(B) + h\nu$	$A_{N_2(C),N_2(B)} = 2.74 \times 10^7\ \mathrm{s^{-1}}$
(30a)		$N_2(a) \longrightarrow N_2(X) + h\nu$	$A_{N_2(a),N_2(X)} = 1.8 \times 10^4\ \mathrm{s^{-1}}$
(30b)		$N_2(a) \longrightarrow N_2(a') + h\nu$	$A_{N_2(a),N_2(a')} = 1.91 \times 10^2\ \mathrm{s^{-1}}$
(31)		$N_2(w) \longrightarrow N_2(a) + h\nu$	$A_{N_2(w),N_2(a)} = 6.5 \times 10^2\ \mathrm{s^{-1}}$
(32)		$N_2^+(B) \longrightarrow N_2^+(X) + h\nu$	$A_{N_2^+(B),N_2^+(X)} = 1.6 \times 10^7\ \mathrm{s^{-1}}$
(33)	Wall reactions	$N_2(X, v) + \mathrm{wall} \longrightarrow N_2(X, v - 1)$	$\gamma'_{N_2(X,v)}$
(34)		$N_2(A, a', a, w) \xrightarrow{\text{diffusion}} N_2(X)$	$D_k N = 5 \times 10^{18}[T_g(\mathrm{K})/300]^{0.5}\ \mathrm{cm^{-1}\ s^{-1}}$

Source: LL Alves et al, PSST 21 045008 (2012)

Chemical kinetic (hybrid) modelling

Closing the calculations

$$\frac{\partial n}{\partial t} = -D\nabla^2 n + n\nu_I = 0 \quad \Rightarrow \quad \frac{\nabla^2 n}{n} = \frac{\nu_I / N}{DN} N^2 \equiv \frac{1}{\Lambda^2}$$

- PDE solution (with boundary condition for the charged-particle density)

$$\frac{\nabla^2 n}{n} = \frac{1}{\Lambda^2} = \text{const}$$

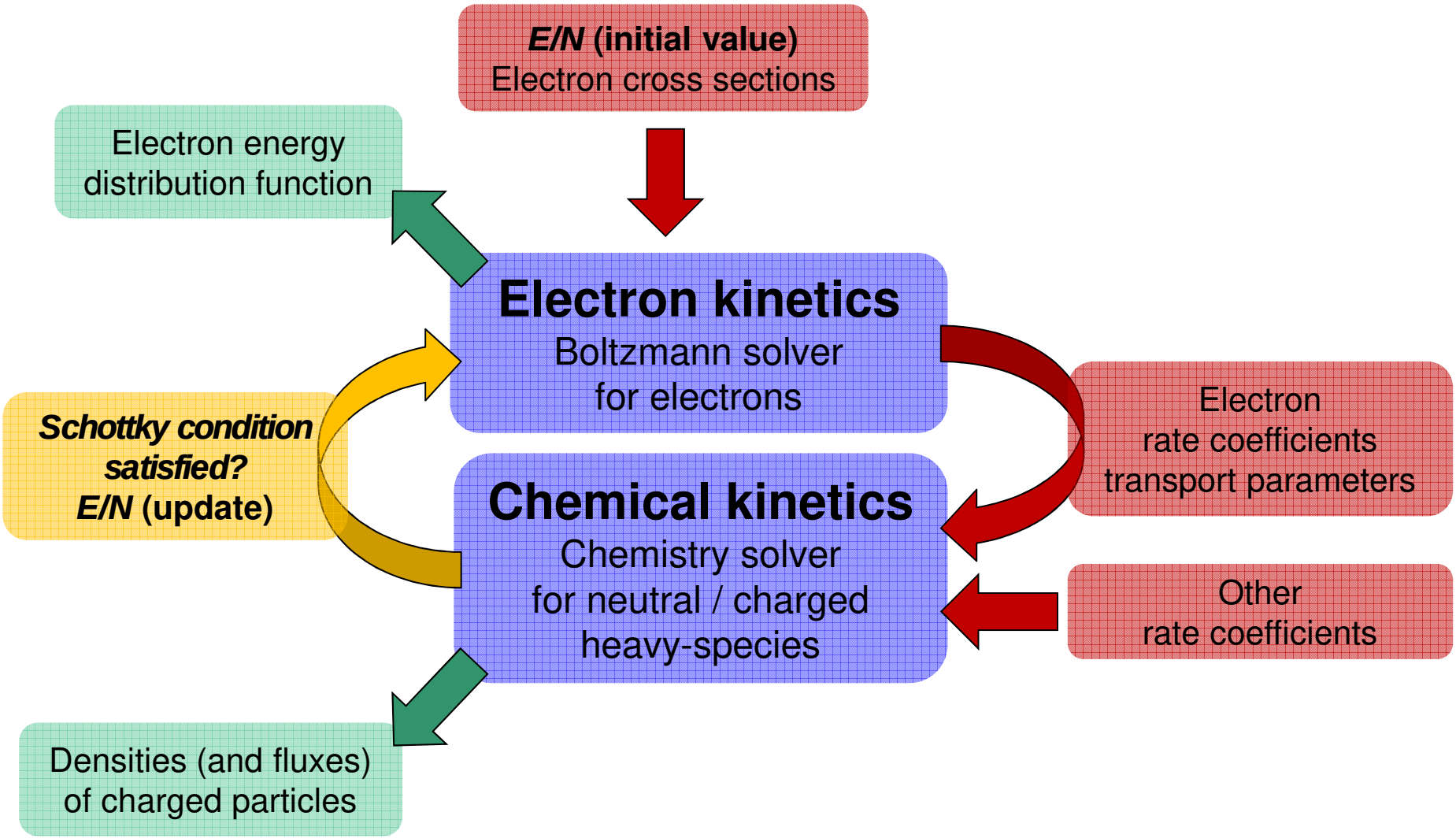
- Electron gain/loss balance **(Schottky condition)**

$$\frac{\nu_I}{N} = \frac{DN}{(N\Lambda)^2}$$

$$\frac{E}{N}$$ **EIGENVALUE**

Chemical kinetic (hybrid) modelling

Joining the electron and chemical kinetics



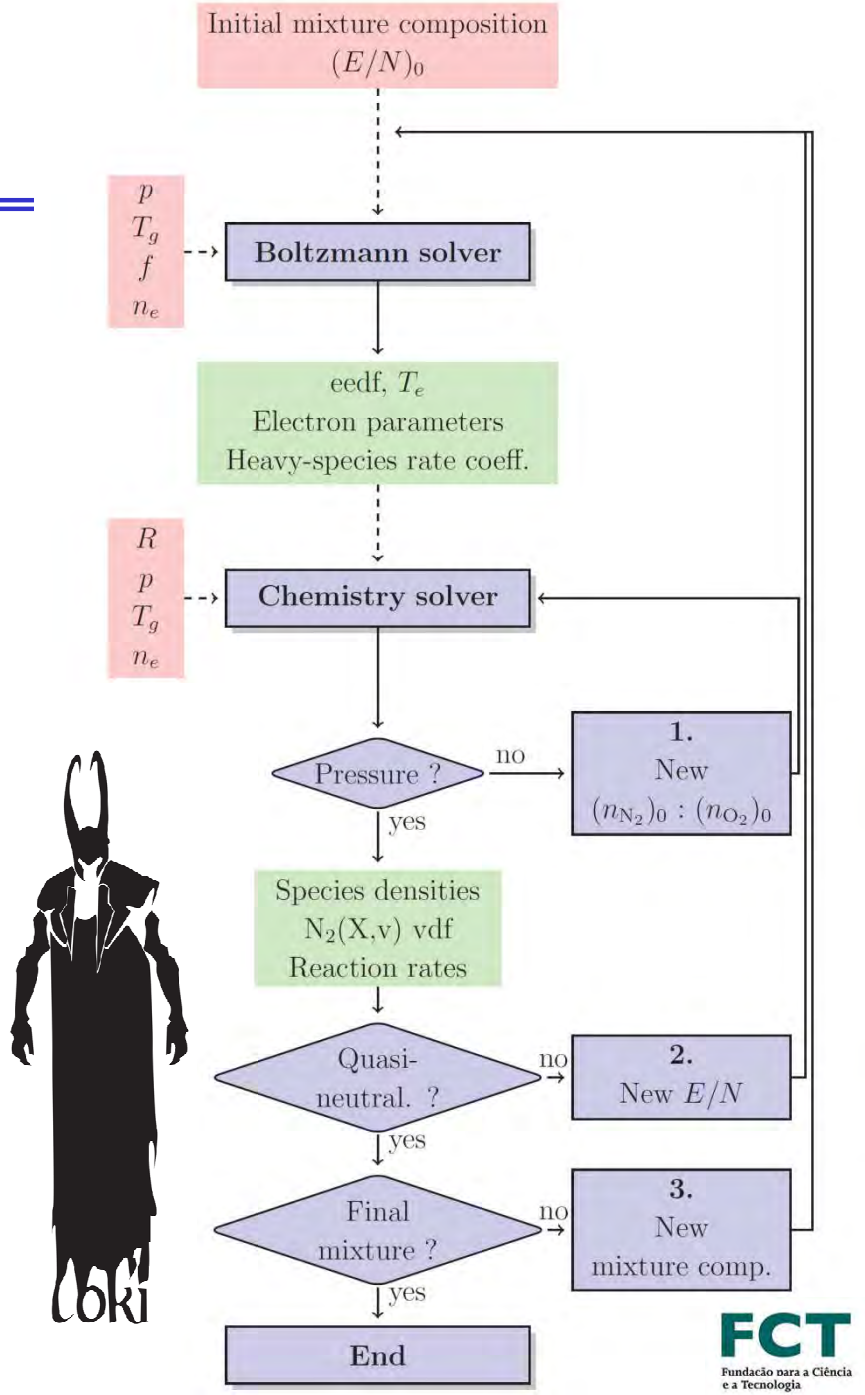
Hybrid modelling

The LisbOn KInetics code (LoKI)

Modular tools with state-of-the-art kinetic schemes and transport description, including

- Boltzmann solver
- Chemistry solver

OPEN SOURCE



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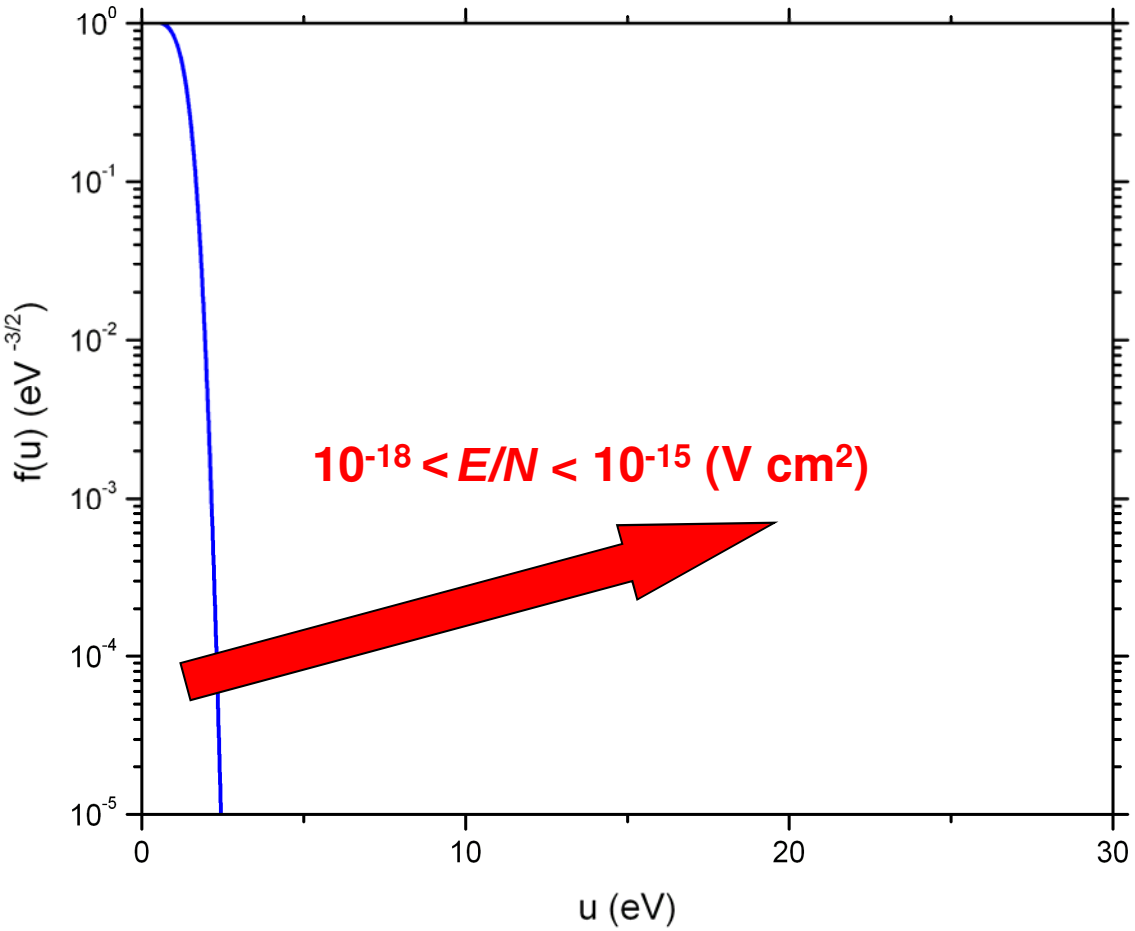
Example results

Electron kinetic calculations

EEDF for argon I

Influence of *E/N*



Electron kinetic calculations

EEDF for argon II

Influence of

- **excitation frequency**
- **e-e collisions**

A:

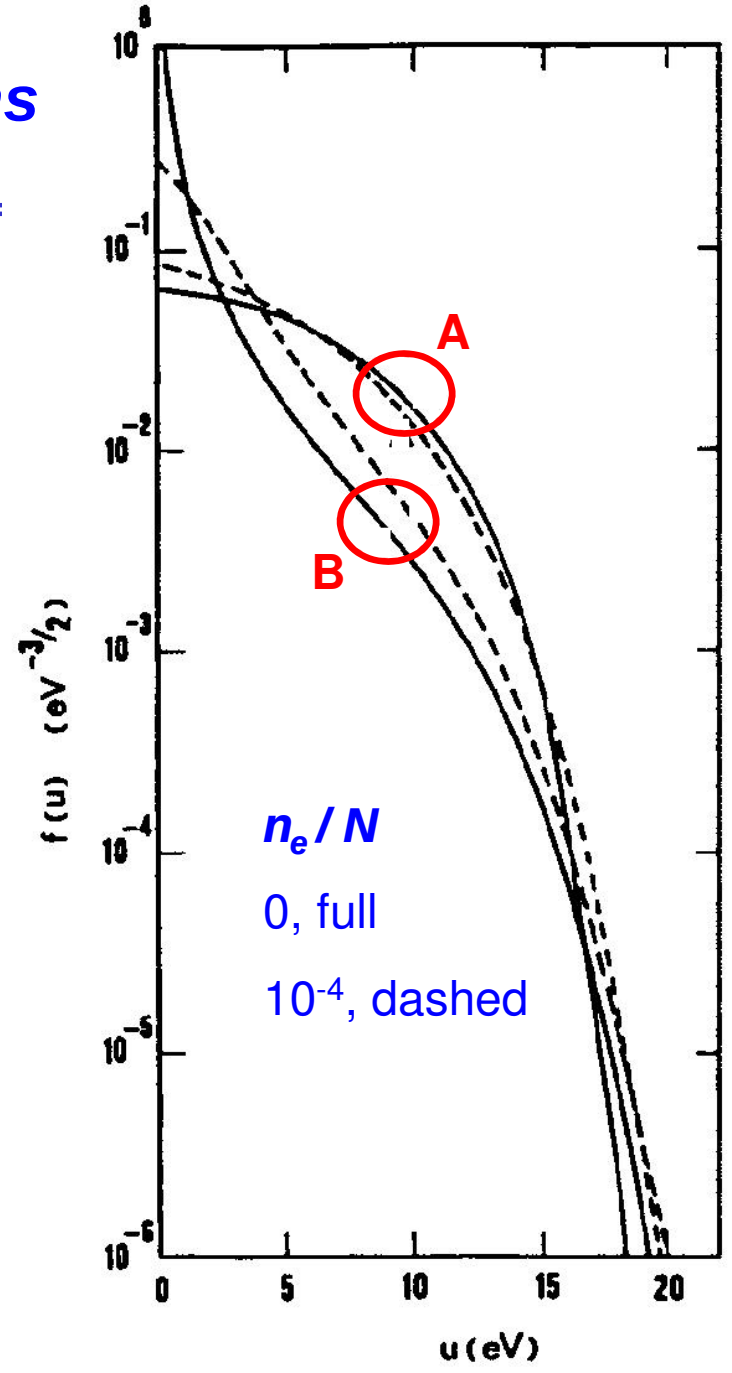
$\omega/N = 0$

$E/N = 3 \times 10^{-16}$ V cm^2

B:

$\omega/N = 2 \times 10^{-6}$ cm^3 s^{-1}

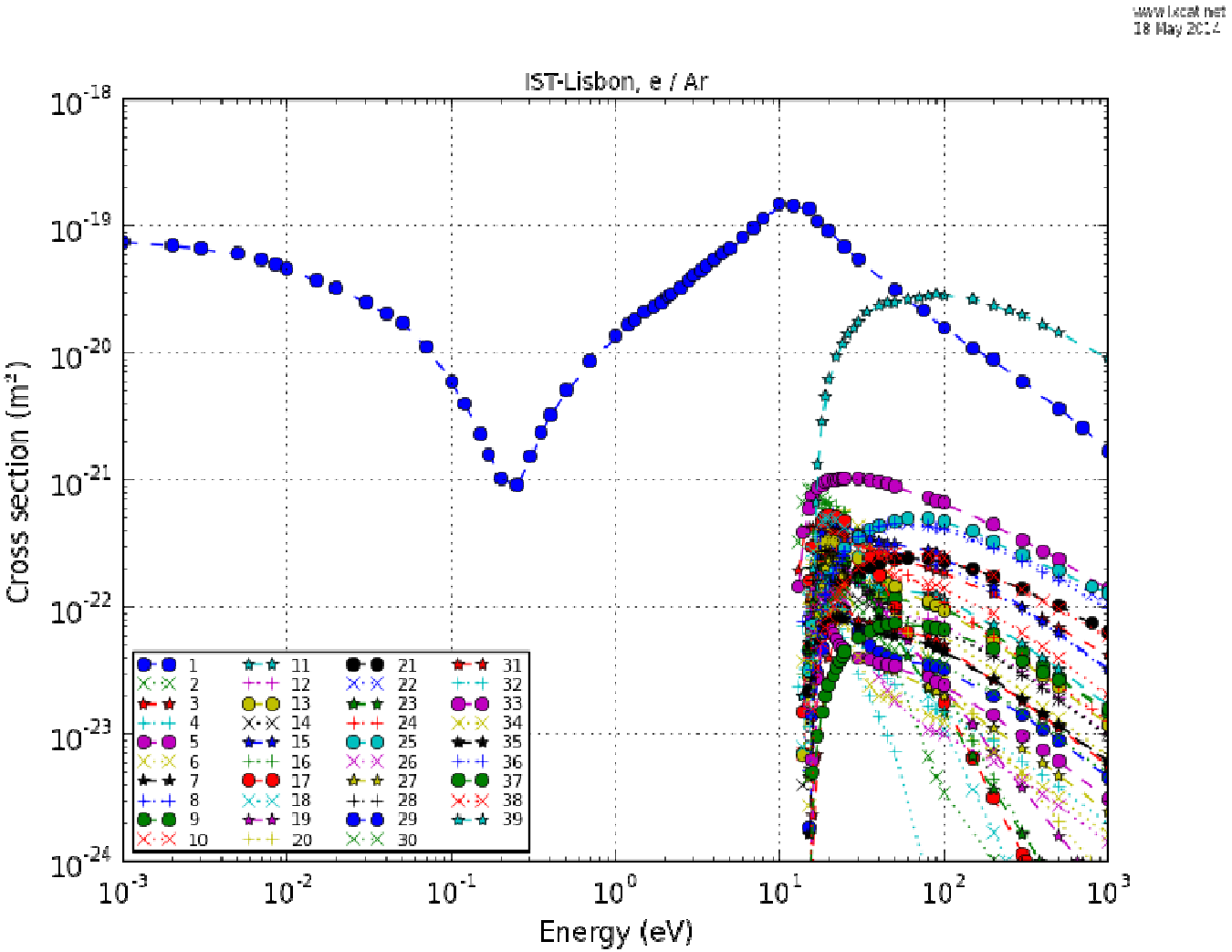
$E/N = 3 \times 10^{-15}$ V cm^2



Source: CM Ferreira and J Loureiro, PSST 9 528 (2000)

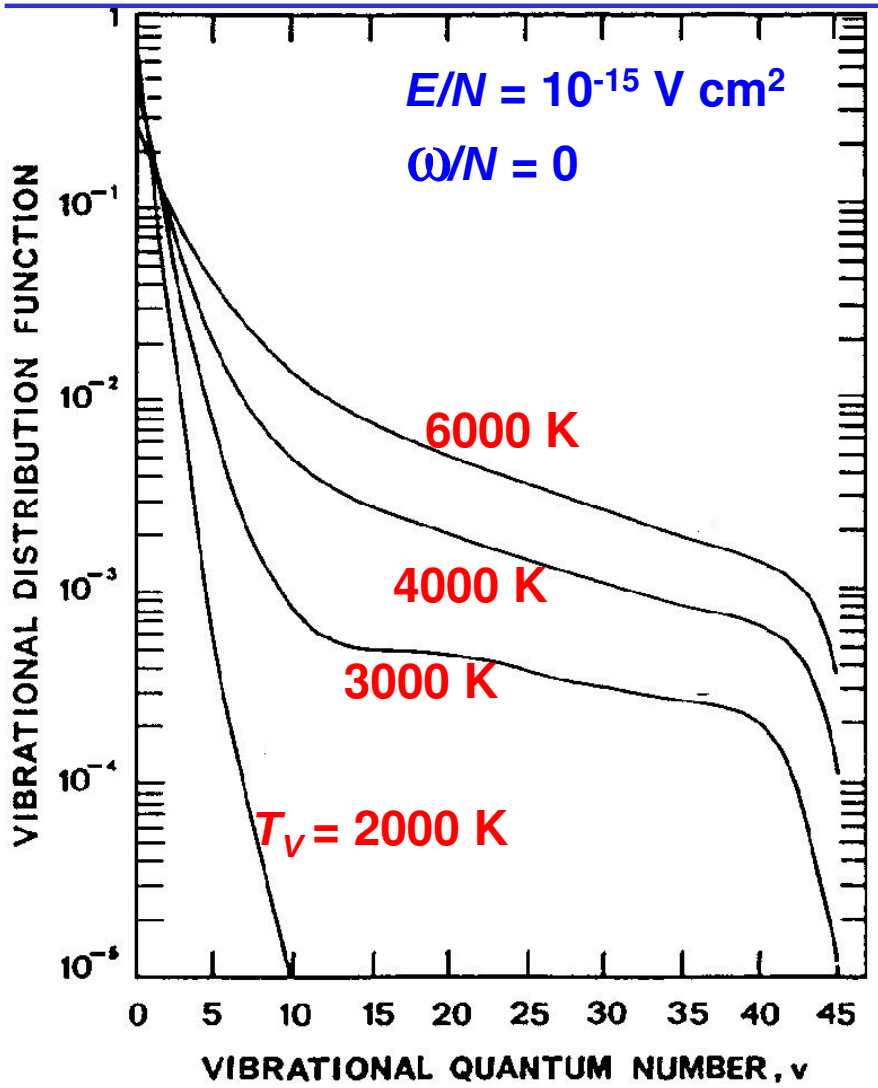
Electron kinetic calculations

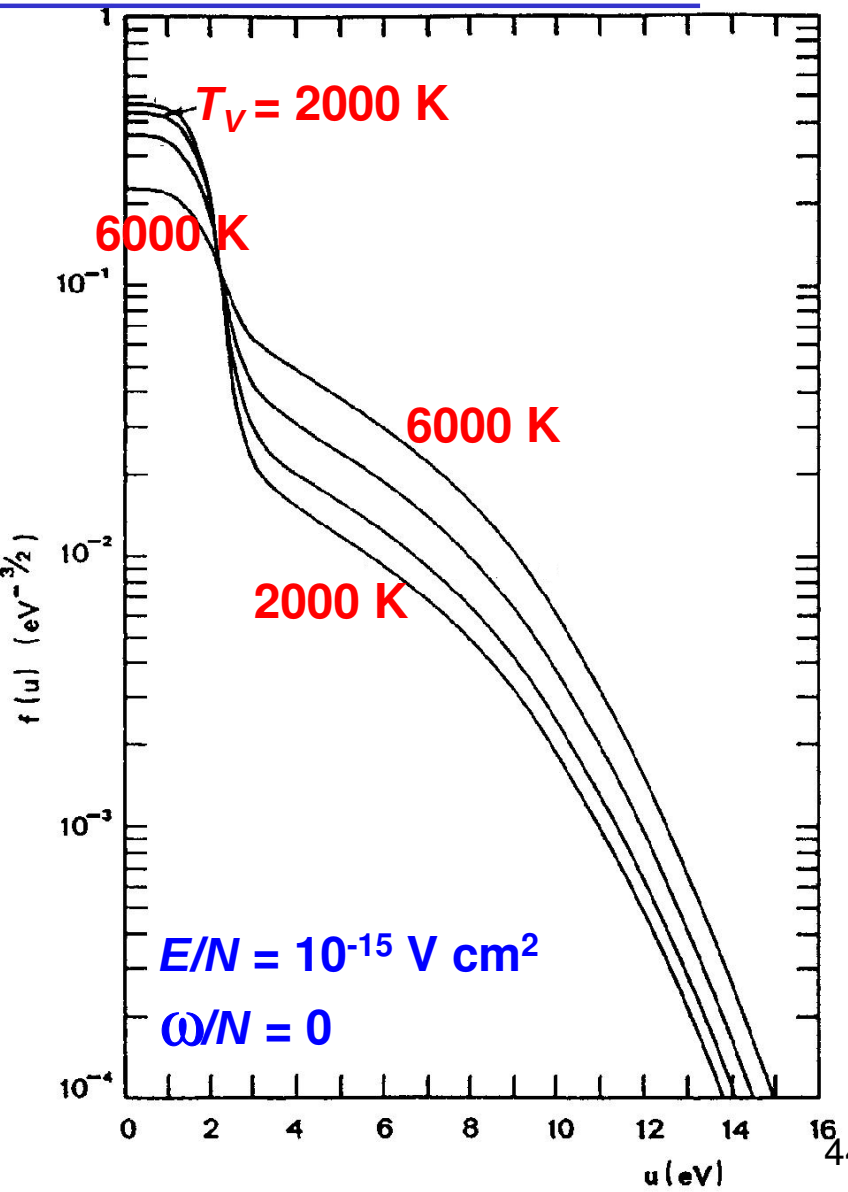
The argon electron momentum-transfer cross section



Electron kinetic calculations

EEDF and VDF for nitrogen



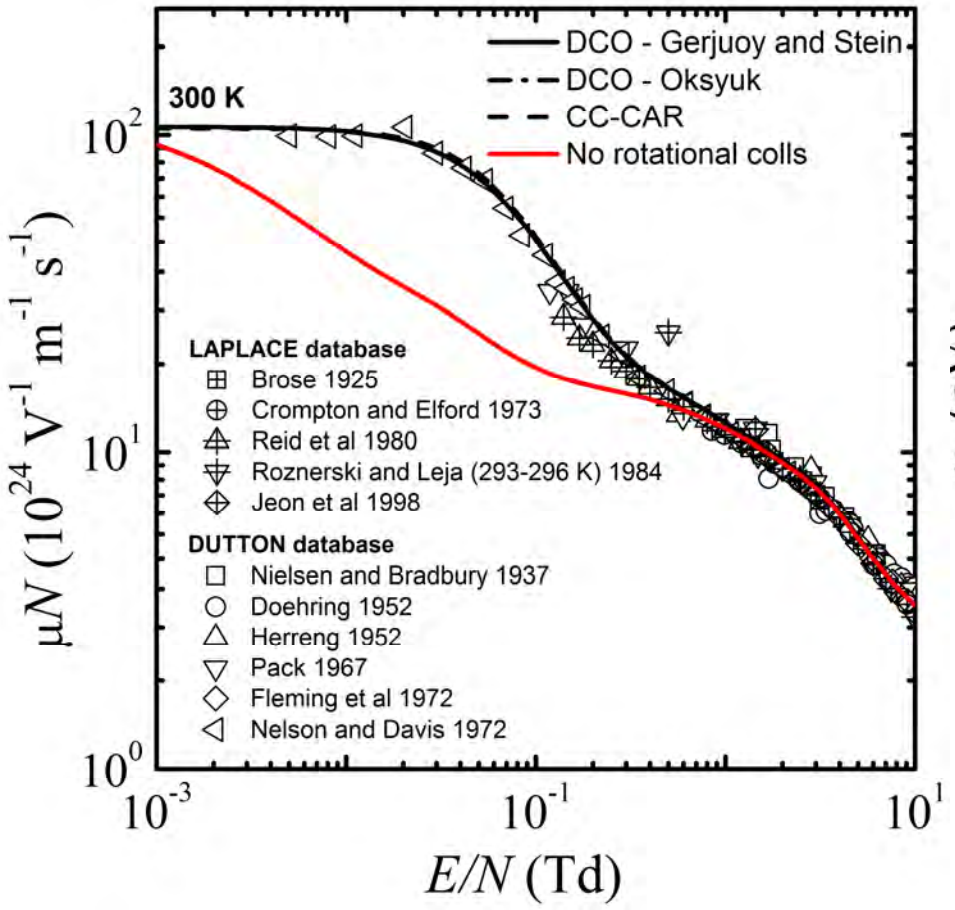


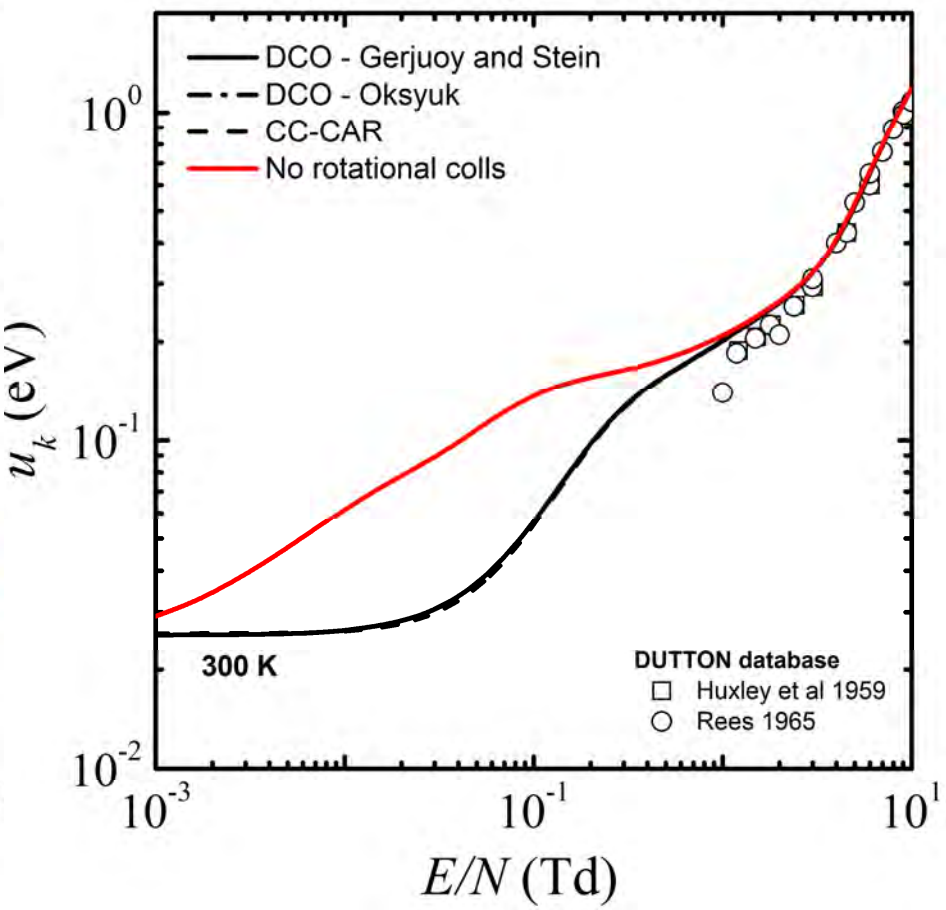
Source: CM Ferreira and J Loureiro, PSST 9 528 (2000)

Electron kinetic calculations

Swarm studies for oxygen (influence of rotational mechanisms)

DCO … discrete collisional operator
CC-CAR … continuous approximation rotations (with Chapman-Cowling correction)

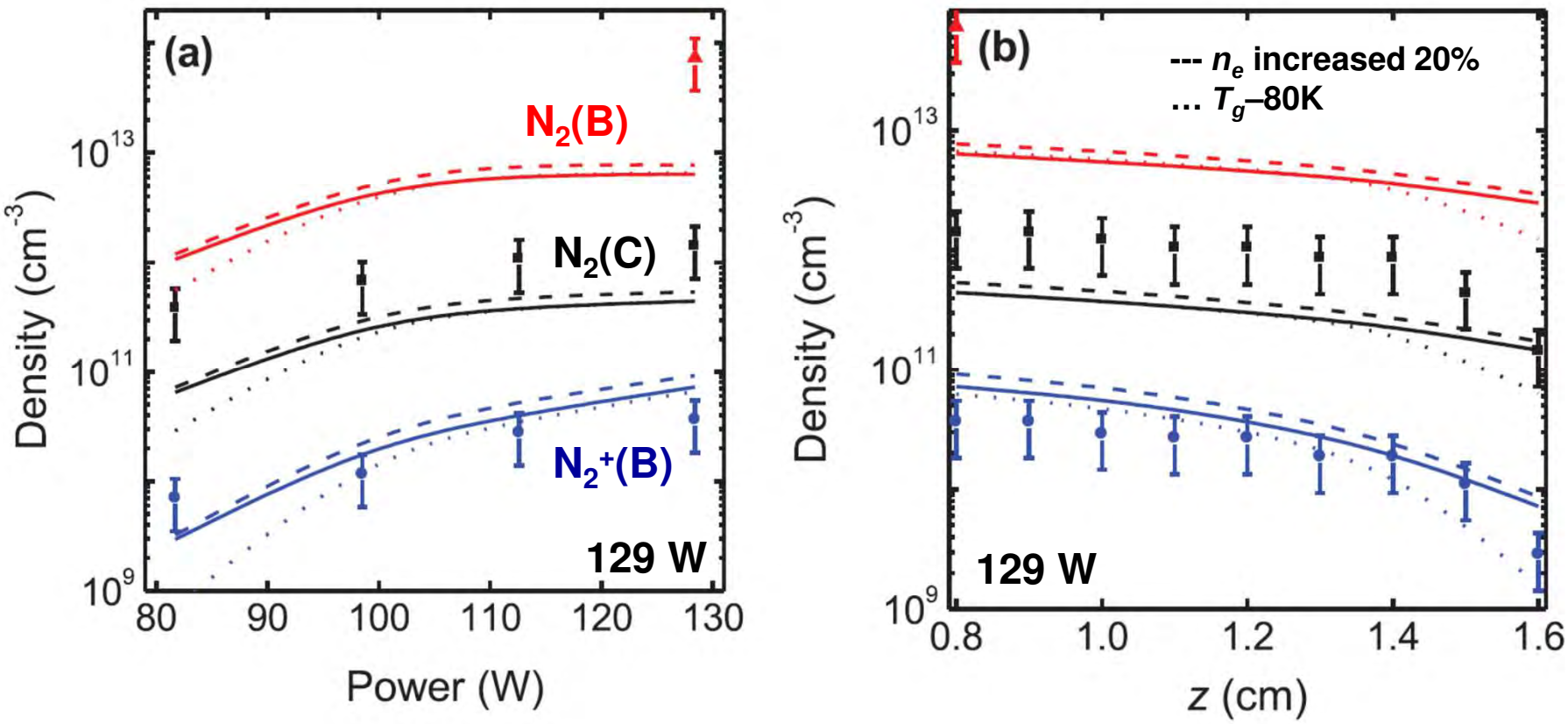




Source: MA Ridenti et al, PSST 24 035002 (2016)

Chemical kinetic calculations

Microwave discharge in air - absolute densities of N_2 species

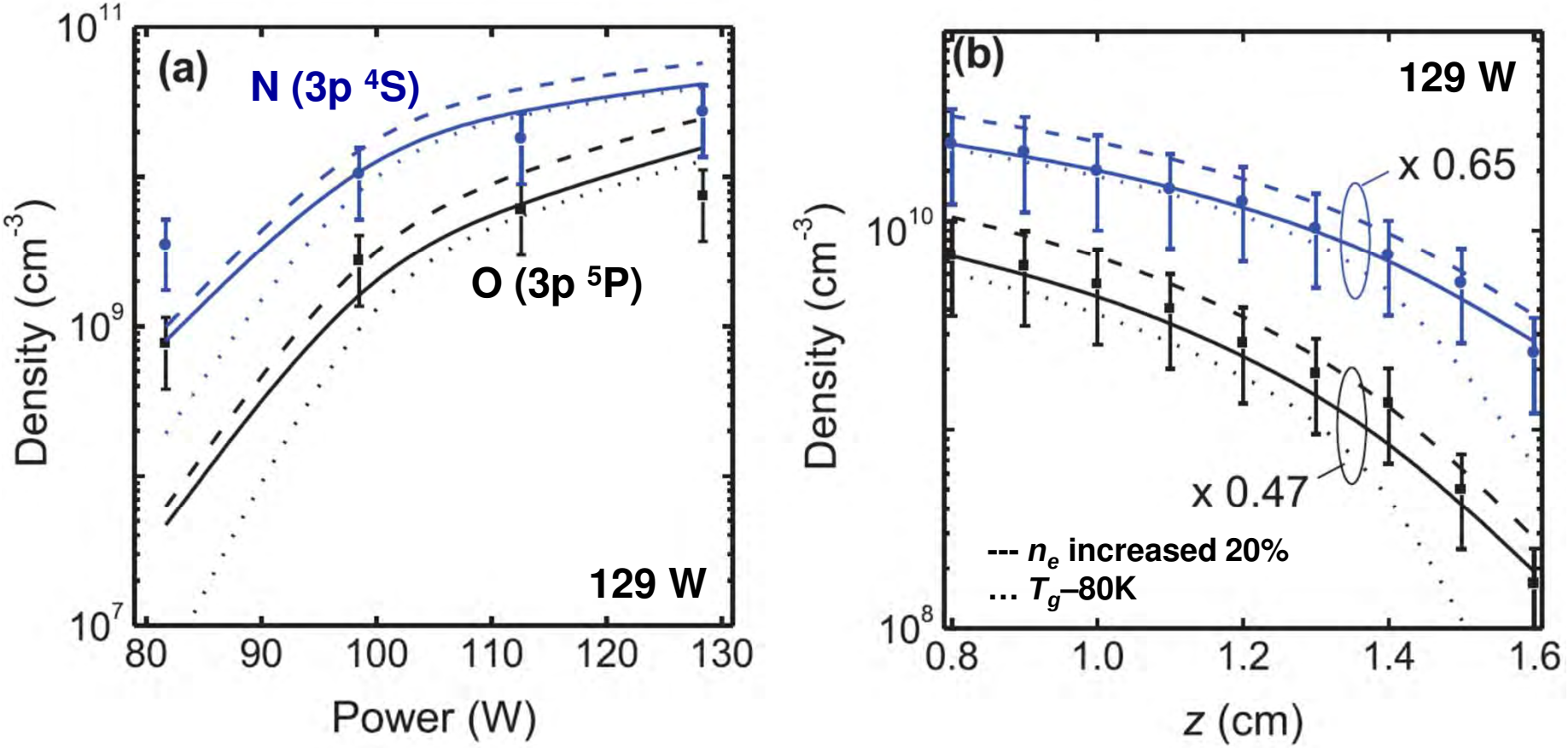


Small radius (345 μm)
Low pressure (300 Pa)

Source: GD Stancu et al, JPD 49 435202 (2016)

Chemical kinetic calculations

Microwave discharge in air - absolute densities of atomic species



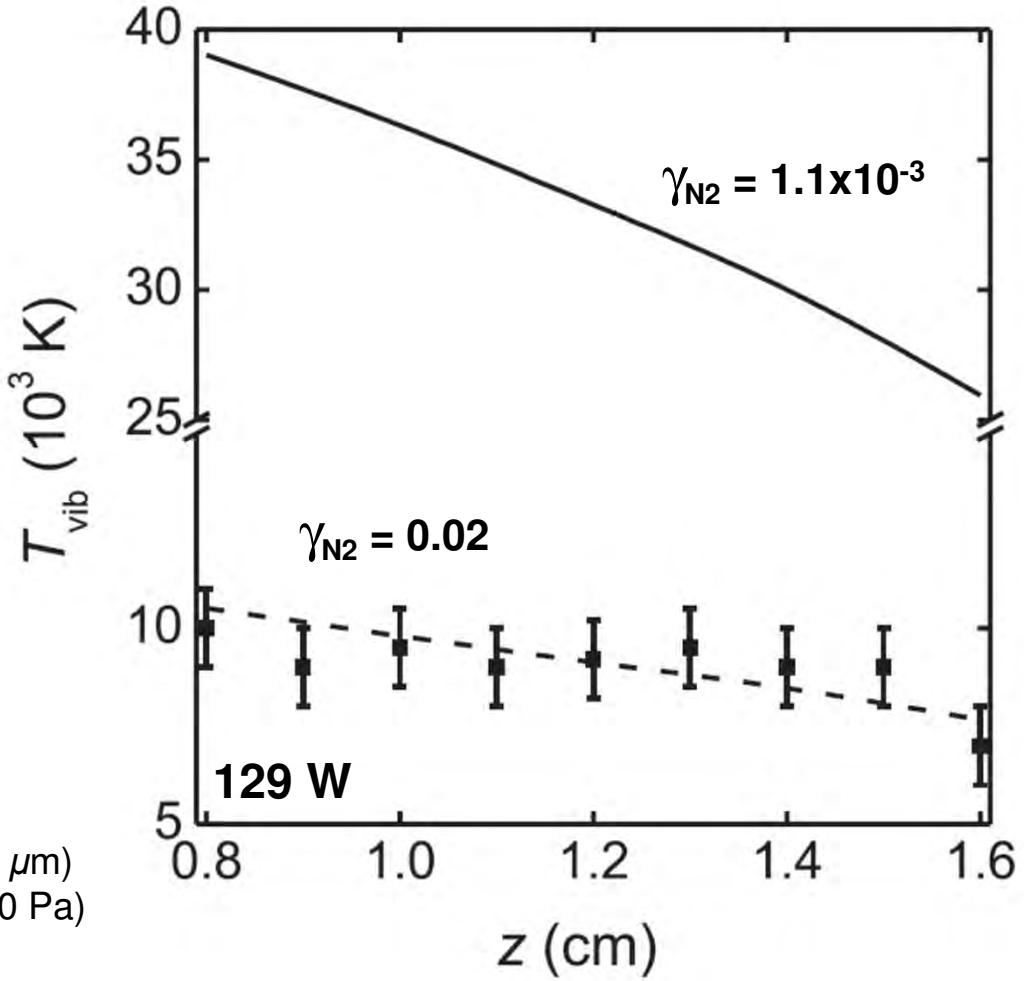
Small radius (345 μm)
Low pressure (300 Pa)

Source: GD Stancu et al, JPD 49 435202 (2016)

Chemical kinetic calculations

Microwave discharge in air - vibrational temperature of the $N_2(C)$ state

Influence of the wall deactivation coefficient



Small radius (345 μm)
Low pressure (300 Pa)

Source: GD Stancu et al, JPD 49 435202 (2016)

Verification of codes

Round-robin call

A **round robin test** is an interlaboratory test (measurement, analysis, or experiment) performed independently several times. This can involve multiple independent scientists performing the test with the use of the same method in different equipment, or a variety of methods and equipment. In reality it is often a combination of the two, for example if a sample is analyzed, or one (or more) of its properties is measured by different laboratories using different methods, or even just by different units of equipment of identical construction.

(***Source: Wikipedia, April 2017***)

Following the GEC16 workshop on LXCat…

The need for a community wide activity on validation of plasma chemical kinetics in commonly used gases has been clearly identified. (…) we would like to propose a round-robin to assess the consistency in results of calculations from different participants in a simplified system.

(***coordination: Sergey Pancheshnyi***)

Verification of codes

Round-robin exercise

General conditions

Gas temperature (constant)	300 K	Species	
Gas pressure (constant)	0.1 bar	e	electrons
Initial density of electrons	1 cm^{-3}	Ar	neutrals
Initial density of ions	1 cm^{-3}	Ar^+	positive ions
Time interval	0 … 0.01 s	Ar*	excited states

Processes and rates

$e + Ar \rightarrow e + Ar$	scattering cross section provided
$e + Ar \rightarrow e + Ar^*$	scattering cross section provided
$e + Ar \rightarrow e + e + Ar^+$	scattering cross section provided
$Ar^+ + e + e \rightarrow Ar + e$	$\boldsymbol{C}$ ($cm^6\ s^{-1}$) = $8.75 \times 10^{-27}\ Te^{-(4.5)}$

Input parameter

$$\frac{E}{N}(\mathrm{Td}) = 43\sqrt{t(\mathrm{ms})}\exp\left[-t(\mathrm{ms})\right]$$

Final remarks

Modelling of LTPs – electron and chemical kinetics

Final remarks

- **Modelling tools are formidable aides for understanding and predicting the behaviour of low-temperature plasmas (LTPs)**

- **The main difficulties in deploying LTP models are**
  - **defining a kinetic scheme for the plasma species**
    (and finding the corresponding elementary data)
  - **describing the plasma excitation and transport**
    (particularly if spatial effects are relevant)

- **Modelling tools need**
  - **verification, e.g. based on crossed-benchmarking, round-robin exercises…**
    (the community is currently starting a collective to meet this goal)
  - **validation of results, by comparing simulations with experiment**
    (collaboration with experimental teams is most welcome)

Modelling of LTPs – electron and chemical kinetics

I need to model a plasma – steps for a recipe

1. **Collect as many information as possible about your system**
   (Dimensions ? Gas pressure ? Gas temperature ? Electron density / power / current ?)
2. **Think about what you want / need**
   (Which quantities / parameters ? For what purpose ?)
3. **Choose the most adequate model approach for your case**
   (Statistical / Kinetic equation / Fluid / CRM & hybrid ?)
4. **Decide about your transport model**
   (check Debye length and mean-free-paths)
5. **Workout your kinetic model**
   (do your bibliography; make educate choices when collecting data)
6. **Choose / develop your simulation tool**
   (when developing, do proper benchmarking and verification of your code)
7. **Validate your modelling results against experimental data**

Questions ?