Steve Biagi's Contributions to Modeling Low Temperature Plasmas (LTPs)

Leanne Pitchford
LAPLACE, Univ. Toulouse III and CNRS, emeritus
pitchford@laplace.univ-tlse.fr

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Outline

1) Low-temperature plasmas
2) Data needs for modeling LTPs
3) The LXCat platform

The take-aways I would like you to have from this talk :

1) The LTP community has benefited tremendously from access to Steve Biagi's compilations of electron/neutral scattering cross sections. These are the best data of their kind available today.
2) Some, but not all, of Steve's data are available on LXCat. I hope we can work together to get more of his data on LXCat.

Low Temperature Plasmas (LTPs)

The properties of plasmas are so remarkable (electrical conductivity, light emission, self-organization, extraordinary chemical activity..) that **"plasma" is considered the 4th state of matter.**

Most of the visible universe is in the plasma state. However, **most of the plasmas on earth are LTPs, created by man** for technical purposes.

In contrast to "fusion" plasmas, **charged particles in LTPs interact with the neutral background gas** and surfaces, as well as with each other.

This **talk will focus on collisional, non-thermal LTPs**, where « $T_{electron}$ » >> $T_{ion} \approx T_g$, with **« $T_{electron}$ » ~ 1 to 10 eV,** and where the degree of ionization is << 10^{-3}.

Much *(but not all!)* of the fundamental physics in LTPs is well established and **much of the research in LTPs is now concerned with the comprehension, development, and optimization of specific plasma configurations for technical applications.**

Technologies based on LTPs – a few examples

Electrical energy

PLASMA

Radiant energy
Source of photons

- Lamps
  - Lighting
  - UV sources for sterlization
- Visualisation
  - Plasma display panels
- Lasers

Kinetic energy
Source of charged particles

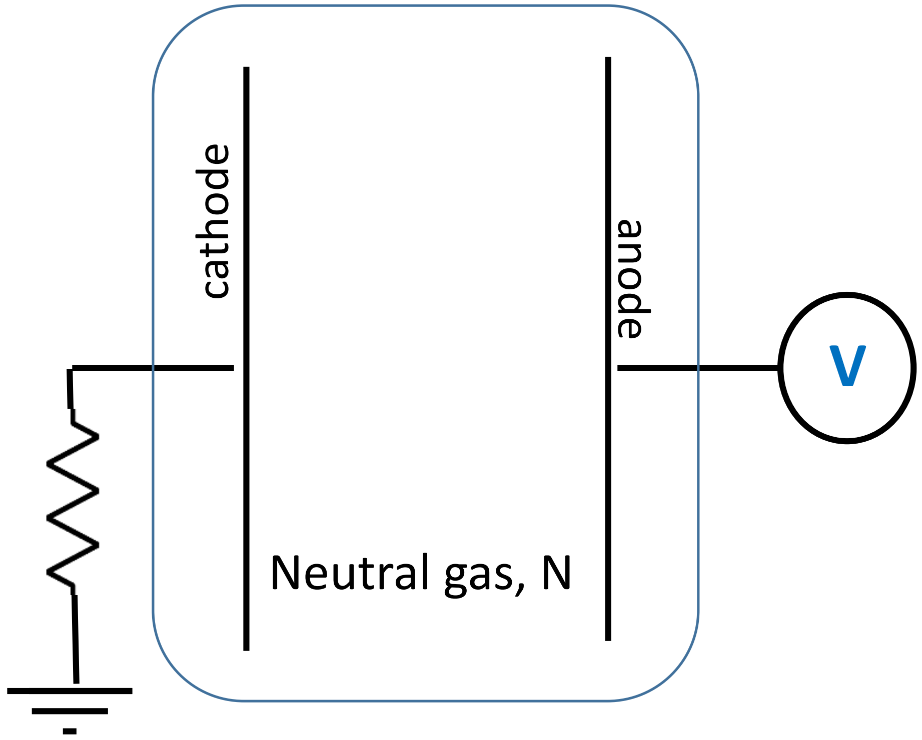
- Ion sources
  - Satellte propulsion
  - Ion sources for ITER
  - Elemental analysis of solids
- Electron beams
  - X-ray sources
- Switches, current interrupters
- Flow control

Chemical energy
Source of reactive species

- Surface processing
  - Microelectronics
  - Functionalization of surfaces
- Volume processes
  - Chemical conversion

Generation of LTPs

LTPs can be generated most simply by applying a voltage (> V_b) beween two electrodes, separated by a gas gap.



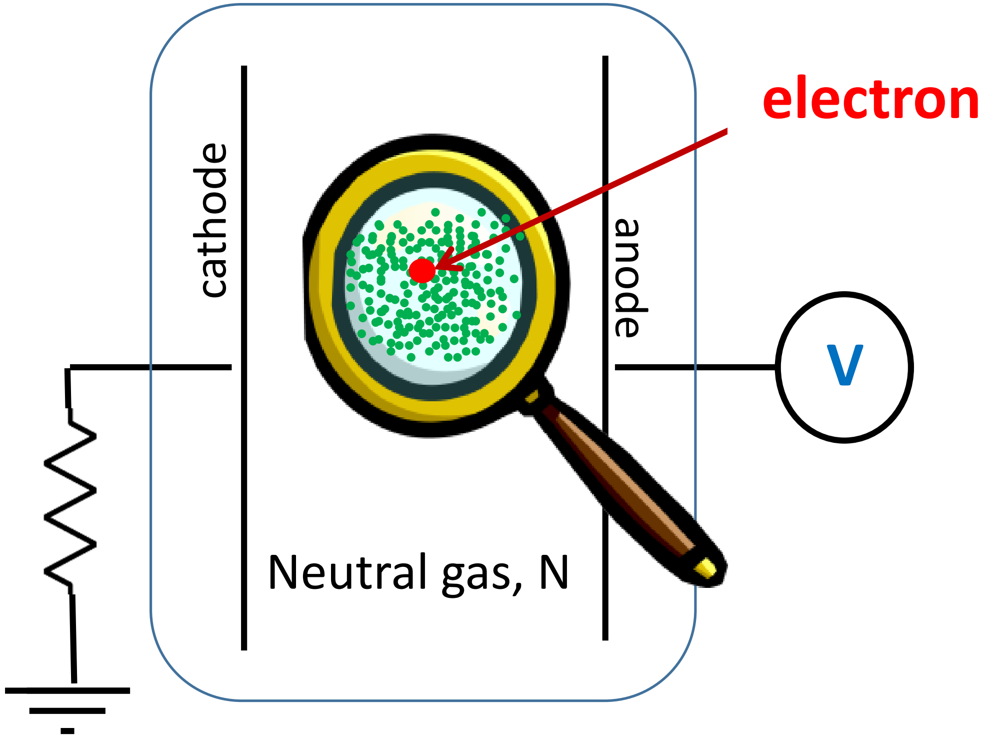
Models of LTPs

INPUT: gas composition and pressure; geometry; circuit; …..

Model

OUTPUT: **E**, n_e, n_{ions}, T_g, species densities,.. as functions of **r** and t

A closer look……



Electrons (very small mass) are easier to accelerate by electric fields than are ions.

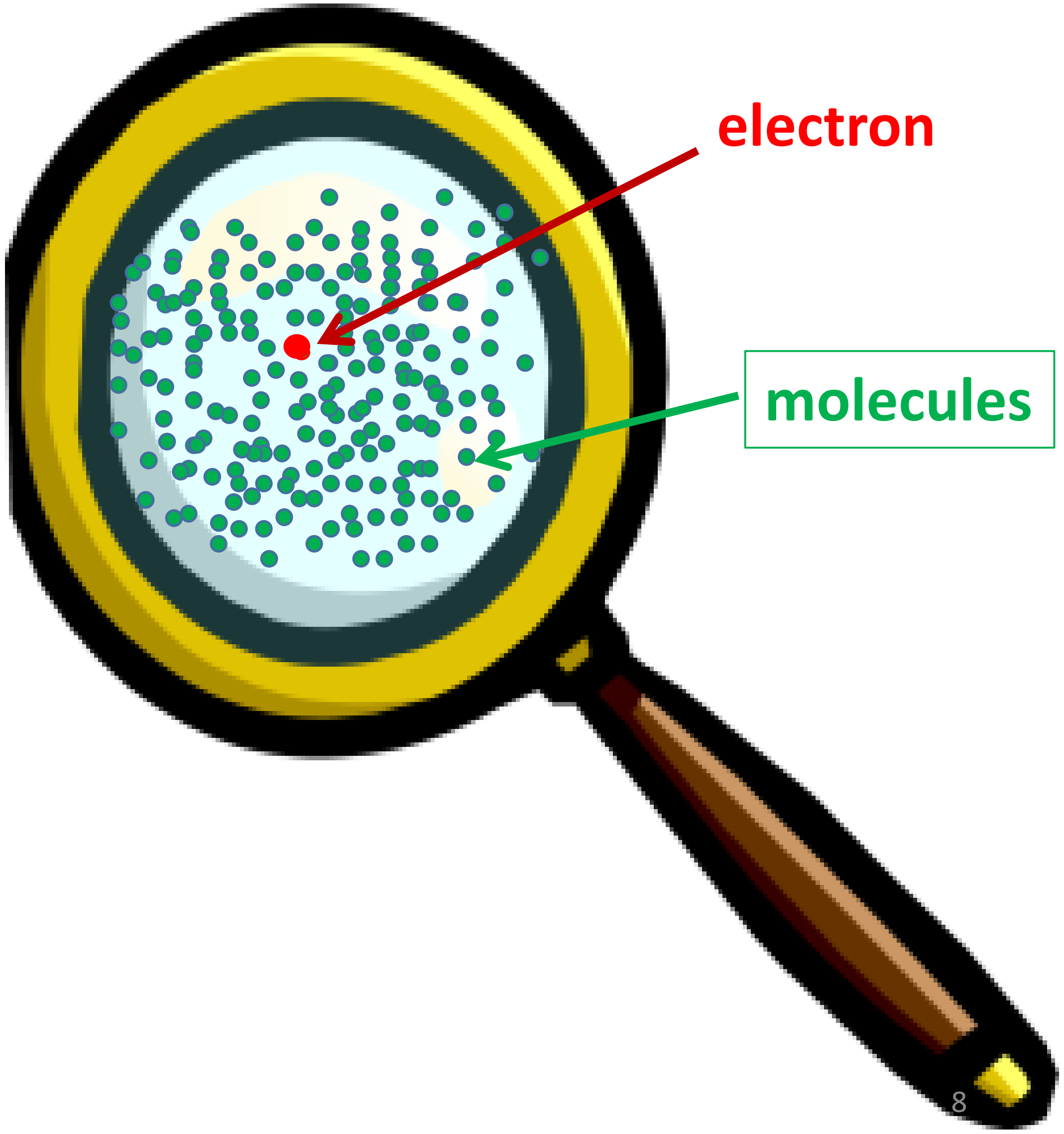
What happens when an energetic electron collides with an $\mathbf{N_2}$ molecule?

elastic collisions : e + $\mathbf{N_2}$=> e + $\mathbf{N_2}$

excitation : e + $\mathbf{N_2}$ => e + $\mathbf{N_2}^*$

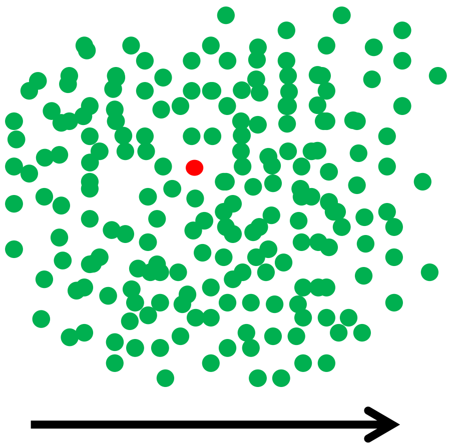
ionization : e + $\mathbf{N_2}$ => e + e + $\mathbf{N_2}^+$

The probability for a collision to happen depends on the electron energy. That is, cross sections depend on electron energy.



Boltzmann equation for electrons

$f(\mathbf{r},\mathbf{v},t)$ = electron velocity distribution function



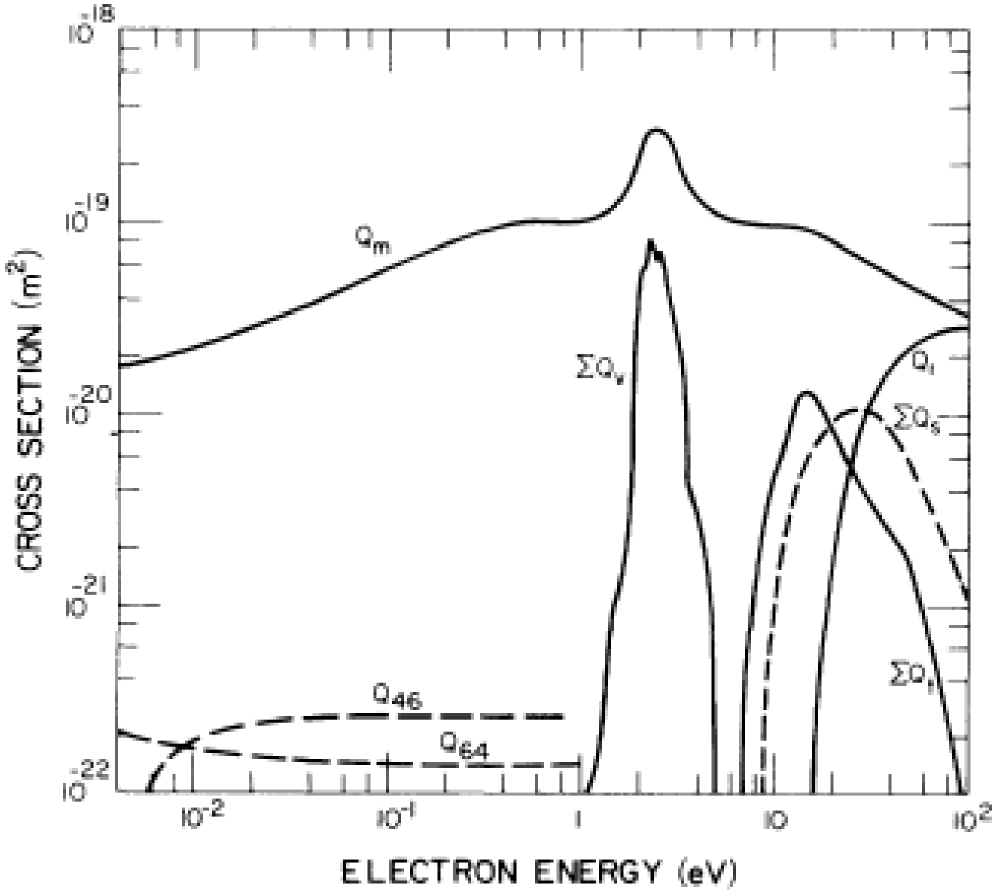
a = -e**E**/m

$$\frac{\partial f}{\partial t} + \underbrace{\vec{v}\cdot\nabla f}_{\text{transport in r}} + \underbrace{\vec{a}\cdot\nabla f}_{\text{transport in v}} = \underbrace{NC[f]}_{\text{collision operator}}$$

where $\int f(\boldsymbol{r},\boldsymbol{v},t)d\boldsymbol{v} = n_e(\boldsymbol{r},t)$

- Electron transport & rate coefficients are integrals over $f(\mathbf{r},\mathbf{v},t)$
- E/N is an important parameter.

Example : electron collisions with nitrogen molecules



MAGBOLTZ – a Fortran code, written by Steve Biagi in 1999 and regularly updated

MAGBOLTZ solves the Boltzmann equation for electrons using a Monte Carlo technique with **E,B** fields at arbitrary angles.

MAGBOLTZ includes Biagi's detailed compilations of electron-neutral scattering cross sections for 56 (!!) different atomic and molecular gases:

Thanks, Marnik!

CF_4	Ar	He	^{3}He	Ne	Kr	Xe	CH_4
C_2H_6	C_3H_8	$i-C_4H_{10}$	CO_2	$C(CH_3)_4$	H_2O	O_2	N_2
NO	N_2O	C_2H_4	C_2H_2	H_2	D_2	CO	$C_3H_8O_2$
C_2H_6O	C_2F_6	SF_6	NH_3	C_3H_6	$c-C_3H_6$	CH_3OH	C_2H_5OH
$i-C_3H_7OH$	Cs	F_2	CS_2	COS	CD_4	BF_3	$C_2H_2F_4$
C_3H_9N	$C_3H_2F_4$	$n-C_3H_7OH$	H_2(para)	D_2(ortho)	CHF_3	CF_3Br	C_3F_8
O_3	Hg	H_2S	$n-C_4H_{10}$	$n-C_5H_{12}$	GeH_4	SiH_4	CCl_4

Such compilations require extensive knowledge of theory, existing measurements with error bars,...

The set of cross sections for each gas, when used in a Boltzmann solver, yields transport and rate coefficients consistent with measurements, which can be very accurate.

Most recent version of MAGBOLTZ

```
C   PROGRAM MAGBOLTZ 2   VERSION 11.19    JANUARY 2024
C -----------------------------------------------------------------------
C   COPYRIGHT 2024   STEPHEN FRANCIS BIAGI
C
C VERSION 11.19     UPDATE OF R134A
C                   SMALL CHANGE IN ELASTIC X-SECTION BETTER FIT
C-----------------------------------------------------------------------
C VERSION 11.18     UPDATE OF R134A C2F4H2   UPGRADE TO 4*
C                   ALSO INTRODUCED A NEW COLLISION TYPE:
C                   ENERGY LOSS = INCIDENT ENERGY - KT
C                   REQUIRED FOR FUTURE HFO ANALYSIS
C-----------------------------------------------------------------------
C VERSION 11.17     UPDATE OF C2F6(1999) BETTER FIT TO ARGON MIXTURE DATA
C-----------------------------------------------------------------------
C VERSION 11.16     UPDATE OF SIH4 FROM   2005  FILE
C                   BETTER FITS TO ARGON AND KRYPTON MIXTURES
C-----------------------------------------------------------------------
C VERSION 11.15     UPDATE OF ETHENE C2H4 FROM  1999 FILE
C                   NOW BETTER THAN 1% ON ARGON/ETHENE MIXTURES 5*
C-----------------------------------------------------------------------
C VERSION 11.14     ADDED CARBON TETRA CHLORIDE TO LIST
C                   CARBON TETRA CHLORIDE HAS THE HIGHEST DIELECTRIC
C                   BREAKDOWN STRENGTH BEING 2.5 TIMES HIGHER THAN
C                   SF6 THE GAS ALSO HAS A LOWER GLOBAL WARMING POTENTIAL
C                   THAN MOST FLOURINE BASED GASES.
C
```

Version 11.19: > 100 000 lines of Fortran code on 1443 pages

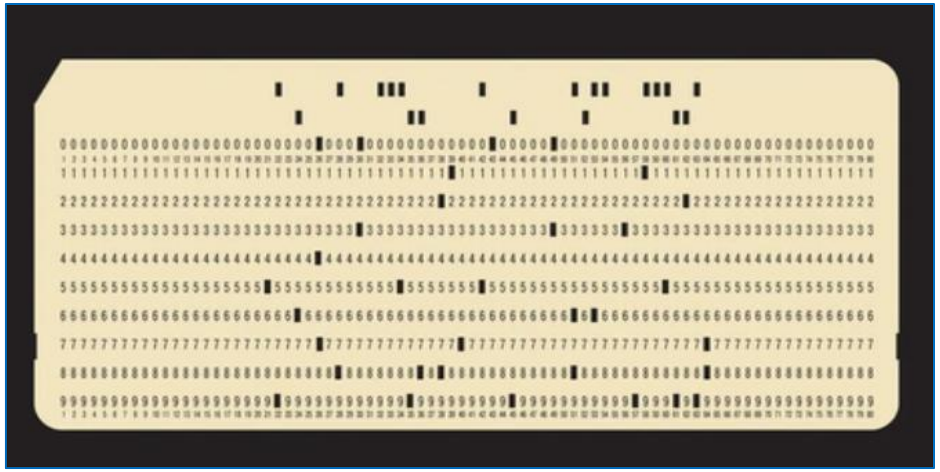
Cross sections for each of gas species are ***hardwired*** into MAGBOLTZ.

MAGBOLTZ input parameters

```
C-----------------------------------------------------------------
C    INPUT CARDS :
C------------------------------------------------------------
C   FIRST CARD: 4I10,F10.5   :  NGAS,NMAX,IPEN,ITHRM,EFINAL
C   NGAS:  NUMBER OF GASES IN MIXTURE
C   NMAX: NUMBER OF REAL COLLISIONS ( MULTIPLE OF 1*10**7 )
C   USE NMAX = BETWEEN 2 AND 5 FOR INELASTIC GAS TO OBTAIN 1% ACCURACY
C       NMAX = ABOVE 10 FOR BETTER THAN 0.5% ACCURACY.
C       NMAX = AT LEAST 10 FOR PURE ELASTIC GASES LIKE ARGON
C       HIGHER VALUES THAN NMAX=214 CAN ONLY BE USED ON COMPUTERS SUCH
C       AS DEC ALPHAS WITH TRUE 64 BIT INTEGERS. PCS ARE LIMITED TO
C       31 BIT INTEGERS...
C     IPEN   = 0 PENNING EFFECTS NOT INCLUDED
C            = 1 PENNING EFFECTS INCLUDED (SEE INSTRUCTIONS ABOVE)
C     ITHRM  = 0 GAS MOTION ASSUMED TO BE AT O KELVIN (STATIC GAS)
C     ITHRM  = 1 GAS MOTION TAKEN TO BE AT INPUT TEMPERATURE
C     EFINAL = UPPER LIMIT OF THE ELECTRON ENERGY IN ELECTRON VOLTS.
C     EFINAL = 0.0 (PROGRAM AUTOMATICALLY CALCULATES UPPER INTEGRATION
C                 ENERGY LIMIT)
C-------------------------------------------------------------
C   SECOND CARD : 6I5    : NGAS1 , NGAS2, NGAS3 , NGAS4 , NGAS5 , NGAS6
C        NGAS1,ETC :  GAS NUMBER IDENTIFIERS (BETWEEN 1 AND 80)
```

MAGBOLTZ input parameters

```
C-----------------------------
C   INPUT CARDS :
C-----------------------------
C  FIRST CARD: 4I10,F10.5
C  NGAS:   NUMBER OF GASES I
C  NMAX: NUMBER OF REAL COI
C  USE NMAX = BETWEEN 2 ANI
C      NMAX = ABOVE 10 FOR
C      NMAX = AT LEAST 10 I
C      HIGHER VALUES THAN I
C      AS DEC ALPHAS WITH T
C      31 BIT INTEGERS...
C    IPEN   = 0 PENNING EFI
C           = 1 PENNING EFI
C    ITHRM  = 0 GAS MOTION
C    ITHRM  = 1 GAS MOTION
C    EFINAL = UPPER LIMIT C
C    EFINAL = 0.0 (PROGRAM A
C                ENERGY LIMIT,
C------------------------------------------------------------
C  SECOND CARD : 6I5    : NGAS1 , NGAS2, NGAS3 , NGAS4 , NGAS5 , NGAS6
C       NGAS1,ETC :  GAS NUMBER IDENTIFIERS (BETWEEN 1 AND 80)
```



IBM 80-column, punched card

The LXCat platform (initiated at LAPLACE in 2009)

LXCat is a web-based, community-wide project for the curation of

data needed in modeling low-temperature plasmas

Electron + neutral
cross sections / oscillator strengths/ swarm parameters

Ion + neutral
cross sections / interaction potentials / swarm parameters

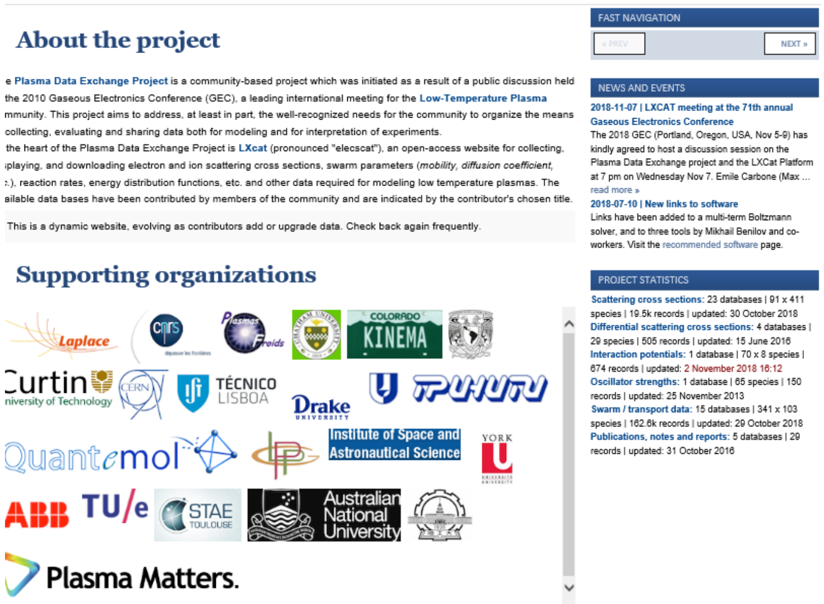
Plasma-surface interactions

Plasma chemistry

Radiation

LXCat

ELECtron (and ion) SCATtering



Availability of data before 2009

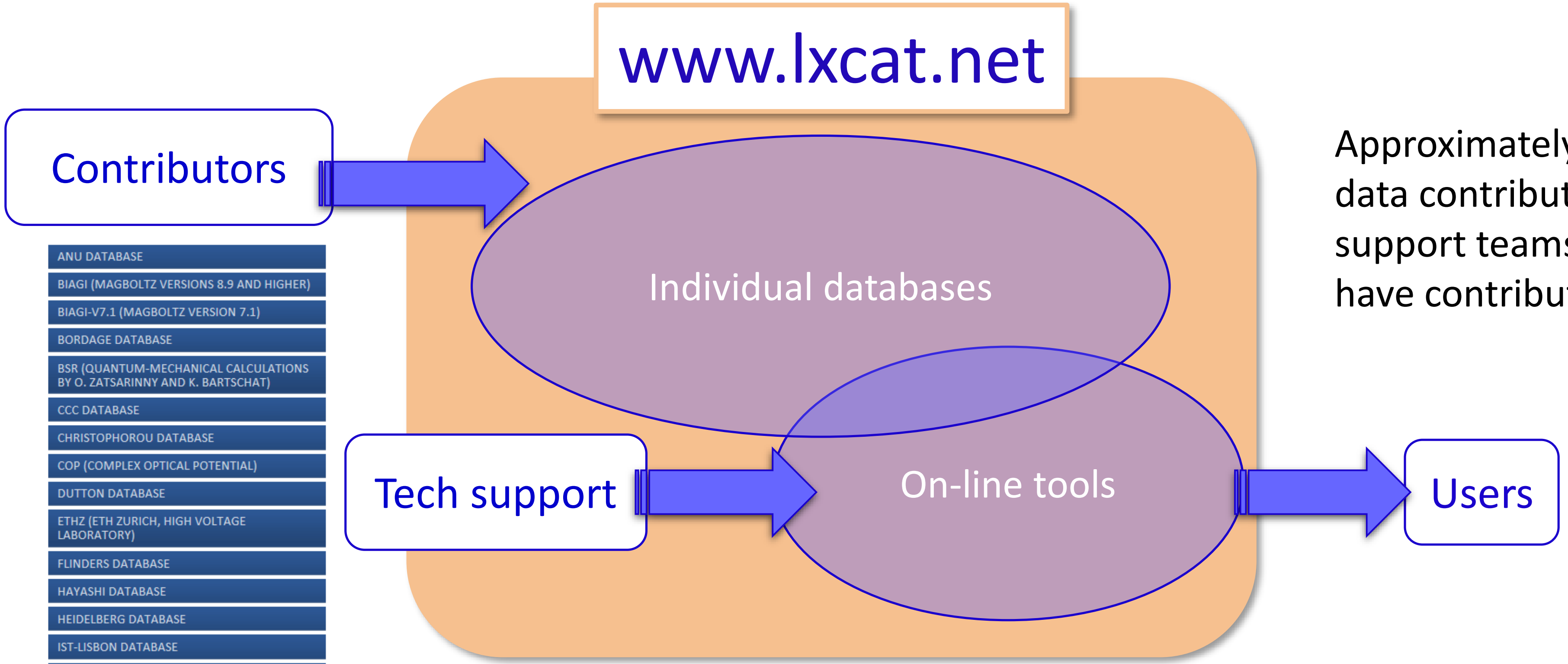
Most people working in the area of modeling LTPs had their own databases, suitable for use in their own codes.

Some on-line compilations of numerical data for electron/neutral scattering cross sections were available, but in different formats, different units, with more or less detail, and of variable accuracy.

People have been generally willing to share their data.

➔ In 2010, the Gaseous Electronics Conference agreed to host a Plasma Data Exchange Project which was largely based on LXCat. In this context we organized 3 workshops at GEC 2011, 2012 and 2013.

LXCat structure – on-line tools



- ANU DATABASE
- BIAGI (MAGBOLTZ VERSIONS 8.9 AND HIGHER)
- BIAGI-V7.1 (MAGBOLTZ VERSION 7.1)
- BORDAGE DATABASE
- BSR (QUANTUM-MECHANICAL CALCULATIONS BY O. ZATSARINNY AND K. BARTSCHAT)
- CCC DATABASE
- CHRISTOPHOROU DATABASE
- COP (COMPLEX OPTICAL POTENTIAL)
- DUTTON DATABASE
- ETHZ (ETH ZURICH, HIGH VOLTAGE LABORATORY)
- FLINDERS DATABASE
- HAYASHI DATABASE
- HEIDELBERG DATABASE
- IST-LISBON DATABASE
- ITIKAWA DATABASE
- LAPLACE (MEASUREMENTS AFTER 1975)
- MORGAN (KINEMA RESEARCH & SOFTWARE)
- NGFSRDW DATABASE
- PHELPS DATABASE
- PUECH DATABASE
- QUANTEMOL DATABASE
- SIGLO DATABASE
- TRINITI DATABASE
- UBC DATABASE
- UNAM DATABASE
- VIEHLAND DATABASE
- BOLSIG+ SOLVER

Approximately 65 volunteers – both data contributors as well as the support teams - from 17 countries have contributed to this project.

LXCat review articles

S Pancheshnyi *et al.,* Chem. Phys. **398** 148 (2012)

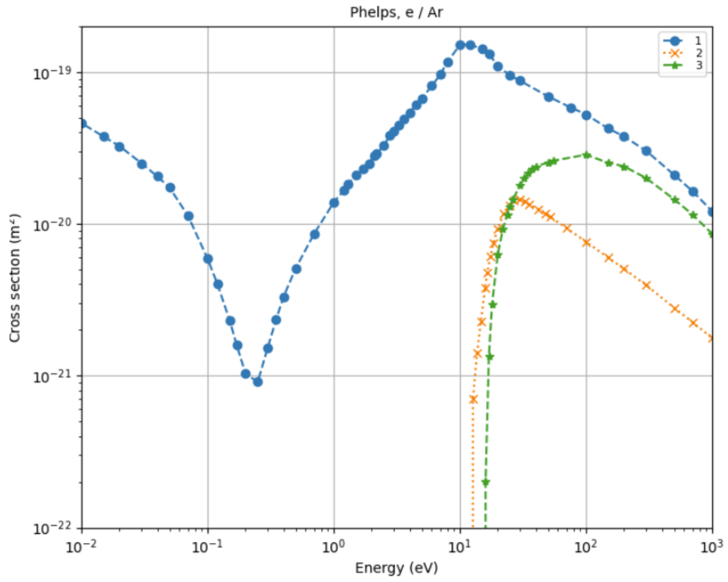
LC Pitchford, *et al.*, Plasma Processes and Polymers, **14** 1600098 (2017)

E Carbone, *et al.,* Atoms ***9*** (1), 16 (2021).

Steve Biagi, one of the first contributors to LXCat, and Luis Alves (IST-Lisbon database) visited Toulouse in 2011 to prepare for the workshop on LXCat at the upcoming Gaseous Electronics Conference. The focus of the workshop was comparisons of data for rare gases on different databases.

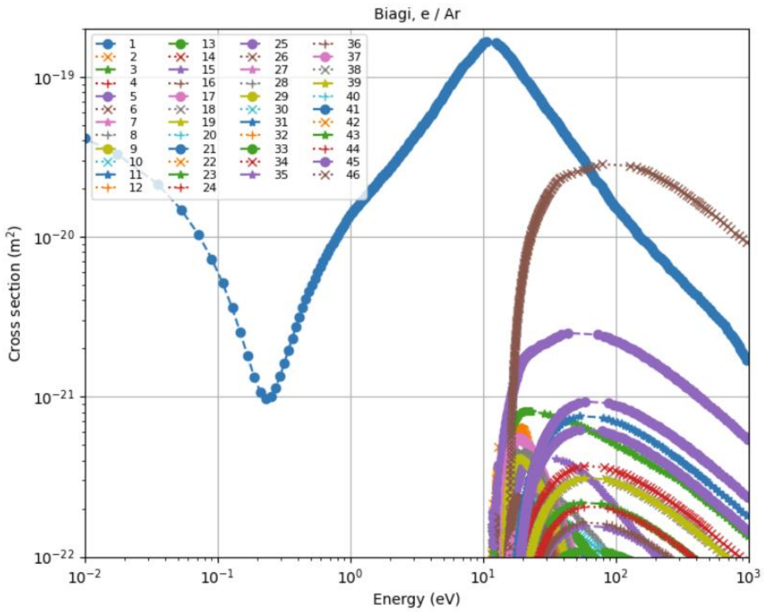
Steve Biagi (UK), Leanne Pitchford, Mairie-Claude Bordage, and Luis Alves

Datasets for e/Ar from two different databases



Phelps

1 excitation levels



Biagi

44 excitation levels

Comparisons of calculated reduced mobility in Argon

J. Phys. D: Appl. Phys. **46** (2013) 334001

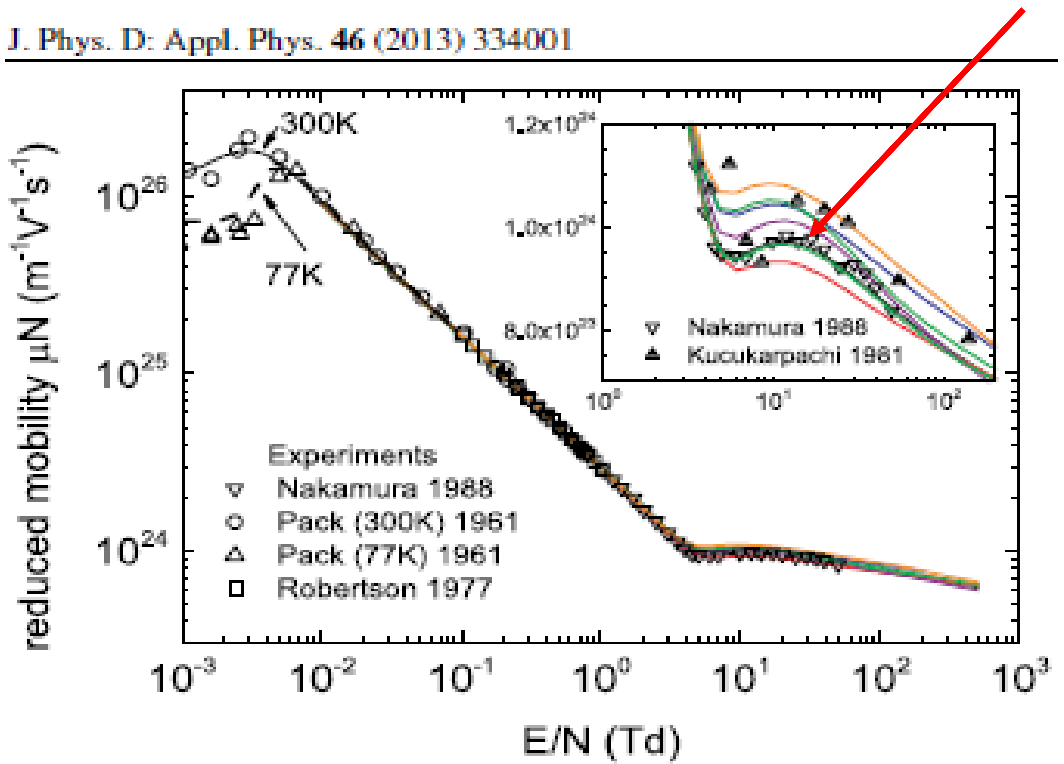


Figure 5. Reduced electron mobility versus E/N. The symbols are experimental data and the solid lines are calculations using the two-term Boltzmann solver, BOLSIG+. The inset is a zoom to illustrate the differences in the calculated results in the region of the knee at $E/N \sim 5$ Td. The colour code is BIAGI-v8.9 (——); BSR (——); HAYASHI (——); IST-LISBON (——); MORGAN (——); PHELPS (——); PUECH (——). The legend refers to the first author and year of publication of references reporting measurements shown in the figure.

See similar comparisons for He, Ne, Kr, Xe, N_2, O_2, H_2, D_2, CO_2 available on the LXCat site.

What data are available on LXCat today?

for electrons

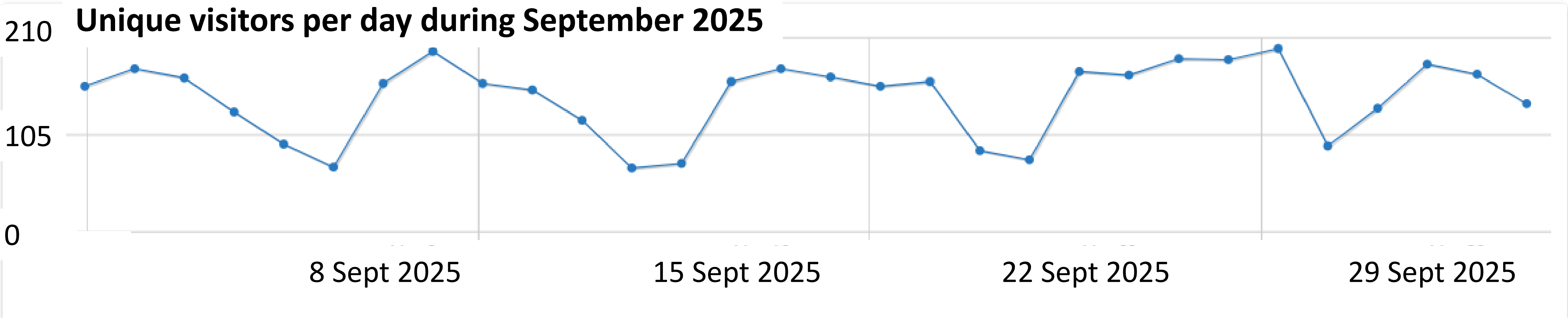
23 databases containing electron/neutral scattering cross sections*
1 database containing optical oscillator strengths for 65 species
5 databases containing differential scattering data
12 databases containing swarm/transport data

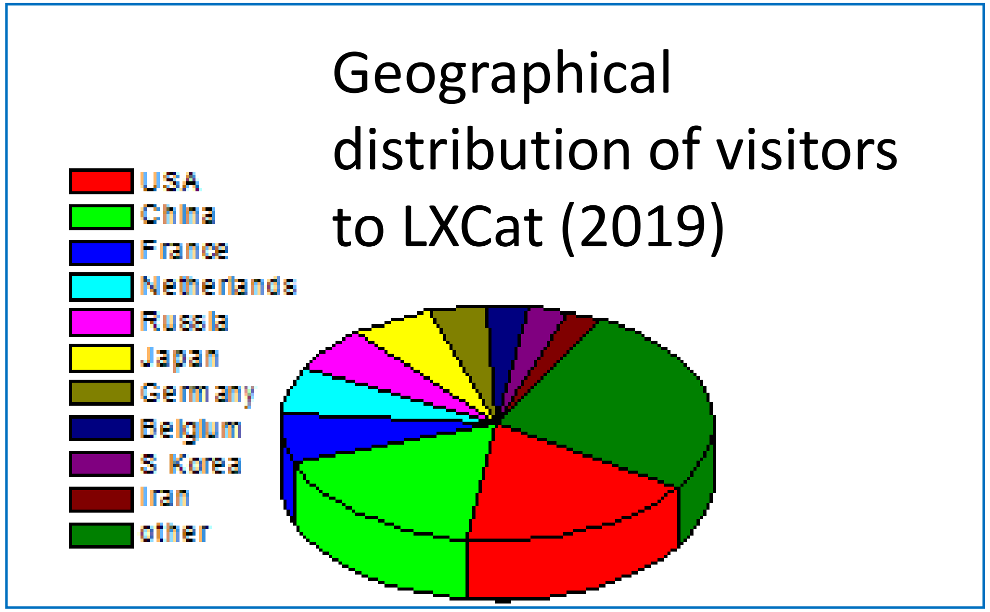
for ions

2 databases containing ion/neutral scattering cross sections
1 database with interaction potentials
3 databases containing swarm/transport data

* The Biagi data are the most downloaded.

Some LXCat statistics





The formal by-laws for the project are available on the LXCat site.
The non-profit organization, « Data for Modeling Plasmas » (DMP), was established in France in 2015.


Remembering Steve, a colleague and a friend,
and his wife, Marie — together again, and
fondly remembered.

Cinque Terre, Italy, 2015