

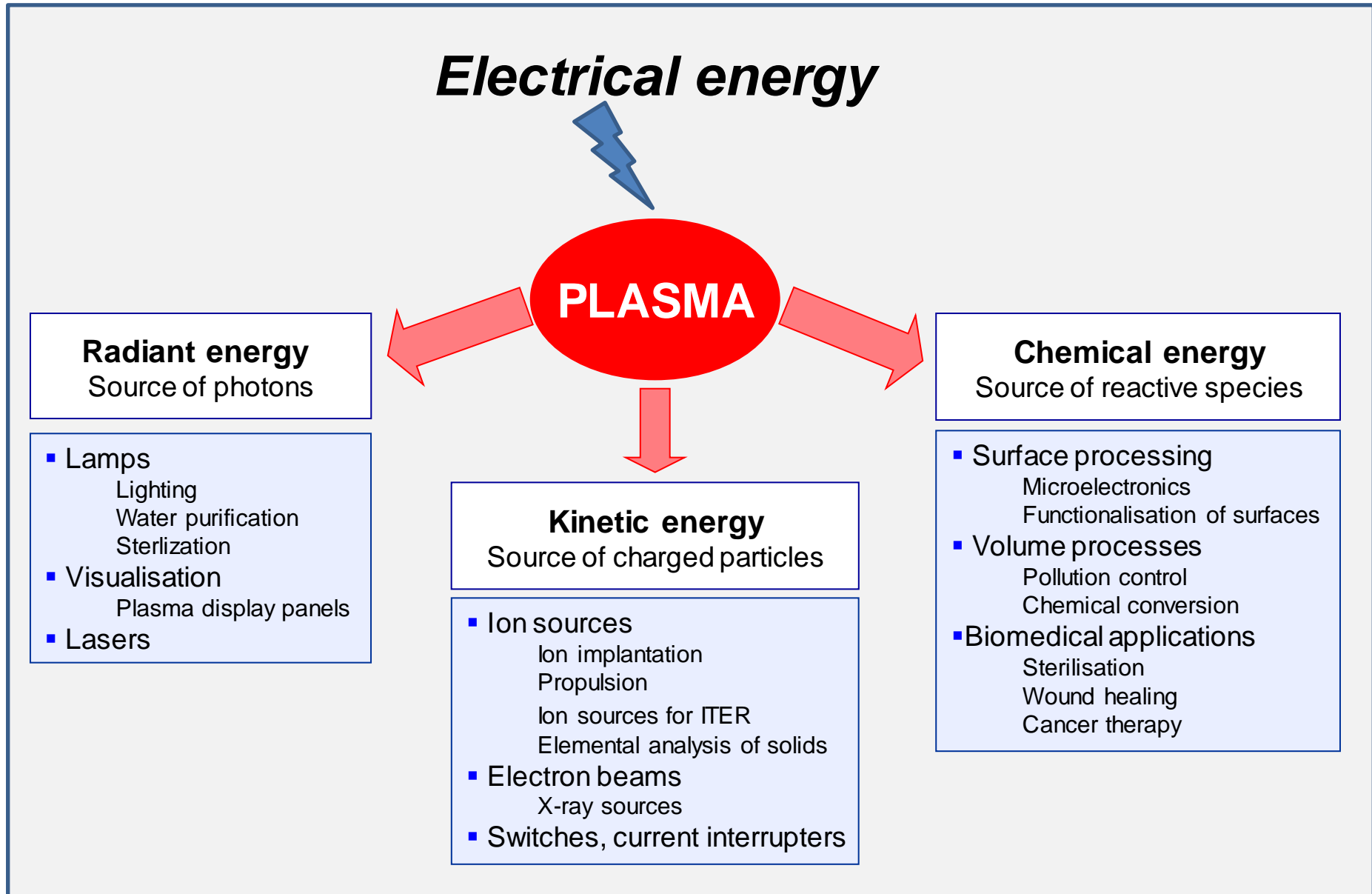
*LXCat : a web-based, community-wide  
project on data needed for modeling  
low temperature, non-LTE plasmas*

***LXCat = ELECtron (and ion) SCATtering***

**www.lxcat.net**

*Presented by Leanne Pitchford, on behalf of the LXCat team  
LAPLACE, Univ Toulouse and CNRS  
Toulouse, France*

# Low-temperature plasma technologies – some examples



# Background and motivation

How to obtain data electron scattering and transport data needed for modeling?

The situation a few years ago (2008):

- Published data are/were usually presented in figure format.
- Some compilations and reviews were available.
- Some on-line compilations of data were available (Morgan, SIGLO, Phelps, NIFS Japan, and others) in different formats and more or less complete, accurate.
- Many other private compilations existed (ex: Biagi, Kushner, Lisbon, Petrovic)
- People are generally willing to share data, if it takes them no time to do so!
- Sergey Pancheshnyi was interested in developing something a bit better....

## Modeling low temperature plasmas : Data needs are extensive.

Electron-neutral (cross sections and/or transport coefficients)

Ion-neutral (cross sections, interaction potentials and/or transport coefficients)

Neutral and ion chemistry

Plasma surface interactions

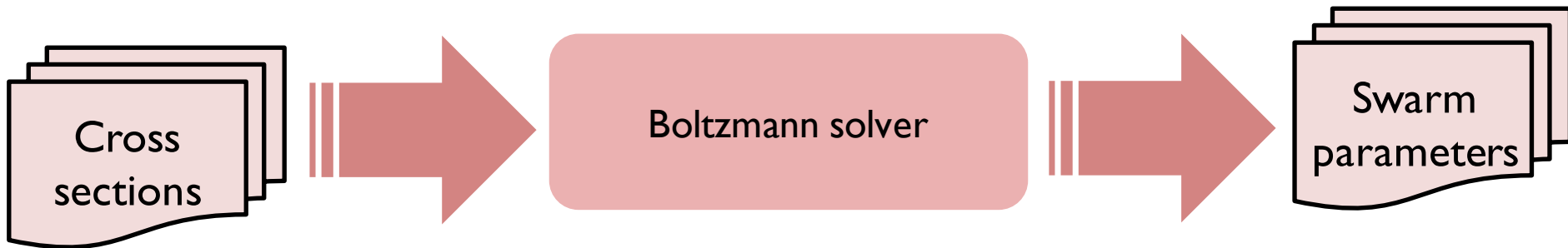
Radiation

....

***Present focus of the LXCat project*** : electron-neutral scattering cross sections from ground state targets, over an energy range from thermal up to some kV.

Data needs depend on the model formulation, but the fundamental data are the cross sections.

**Complete sets of cross sections:** electron-neutral (ground state) describing momentum-loss, energy-loss processes, and electron number changing processes (ionization, attachment, ...)



**Swarm parameters:** electron transport (mobility, diffusion), rate coefficients as functions of  $E/N$  (if non-Maxwellian) or average energy

Consistency of measured and calculated swarm parameters is a minimum requirement for validation of the cross section data set.

# LXCat in 2015

www.lxcat.net

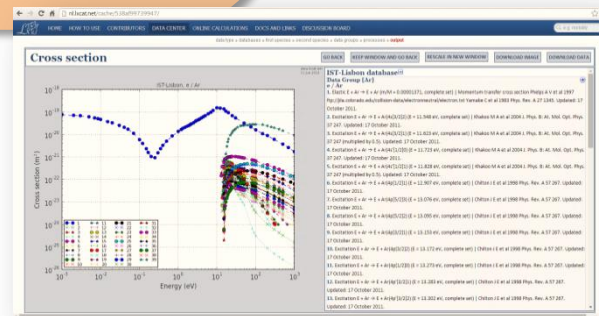
Contributors

Individual databases  
~22 at present  
(~ 30 people from 12 countries)

On-line tools

Users

BSR (QUANTUM-MECHANICAL CALCULATIONS BY O. ZATSARINNY AND K. BARTSCHAT)
BIAGI-V7.1 (MAGBOLTZ VERSION 7.1)
BIAGI-V8.9 (MAGBOLTZ VERSION 8.9)
BORDAGE DATABASE
BRAY DATABASE
DUTTON DATABASE
FLINDERS DATABASE
HAYASHI DATABASE
IST-LISBON DATABASE
ITIKAWA DATABASE
LAPLACE (MEASUREMENTS AFTER 1975)
MORGAN (KINEMA RESEARCH & SOFTWARE)
NGFSRDW DATABASE
PHELPS DATABASE
PUECH DATABASE
QUANTEMOL DATABASE
SIGLO DATABASE
TRINITY DATABASE
URQUIJO (DE URQUIJO DATABASE, UNAM)
VIEHLAND DATABASE
UBC DATABASE
ETHZ (ETH ZURICH, HIGH VOLTAGE LABORATORY)
BOLSIG+ SOLVER



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

# Contributors to the LXCat project

(updated October 2015)

**Website conception and development:** S Pancheshnyi, France /Switzerland

**Electrons: Compilations of cross section data :** MC Bordage, V. Puech, LC Pitchford, France; SF Biagi, UK; WL Morgan, AV Phelps\*, USA; LL Alves and CM Ferreira\*, Portugal; Kochetov and Napartovich, Russia; Y. Itikawa, M Hayashi\*, Japan; L Campbell and M Brunger, Australia ; C Brion (measured oscillator strengths), Canada

**Quantum calculations:** J. Tennyson and D. Brown, UK; O. Zatsarinny and K. Bartschat USA; I. Bray and D. Furst, Australia; Al Stauffer, Canada

**Compilations of experimental transport coefficients:** transcription of data from publications S. Chowdhury, France/India; J. de Urquijo, Mexico; LL Alves, Portugal; A. Chachereaun Switzerland

**Ions:** L Viehland, AV Phelps, USA; J. de Urquijo, Mexico

**On-line Boltzmann solver for electrons:** GJM Hagelaar, France

**Technical assistance:** S. Chowdhury and B Chaudhury, France/India;

**Mirror site :** J van Dyke, the Netherlands

\*deceased

Demonstration of the LXCat website



# The LXCat platform

- **Considerations**

- Contributors and users are typically not experts in curation of data:

- User-specific data tables (different complexity, functionalities, formats, etc.) for contributors
- Simple and straightforward web interface for users
- Server-to-server interface for external projects (VAMDC)

- Community project, no solid funding:

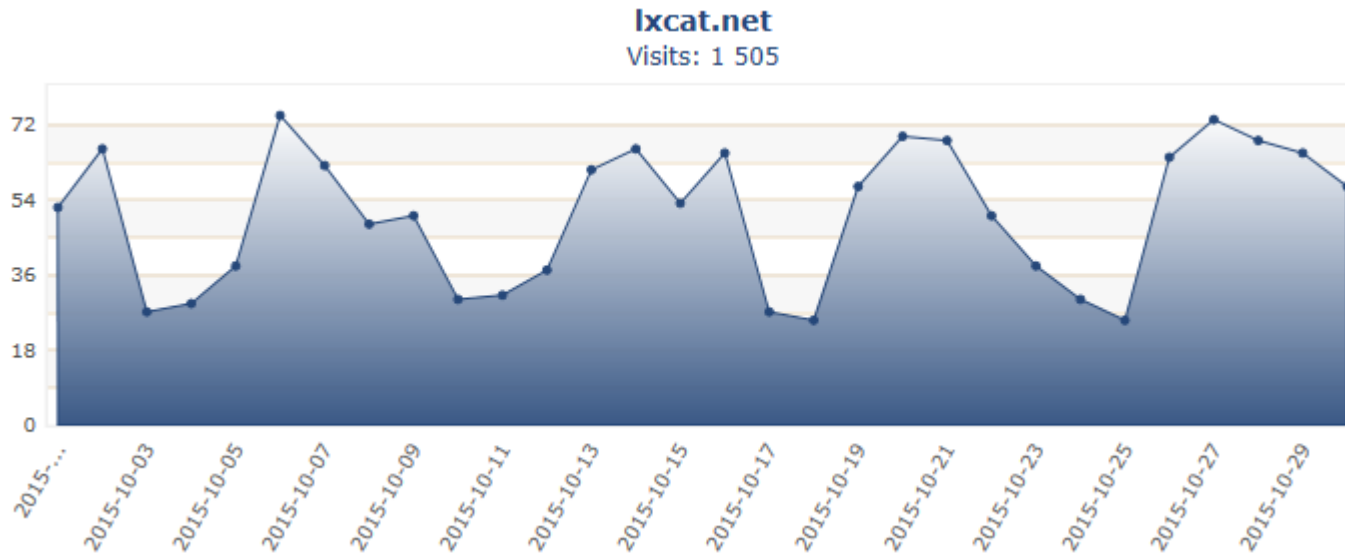
- High reliability with low maintenance need

- **Final structure**

- Standard LAMP system: Linux (operating system), Apache (web server), MySQL (database), PHP & Python (script languages)

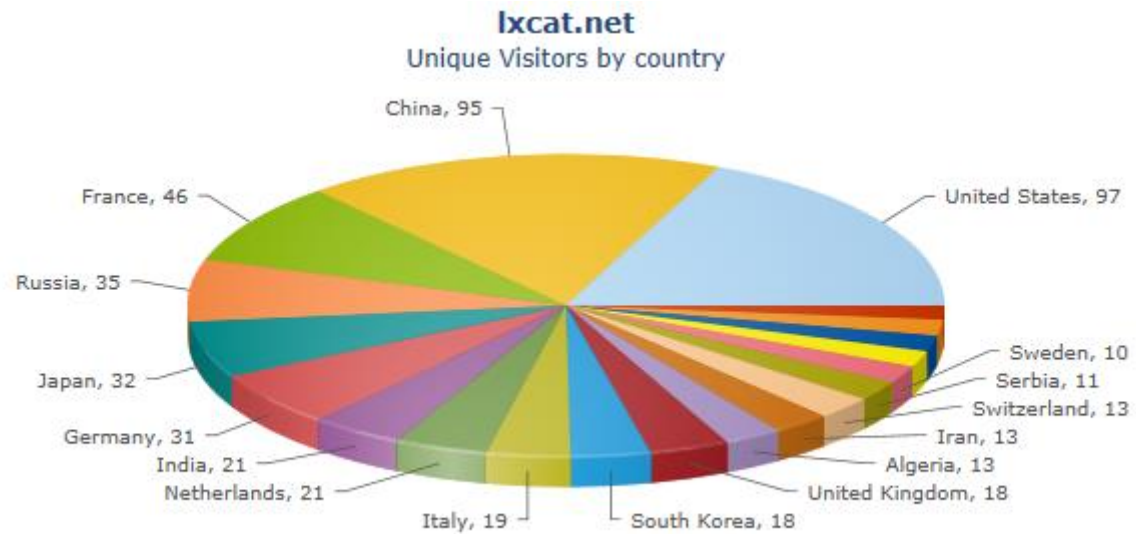
- One master server (LAPLACE, 2010) and (multiple) mirroring nodes (TU/e, 2013) separated geographically

# LXCAT: some statistics



**Number of unique visitors per day over the last month**

**Where are they from?**



# GEC Plasma Data Exchange Project => evaluation

## Cluster issue : 2013 *J. Phys. D: Appl. Phys.* **46** Issue 33

*Paper I: Comparisons of sets of electron-neutral scattering cross sections and swarm parameters in noble gases I. Argon* LC Pitchford, Alves LL, Bartschat K, Biagi SF, Bordage MC, Phelps AV, Ferreira CM, Hagelaar GJM, Morgan WL, Pancheshnyi S, Puech V, Stauffer A and Zatsarinny O

*Paper II: Comparisons of sets of electron-neutral scattering cross sections and swarm parameters in noble gases II. Helium and Neon* LL Alves, Bordage MC, Biagi SF, Pitchford LC, Zatsarinny O, Bartschat K, Hagelaar GJM, Pancheshnyi S, Ferreira CM, Puech V, Morgan WL and Phelps AV

*Paper III: Comparisons of sets of electron-neutral scattering cross sections and swarm parameters in noble gases III. Krypton and Xenon* MC Bordage, SF Biagi, LC Pitchford, K Bartschat, S Chowdhury, GJM Hagelaar, WL Morgan, V Puech, O Zatsarinny

*Paper IV: Computational Methods for Electron-Atom Collisions in Plasma Applications*  
K. Bartschat

# Looking to the future.....

- **Continuing development of on-line tools, expansion of databases, and "evaluation" of data:** new on-line tools, new contributors, new data types; some "evaluations" have been published, others have been presented at the conferences and will be published, further work is in progress.
- **Assuring proper credit to all contributors:** we need a consistent format for referencing websites; journals should ask referees to be especially attentive to references for sources of data in articles reporting results of calculations. Traceability!
- **Coordination with model developers and with other on-going data activities:** users of some commercial codes are referred to LXCat for data; data from external sources could be imported temporarily to the LXCat platform to make use of the existing on-line tools – is this of interest?
- **Setting up a structure to assure survivability:** in July 2015, we created a non-profit association in France (DMP = Data for Modeling Plasmas) which can be used for community-funding & community-management of data related projects. See [http: //assoc.lxcat.net](http://assoc.lxcat.net) for details.

**to participate, contact [lxcat.info@gmail.com](mailto:lxcat.info@gmail.com)**