LXCat 3 and beyond

Towards reproducible plasma modeling studies

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Jan van Dijk

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Reproducibility of results

Reproducibility of results

We have a problem

- Modeling results are very hard to reproduce
- Sometimes even for the author…

Finally, it is also important to underline the need for accurate input data (cross sections, rate coefficients, surface coefficients, etc), see section 20. Efforts to develop a database as LXCAT with standardized input data, accompanied with papers [243] and sessions in conferences have to be pursued.

20. Atomic, molecular and transport data

Luís Lemos Alves[1] *and Annarita Laricchiuta*[2]

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[2] CNR Institute for Plasma Science and Technology (ISTP) Bari Section, Bari, Italy

Status

LTPs are at the basis of key-enabling technologies (e.g. material synthesis and processing and energy and environment), they have been used in biological and medical applications, and they are essential to pave the way to Space exploration. Modeling studies and experimental analyses are

[1] Adamovich et al. The 2022 Plasma Roadmap: low temperature plasma science and technology. *Journal of Physics D: Applied Physics*, *55*(37). https://doi.org/10.1088/1361-6463/ac5e1c

VIII. PLASMA AND RELATED DATABASE

A. Introduction

In the study of any of the different plasmas discussed in this review a common challenge is to obtain a thorough understanding of the physical and chemical properties of plasmas. In order to determine such properties, it is essential to assemble authoritative databases that allow the design, diagnostics and monitoring of the plasma.

[2] Anirudh, R. et al. *2022 Review of Data-Driven Plasma Science*. http://arxiv.org/abs/2205.15832

4. Data and mechanisms

Over the past decade, the topic of input data for computational models and simulations of LTPs has taken on greater importance and experienced increased activity within the LTP community. The community has realized that reliable and validated data is critical to the use of models in both investigating processes in established parameter spaces and extending models into yet-to-be-experimentally investigated parameter spaces. This increased interest has

[3] Alves, L. L. et al. (2023). Foundations of plasma standards. *Plasma Sources Science and Technology*, *32*(2). https://doi.org/10.1088/1361-6595/acb810

Reproducing modeling results

Two main components

- Simulation code
- Input data

Reproducing modeling results

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- Input data

=> Open source development

Reproducing modeling results

Two main components

- Simulation code => Open source development
- Input data => Advanced **data platforms**

Reproducing modeling results

Two main components

- Simulation code => Open source development
- Input data => Advanced **data platforms**

Do not exist for plasma chemistry data

- Where to start?

State of the art: LXCat ("elecscat") [4]

Electron (and ion) collisional processes in plasmas

- **Cross sections**
- Potentials
- Swarm parameters

[4] Carbone, E., Graef, W., Hagelaar, G., Boer, D., Hopkins, M. M., Stephens, J. C., Yee, B. T., Pancheshnyi, S., van Dijk, J., & Pitchford, L. (2021). Data Needs for Modeling Low-Temperature Non-Equilibrium Plasmas: The LXCat Project, History, Perspectives and a Tutorial. *Atoms*, *9*(1), 16. https://doi.org/10.3390/atoms9010016

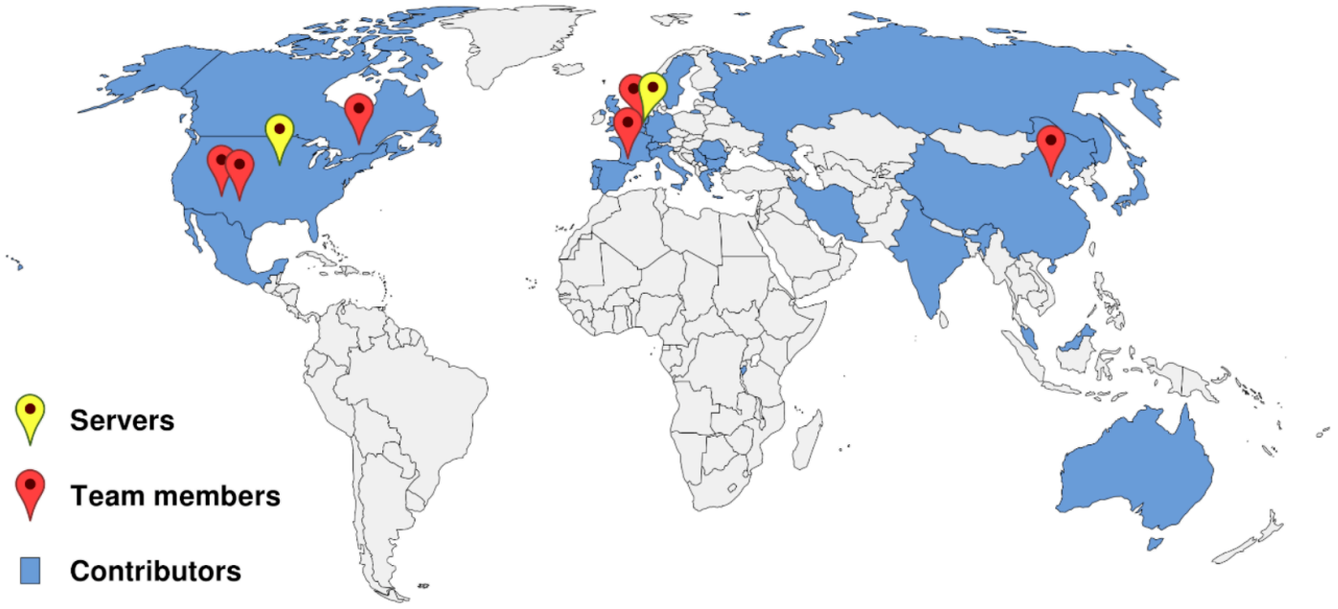
State of the art: LXCat ("elecscat") [4]

Electron (and ion) collisional processes in plasmas

- **Cross sections**
- Potentials
- Swarm parameters

Statistics

- ≈ 120 visitors/day
- ≈ 30000 cross sections
- International



[4] Carbone, E., Graef, W., Hagelaar, G., Boer, D., Hopkins, M. M., Stephens, J. C., Yee, B. T., Pancheshnyi, S., van Dijk, J., & Pitchford, L. (2021). Data Needs for Modeling Low-Temperature Non-Equilibrium Plasmas: The LXCat Project, History, Perspectives and a Tutorial. *Atoms*, *9*(1), 16. https://doi.org/10.3390/atoms9010016

Recap: LXCat 2

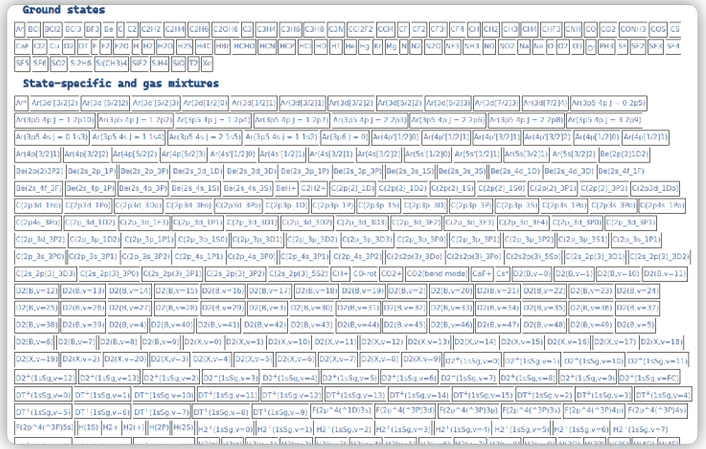
Data format & Semantics

```
EXCITATION
N2 -> N2 (v=0 - v=1)
 3.000000e-1
SPECIES: e / N2
PROCESS: E + N2 -> E + N2 (v=0 - v=1), Excitation
PARAM.:  E = 0.3 eV, complete set
COMMENT: [e + N2(X,v=0) <-> e + N2(X,v=1), Vibrational]
COMMENT: Pitchford L C and Phelps A V 1982
UPDATED: 2017-09-03 03:54:40
COLUMNS: Energy (eV) | Cross section (m2)
-----------------------------
 3.000000e-1    0.000000e+0
 4.000000e-1    3.000000e-23
 <omitted lines>
-----------------------------
```

Data storage

Particle	Charge	e	S	L	Parity	J
e	-1	NULL	NULL	NULL	NULL	NULL
Ar	0	*	NULL	NULL	NULL	NULL
Ar	0	NULL	0	0	Even	0

Design & Implementation



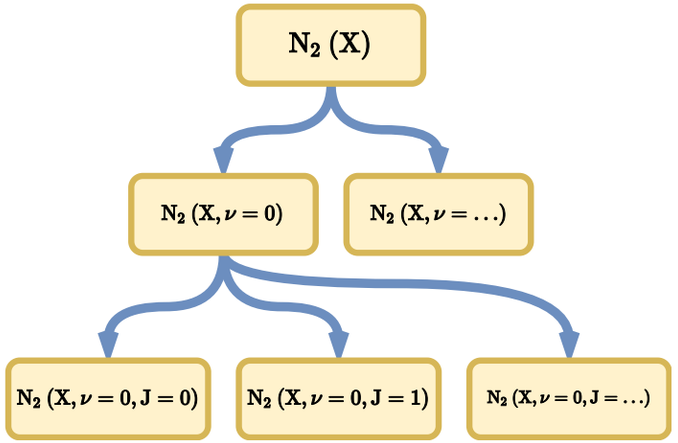
Recap: LXCat 3

Data format & Semantics

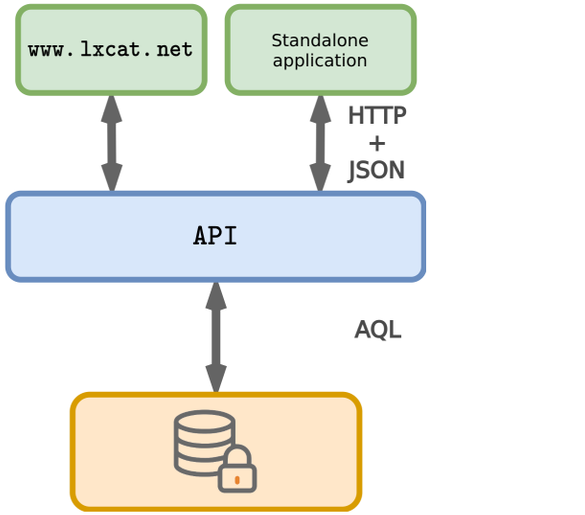
$\mathrm{He}^{+}\ (^{2}\mathrm{S}_{1/2})$

```
{
  "particle": "He",
  "charge": 1,
  "type": "AtomLS",
  "electronic": {
    "config": [],
    "term": {
      "S": 0.5,
      "L": 0,
      "P": 1,
      "J": 0.5
    }
  }
}
```

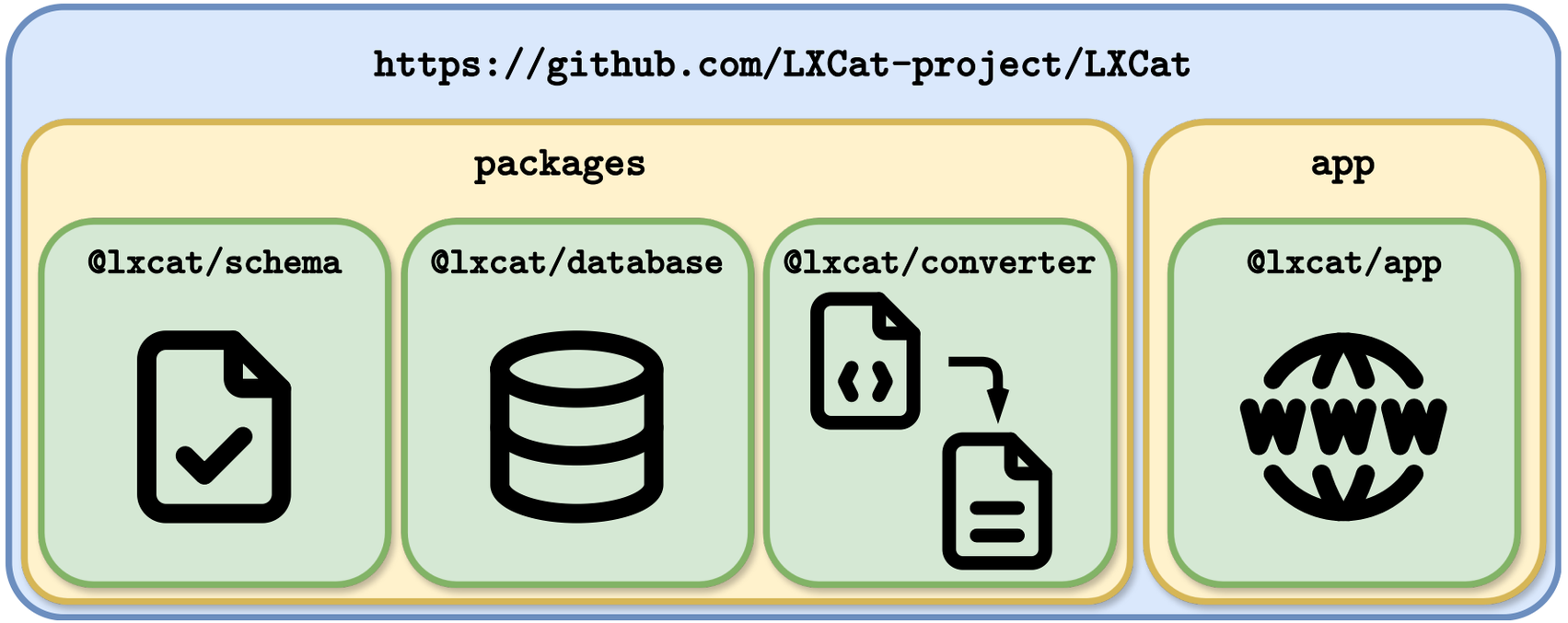
Data storage



Design & Implementation



Project architecture



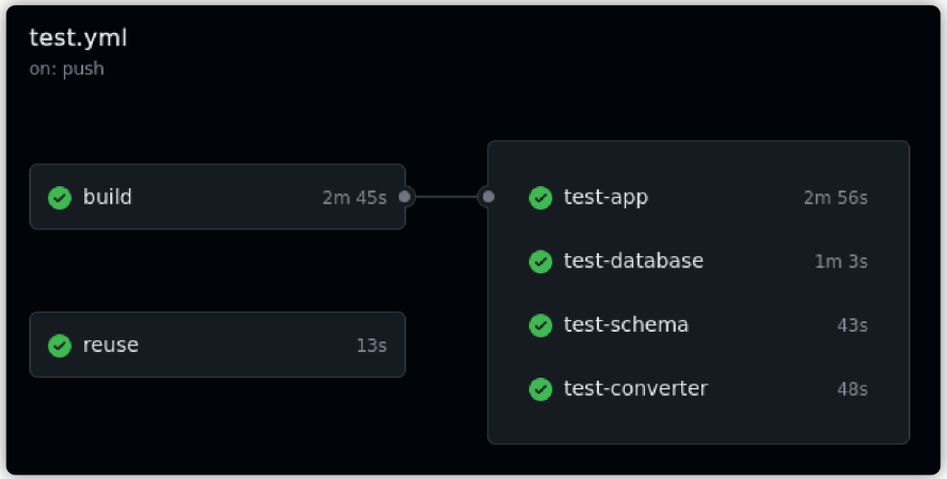
Open source!

Zod ArangoDB NEXT.JS TU/e

Testing & Code coverage

Test suite

- Unit, regression, end-to-end
- Needs to succeed before code is accepted



Dependabot

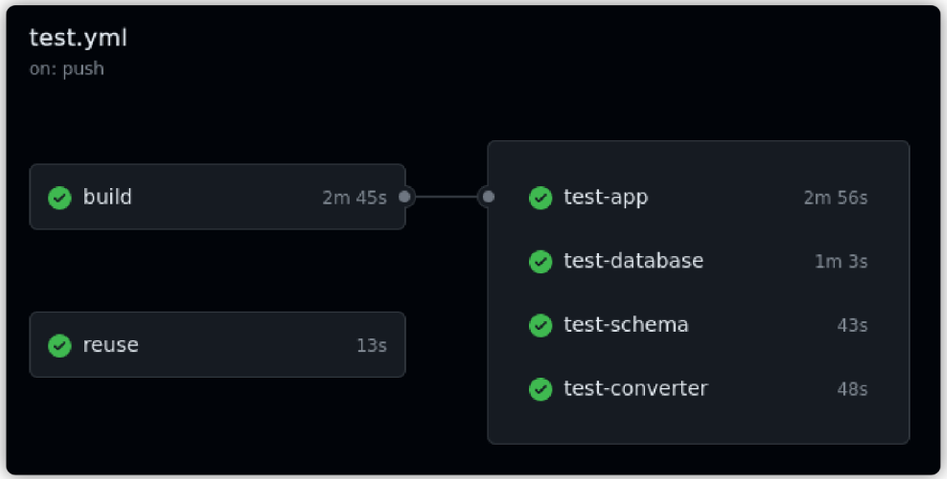
TU/e

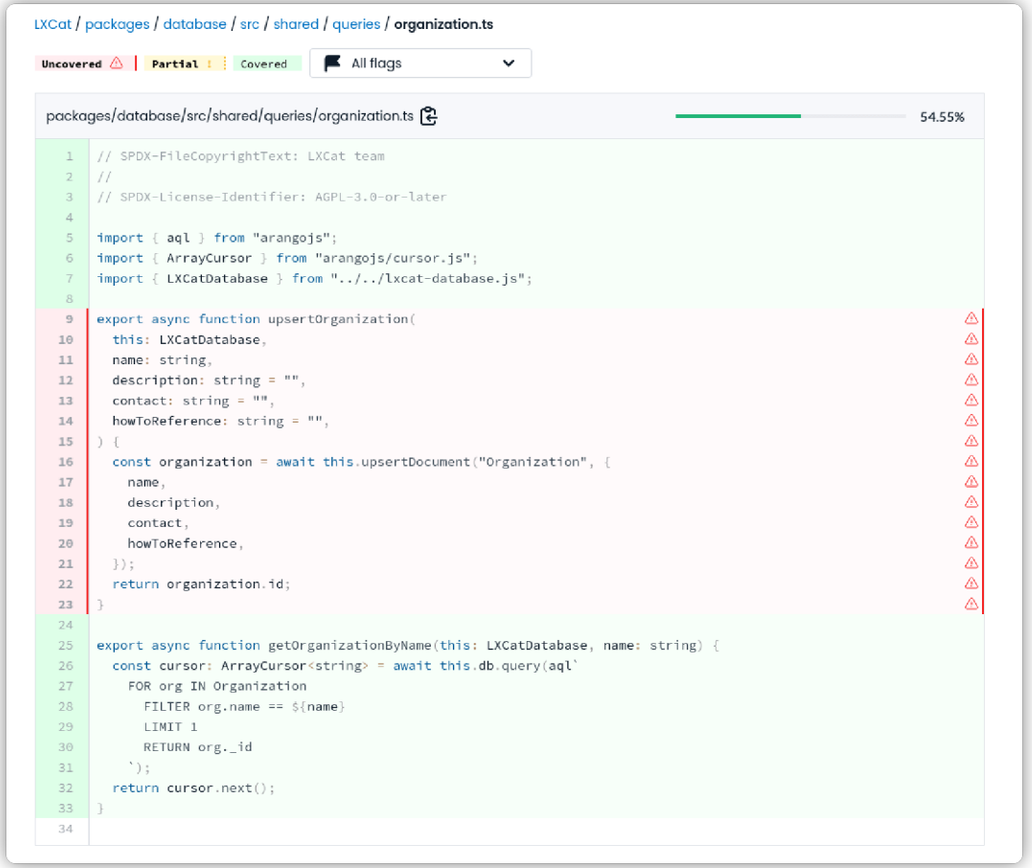
Testing & Code coverage

Test suite

- Unit, regression, end-to-end
- Needs to succeed before code is accepted

Code coverage (~80%)



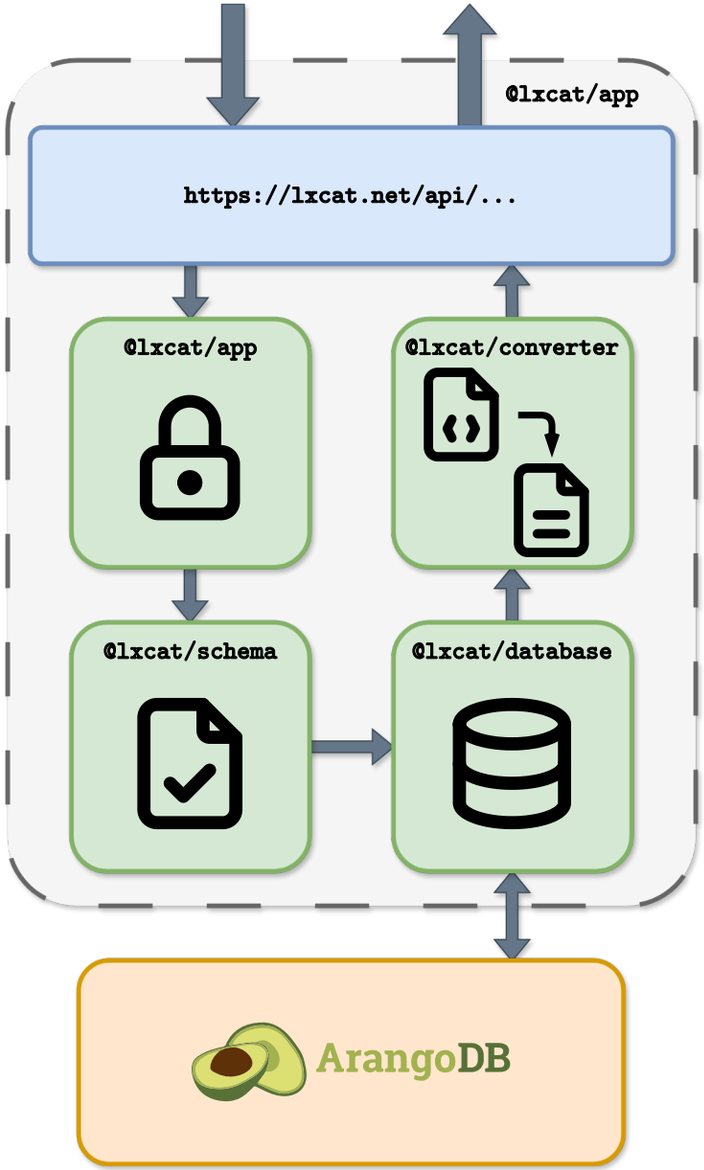


Dependabot Codecov TU/e

Data flow

API Request handling

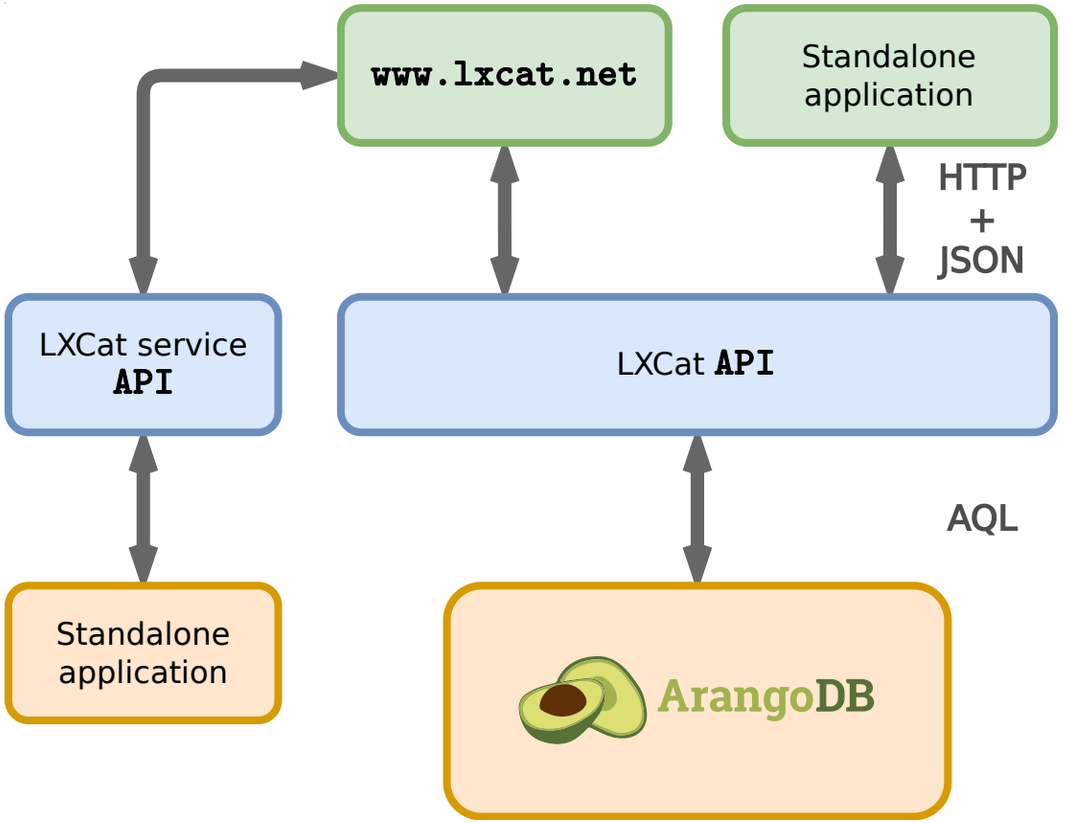
- Authorize
- Validate
- Query
- Convert



Interacting with simulation software

Simulation software

- Integrated
- External application



[5] Hagelaar, G. J. M., & Pitchford, L. C. (2005). Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models. Plasma Sources Science and Technology, 14(4), 722–733.
[6] Tejero-del-Caz, A., Guerra, V., Gonçalves, D., da Silva, M. L., Marques, L., Pinhão, N., Pintassilgo, C. D., & Alves, L. L. (2019). The LisbOn KInetics Boltzmann solver. Plasma Sources Science and Technology, 28(4), 043001.

Interacting with simulation software

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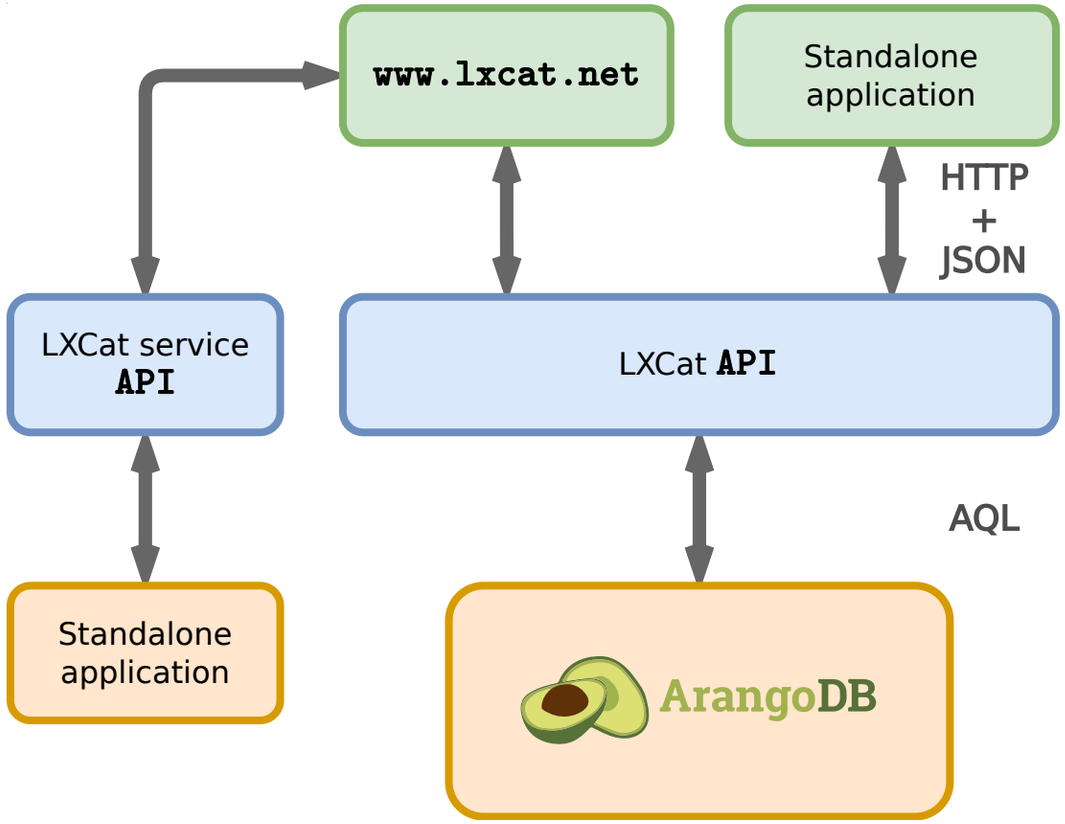
Boltzmann solver example

- BOLSIG+ [5]
- LoKI-B [6]



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Demo

Chemistry

Schema updates

- Rate coefficients
- Transport parameters

Flexible infrastructure

- Species
- Data type

```
{
  "reaction": {
    ...
  },
  "info": [
    {
      "type": "RateCoefficient",
      "references": ["main"],
      "threshold": { "value": 0, "unit": "eV" },
      "data": {
        "type": "Expression",
        "expression":
          "0.25*0.8*8.1e-13*(Te/300)^(-0.64)*(Tgas/300)^(-0.86)",
        "unit": "m^3/s",
        "parameters": ["Te", "Tgas"]
      }
    }
  ]
}
```

The MCPlas toolbox

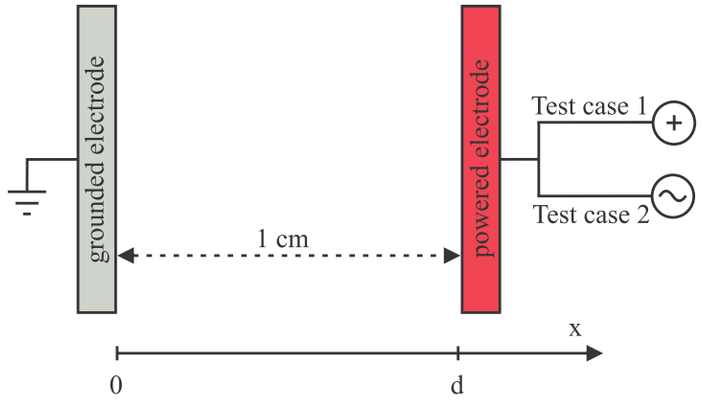
Complex chemistry

- JSON
- COMSOL

Fluid-Poisson model

- Simple geometry
- 1D and 2D
- DC and RF

PLASIMO [7] comparison



[7] van Dijk, J., Peerenboom, K., Jimenez, M., Mihailova, D., & van der Mullen, J. (2009). The plasma modelling toolkit Plasimo. Journal of Physics D: Applied Physics, 42(19), 194012. https://doi.org/10.1088/0022-3727/42/19/194012

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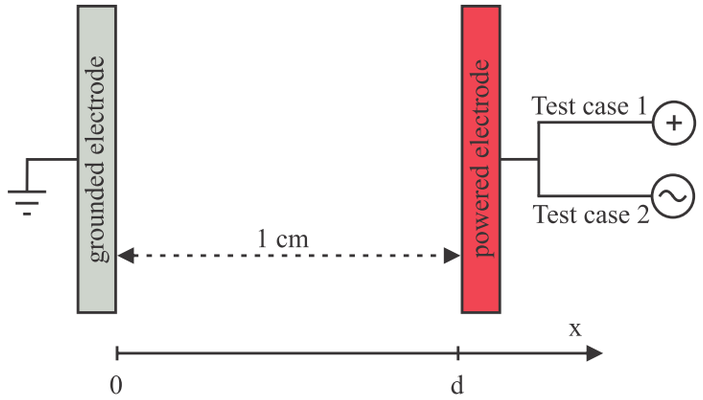

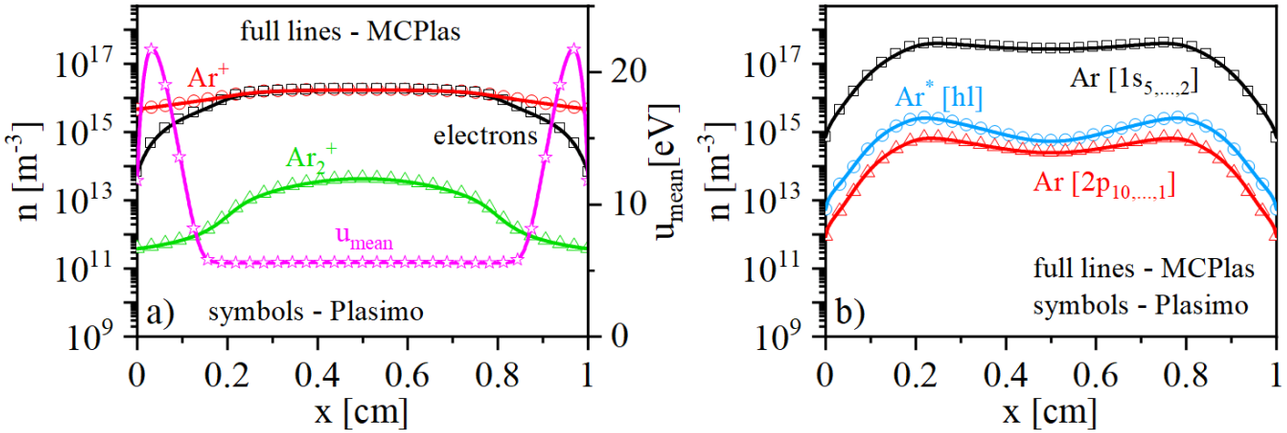

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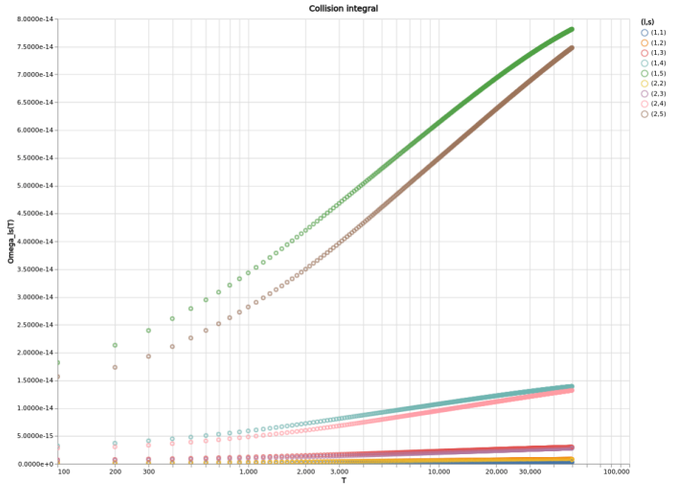
Ecosystem overview

Potential integrator

- MagnumPI [8]



[8] https://gitlab.com/magnumpi/magnumpi

[9] https://plasimo.phys.tue.nl/

Ecosystem overview

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Boltzmann solver

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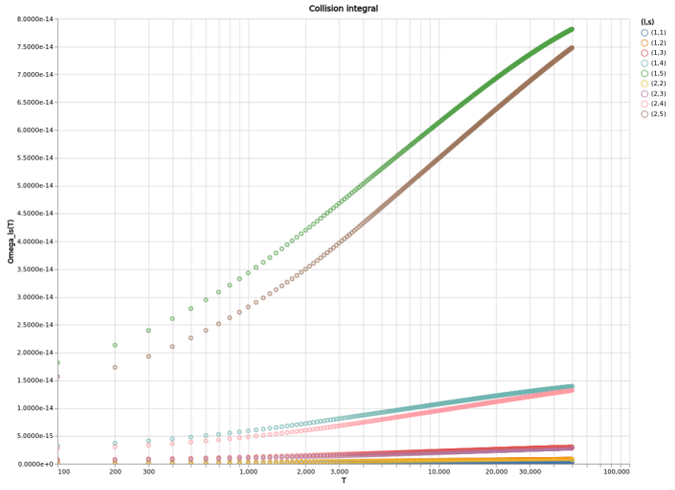

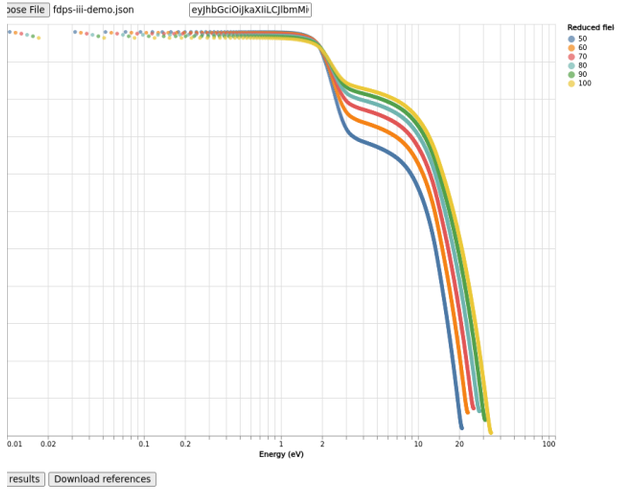

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Ecosystem overview

Potential integrator

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Boltzmann solver

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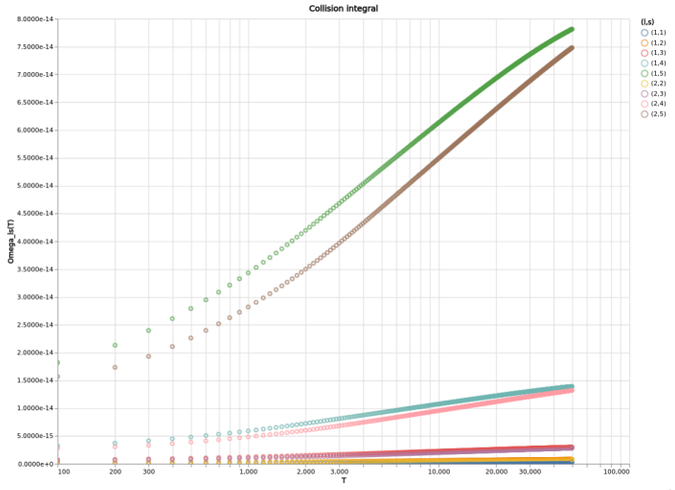
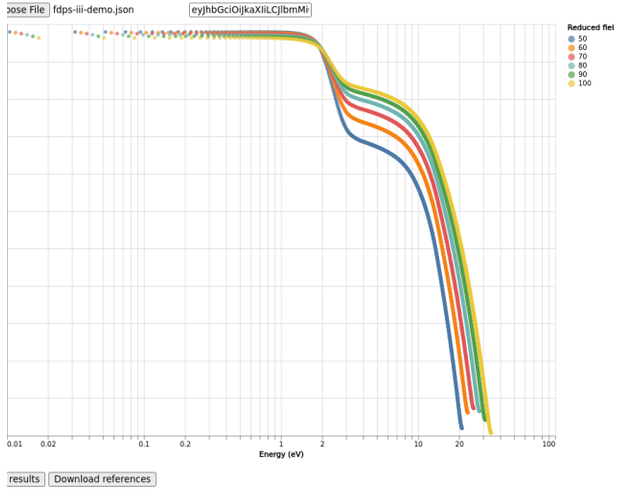
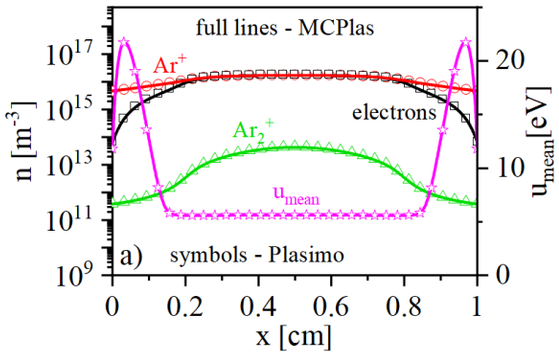
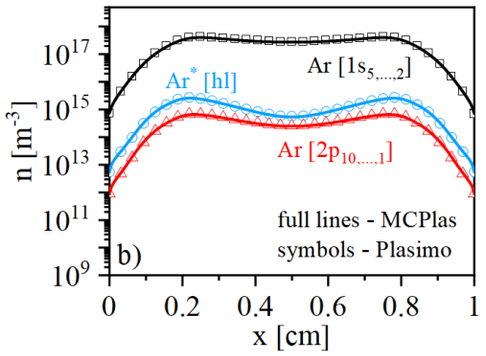
General plasma modeling

- MCPlas (COMSOL)
- PLASIMO [9]
- (Global model)









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Ecosystem: infrastructure

Ecosystem: infrastructure