Making a case for open-source codes

the LisbOn KInetics simulation tool

L.L. Alves
llalves@tecnico.ulisboa.pt

Instituto de Plasmas e Fusão Nuclear
Instituto Superior Técnico, Universidade de Lisboa
Lisboa, Portugal
https://www.ipfn.tecnico.ulisboa.pt
https://www.ipfn.tecnico.ulisboa.pt/nprime/

TORINO 2023 FUNDAMENTAL PLASMA PHYSICS

Software development in LTP

A G Smart *Phys. Today* (2018)
R Bast *Nat. Phys.* (2019)

Software development, computational calculations

prominent research activities in LTP science

However, the community has not been driven

- to define clear standards for the various steps of the workflow
- to adopt the (good) practice of systematic publishing the codes used in computational calculations.

Accessing software
as *publicly available* or *open-source* code

- is desirable to ensure the quality standards of published material
  (the code allows reproducing / validating / confirming / challenging the calculations and the research findings)
- it can accelerate and inspire advances in the scientific work
  (especially in the small LTP community)

Open source / Publicly available

A M St. Laurent O'Reilly Media (2008)

'open-source code'

any computer software under a license
in which the copyright holder grants users the rights to use, analyze, modify and distribute the source code to anyone and for any purpose

'publicly available code'

- any software that contains or is derived (in whole or in part) from 'free software', 'open-source software', 'copyleft' or similar licensing and distribution models
- any software redistributable at no charge for the purpose of making derivative works
  (*open-source codes* are *publicly available codes*)

Outline

- **Making a case for open-source codes**

  Open-source codes: advantages and barriers

  Status of LTP codes

- **Example of the LisbOn KInetics simulation tool**

  Workflow, main features

  Development, following good practices for open-source codes

- **Final remarks**

Alves et al., “Foundations of plasma standards” 2023 *Plasma Sources Sci. Tech.*

Making a case for open-source codes

Open-source codes : why not ?

Complex codes

multidimensional / multiscale / multispecies

(collaborative) Code review

- Facilitates debugging and verification activities
- Improves code quality and correctness
- Provides continuity of the research work
- Promotes knowledge transfer within and between research groups

Open-source codes : still not convinced ?

Closed-source usually leads to NEGATIVE answers

- Could you rewrite the same code built some years ago, reproducing the same computational results that were then published ?
- Can you easily find the old version of the code used for that publication ?
- How many versions of the software can you find simultaneously being used in your research group ?
- Do you know the differences between these versions?
- What is the best/most recent version to distribute to a new student ?
- Is there any related documentation ?
- Are you confident about the set of input data to use in the simulations ?

Open-source codes : barriers

Main barriers related to the LTP community

- The lack of a common programming language and architecture
- Restrictions by government and industry on distribution of codes
- Lack of funding for software development
- The large effort to update or rewrite codes
- Little credit to reward this effort and for tool sharing
- Little tradition of using (recent) collaborative frameworks (e.g., OpenFOAM, MOOSE) to develop “foundation libraries”
- Difficulty in embracing an ontology that separates (open-source) ‘tools’ from FAIR ‘data’

Codes vs data

Codes and data “live” through each other

80% of researchers are in favor of open-access data

- due to impact on citations (67%)
- due to visibility of research (61%)
- for public benefit (56%)
- due to or journal/publisher mandate (56%)

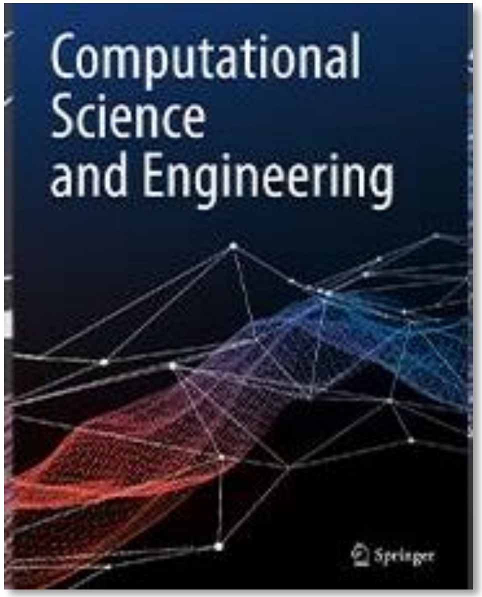
SPRINGER NATURE

Computational Science and Engineering

A new journal from Springer, very recently launched

Computational Science and Engineering publishes research on the use of computational methods to solve scientific problems across natural and engineering sciences.

Special attention is paid to the **reproducibility of code and to the FAIR principles of research data**. The journal is **fully open access** and **encourages authors to make their code and data openly available**.



Springer

Situation of LTP codes

Boltzmann solvers: “comfortable” situation

- several open-source codes
  BOLOS, MultiBolt, Magboltz, METHES, LoKI-B, LoKI-MC
- some publicaly available codes
  BOLSIG+, EEDF

Chemistry solvers: lack of open-source codes

- some publicaly available and “available on request” codes
  ZDPLASKIN, GlobalKIN
  (LisbOn KInetics – LoKI to be released as open-source code)

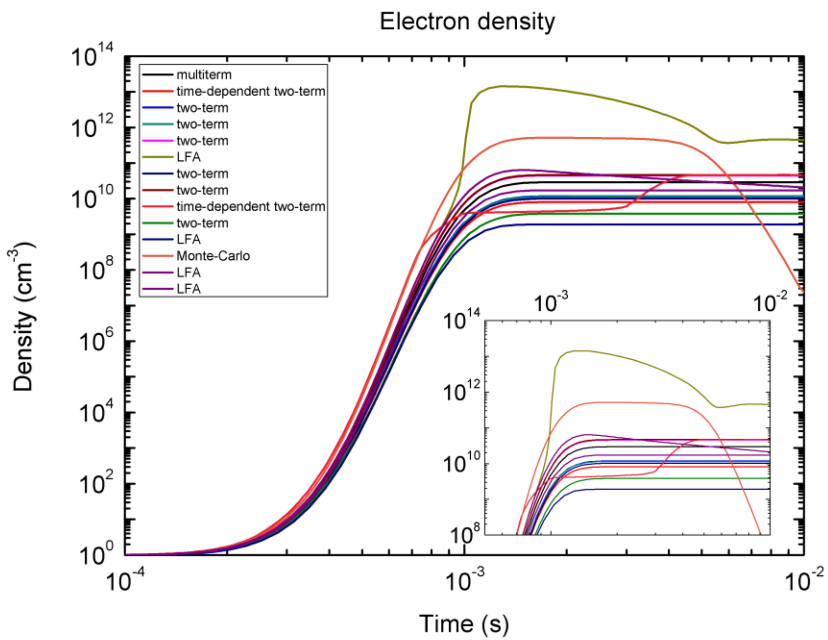
Fluid codes and platforms

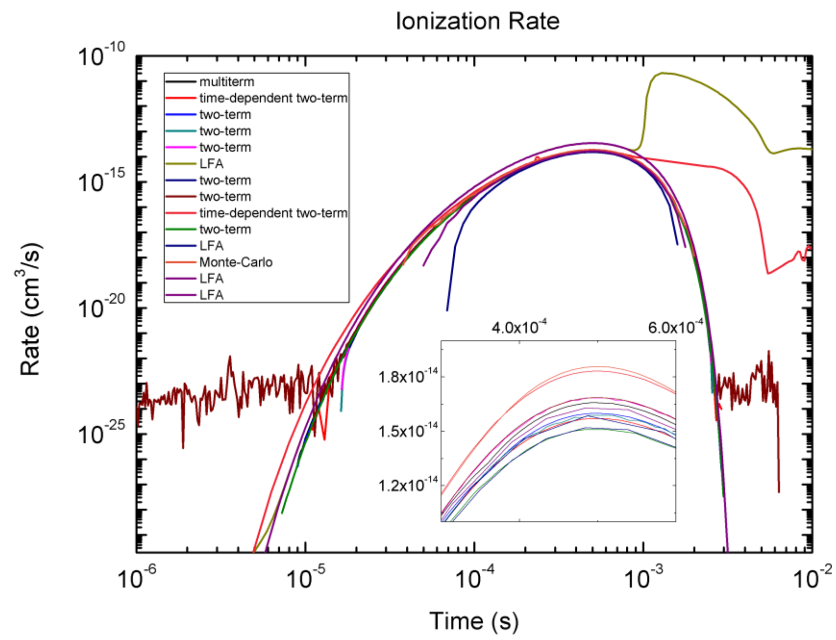
- some “available on request” codes
  HPEM, non-PDPSIM
- several commercial codes / platforms
  Quantemol, PLASIMO, COMSOL
- some open-source platforms
  MOOSE, OpenFOAM

+ many other in-house codes

Results of round-robin exercise (2017-2018)

Modelling of an argon plasma (0.1 bar and 300 K), excited by an electric field pulse for initial electron and ion densities of 1 cm^{-3}





Differences in results

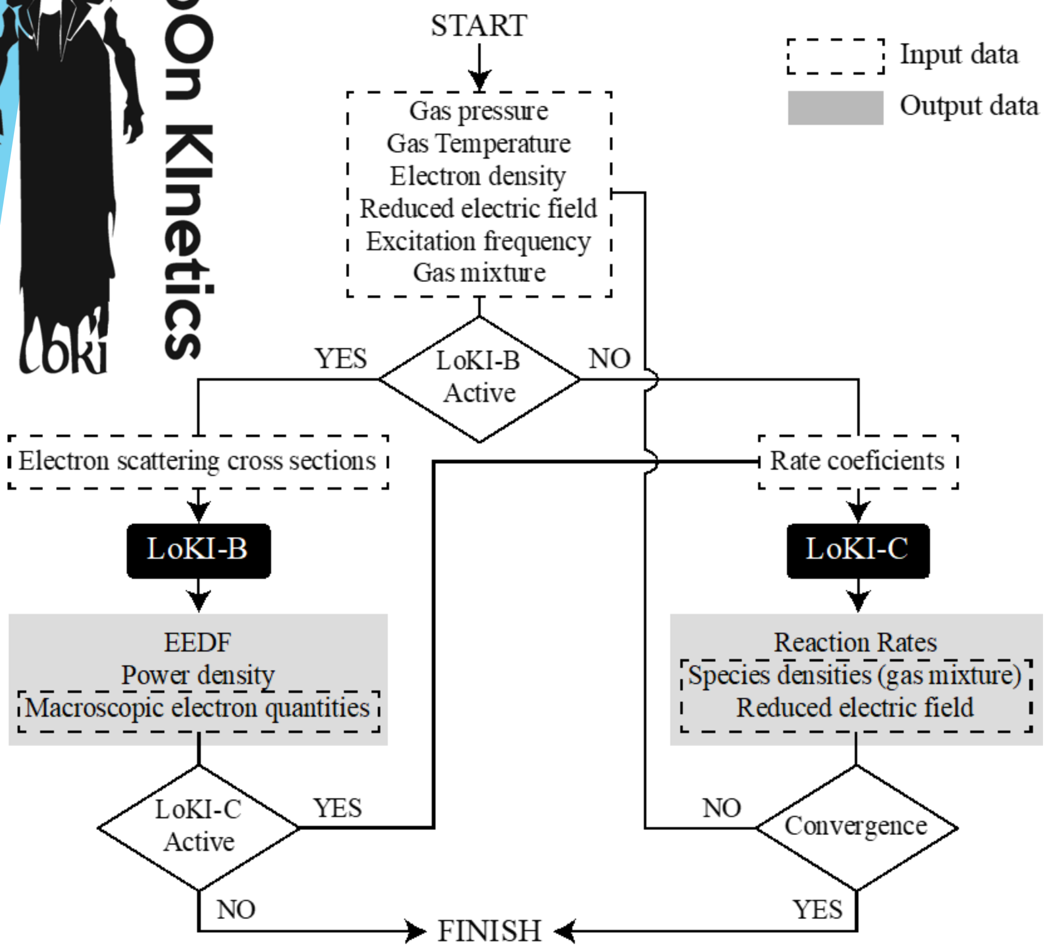
- different implementations of the same publicly available code (versions / setups)
- different deployments of the physical models and the input data in in-house codes

The example of the LisbOn KInetics simulation tool

The LisbOn KInetics (LoKI) simulation tool

(developed under MATLAB®)

LisbOn KInetics



OPEN SOURCE

LoKI-B

https://github.com/IST-Lisbon/LoKI

- solves the space independent form of the two-term electron Boltzmann equation, for DC/HF or time-dependent (non-oscillatory) electric fields.
- includes e-e collisions, CAR operator, and growth models for the electron density.

LoKI-C

- solves the system of 0D rate balance equations for the heavy particles.
- includes modules to describe
  (i) the collisional, radiative and transport mechanisms controlling the creation / destruction of volume and surface species
  (ii) the thermal heating of the neutral gas

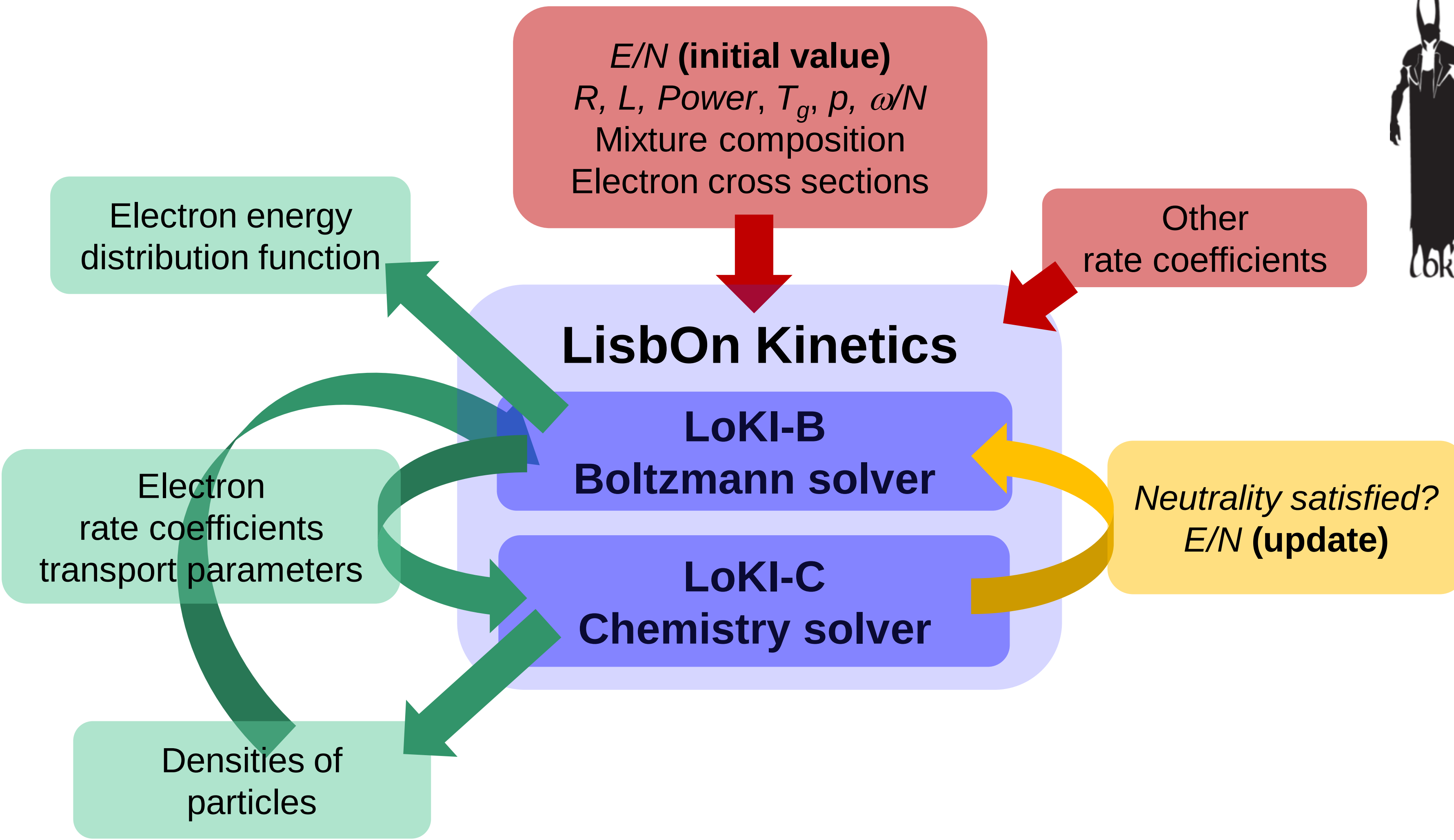
ipfn INSTITUTO DE PLASMAS E FUSÃO NUCLEAR

N-PRiME

loki@tecnico.ulisboa.pt

LoKI workflow

A Tejero, L L Alves *et al Plasma Sources Sci. Technol.* (2019)
V Guerra *et al Plasma Sources Sci. Technol.* (2019)



LisbOn KInetics

LoKI main features

A Tejero, L L Alves *et al Plasma Sources Sci. Technol.* (2019)
V Guerra *et al Plasma Sources Sci. Technol.* (2019)

LisbOn KInetics

Focus on…

- plasma chemistry
  described by a spatially averaged (global) model

Valid for…

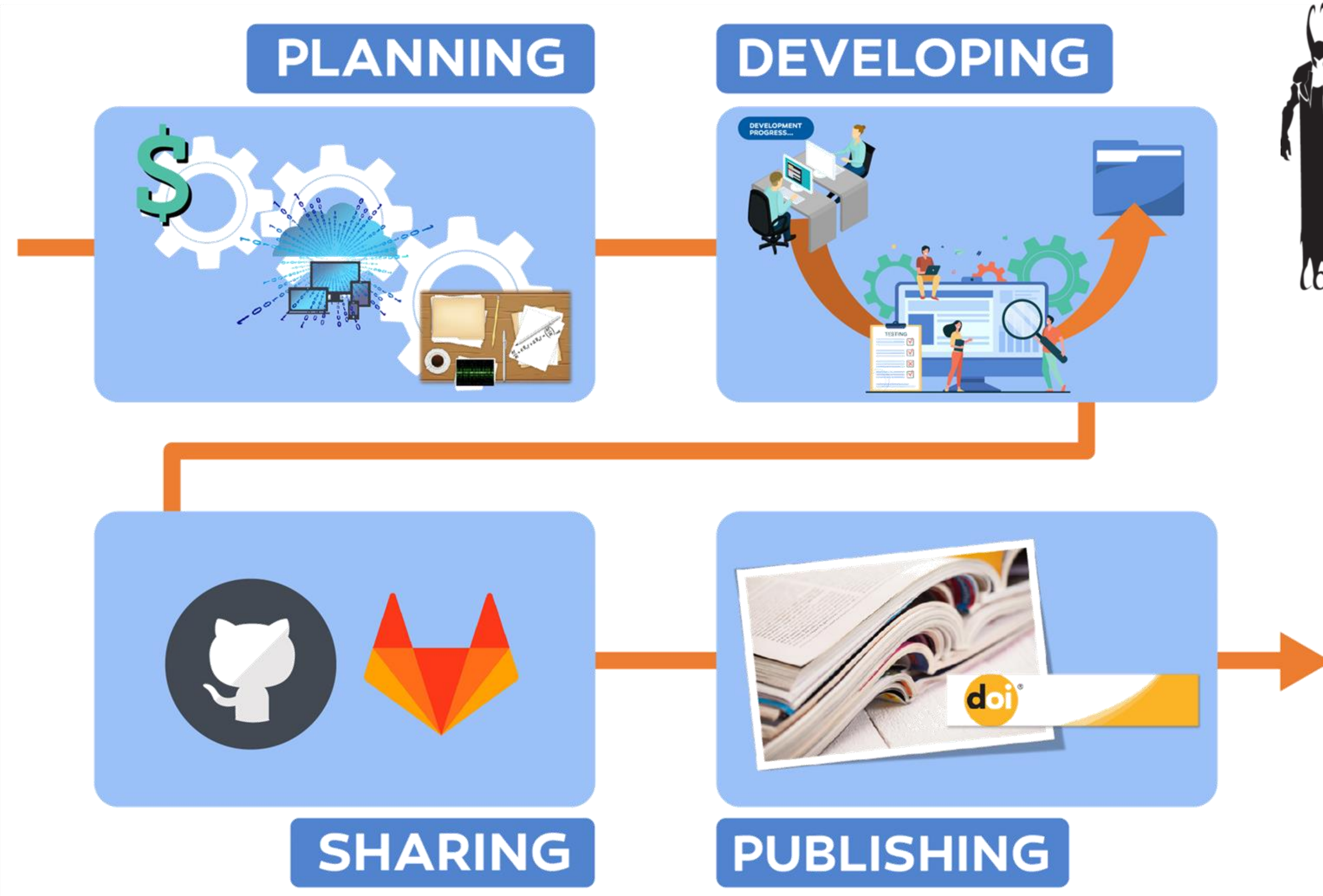
- homogeneous plasmas (dc / mw)
- intermediate to high pressures (p > 10 Pa → λ_i < 1 cm)
- dense plasmas (n_e > 10^{16} m^{-3} → λ_D < 100 μm)

Main features…

- Collisional interactions
  - in **any atomic / molecular gas mixture**
  - of **any charged (electrons / ions) or neutral species**
  - with **any target state (electronic, vibrational or rotational)**
- I/O allowing easy comparison with experiments
  (power / currents ; densities of species)

LoKI development

L L Alves *et al Plasma Sources Sci. Technol.* (2023)



LisbOn KInetics

LoKI development

planning

Financial

securing the necessary resources for the task

Technical

deciding about

- the programming language
- the ontology, e.g. separation of tools from data

Scientific

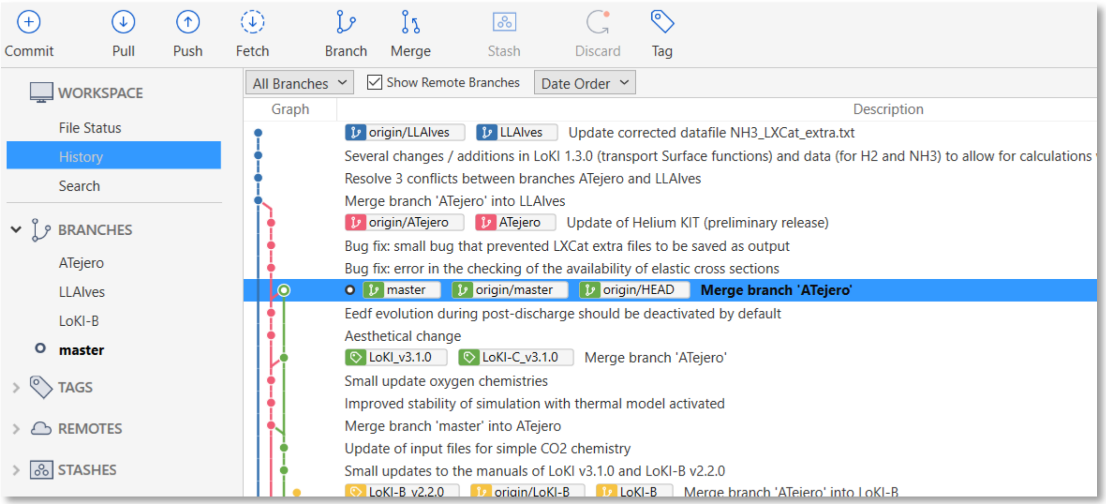
- formalizing / structuring the problem
  LoKI-B / LoKI-C coupling ; closure
- preparing the numerical implementation
  I/O management ; compatibility to popular databases - LXCat
- choosing numerical methods and algorithms for the solution

LoKI development

developing, reviewing, verifying

Review during code development

- collaborative development
- debugging of transcription from old codes
- modular development
  (e.g .transport, thermal, scattering operators)
- version control



Verification

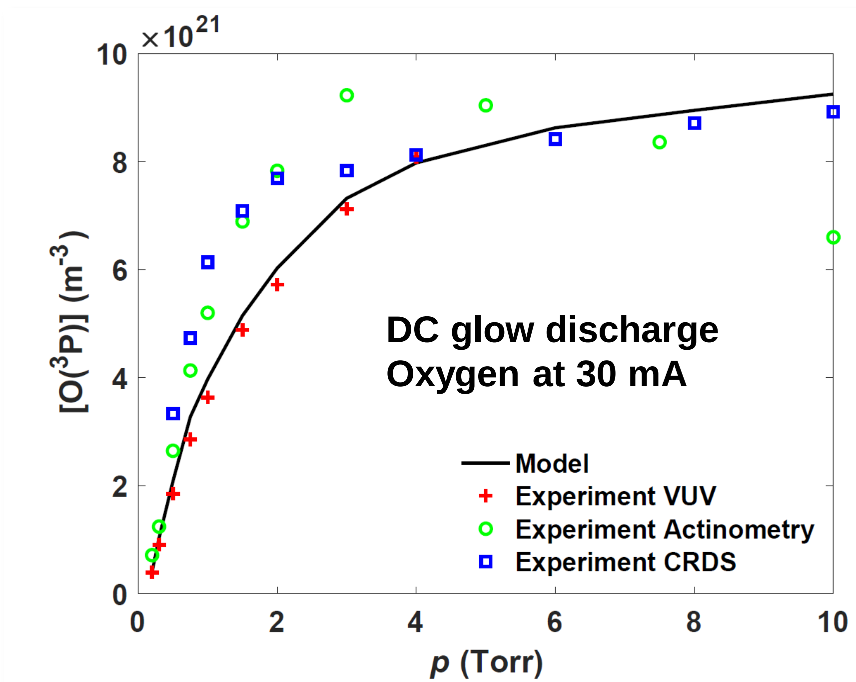
- asymptotic limits
- conservation laws
- benchmark against analytical solutions, other codes
- regression tests

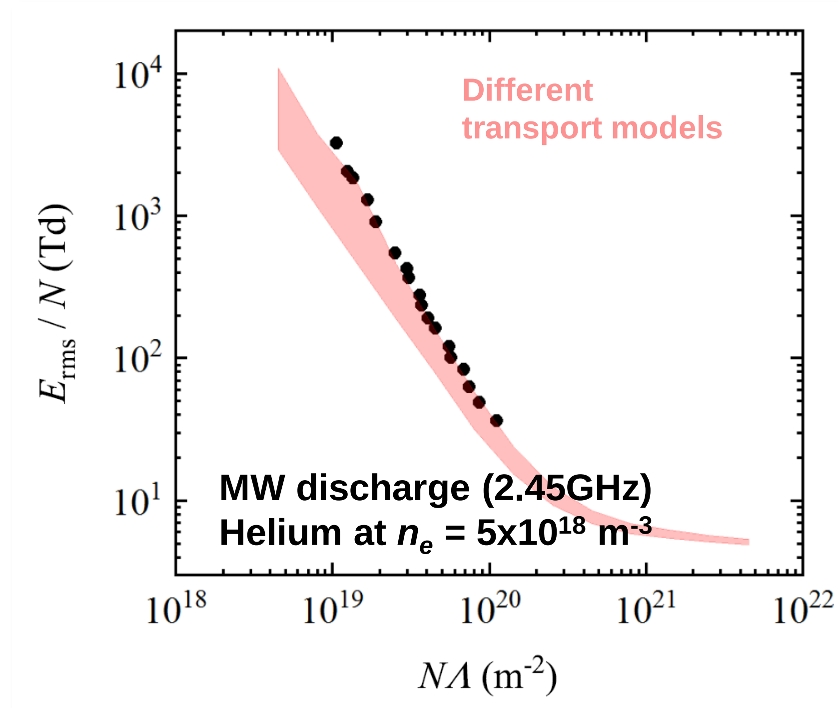
LoKI development
validating

L L Alves and A Tejero *Plasma Sources Sci. Technol.* (2023)
T C Dias *et al Plasma Sources Sci. Technol.* (submitted)

Validation

- of cross section sets
  by performing swarm analyses
- of kinetic schemes
  by comparing calculations with experimental measurements
  by assessing uncertainties in the calculations





LoKI development

"plug and play" reaction mechanisms for plasma chemistry

Extract of .chem file

```
%---- electron impact excitation/deexcitation ----
e + N2(X,v=0) <-> e + N2(A3Su+)                                  | eedf
e + N(4S) <-> e + N(2D)                                          | eedf

%---- e-V processes ----
e + N2(X,v=0) <-> e + N2(X,v=1)                                  | eedf
e + N2(X,v=1:9) -> e + N2(X,v=v+1)                               | nitrogenEVscaling

%---- electron impact dissociation ----
e + N2(X,v=0) -> e + 2N(4S)                                      | eedf

%---- electron impact ionization ----
e + N2(X,v=0) -> 2e + N2(+,X)                                    | eedf
e + N2(A3Su+) -> 2e + N2(+,X)                                    | eedf
e + N(4S) -> 2e + N(+,gnd)                                       | eedf

%---- electron recombination ----
e + N2(+,X) -> 2N(4S)                                            | powerElectronTemp

%---- heavy species collisions ----
N2(B3Pg) + N2(X) -> N2(A3Su+) + N2(X)                            | constantRateCoeff
N(2D) + N(4S) + N2(X) -> N2(B3Pg) + N2(X)                        | constantRateCoeff
N(2D) + N2(X) -> N(4S) + N2(X)                                   | arrheniusGasTemp
N2(+,X) + N2(X,v=0) + N2(X) -> N4(+,X) + N2(X)                   | powerGasTemp
N(4S) + N(4S) + N2(X) -> N2(a1Pg) + N2(X)                        | arrheniusGasTemp
N2(C3Pu) -> N2(B3Pg)                                             | constantRateCoeff

%---- V-V processes ----
N2(X,v=1:10) + N2(X,w=0:v-1) <-> N2(X,v=v-1) + N2(X,v=w+1)       | nitrogenMolecularVV
N2(X,v=1:10) + N2(X,v=10) -> N2(X,v=v-1) + 2N(4S)                | nitrogenMolecularVVDis

%---- Molecular V-T processes ----
N2(X,v=1:10) + N2(X) <-> N2(X,v=v-1) + N2(X)                     | nitrogenMolecularVT
N2(X,v=10) + N2(X) -> 2N(4S) + N2(X)                             | nitrogenMolecularVTDis

%---- Atomic V-T processes ----
N2(X,v=7:10) + N(4S) <-> N2(X,v=v-1) + N(4S)                     | nitrogenAtomicVT
```

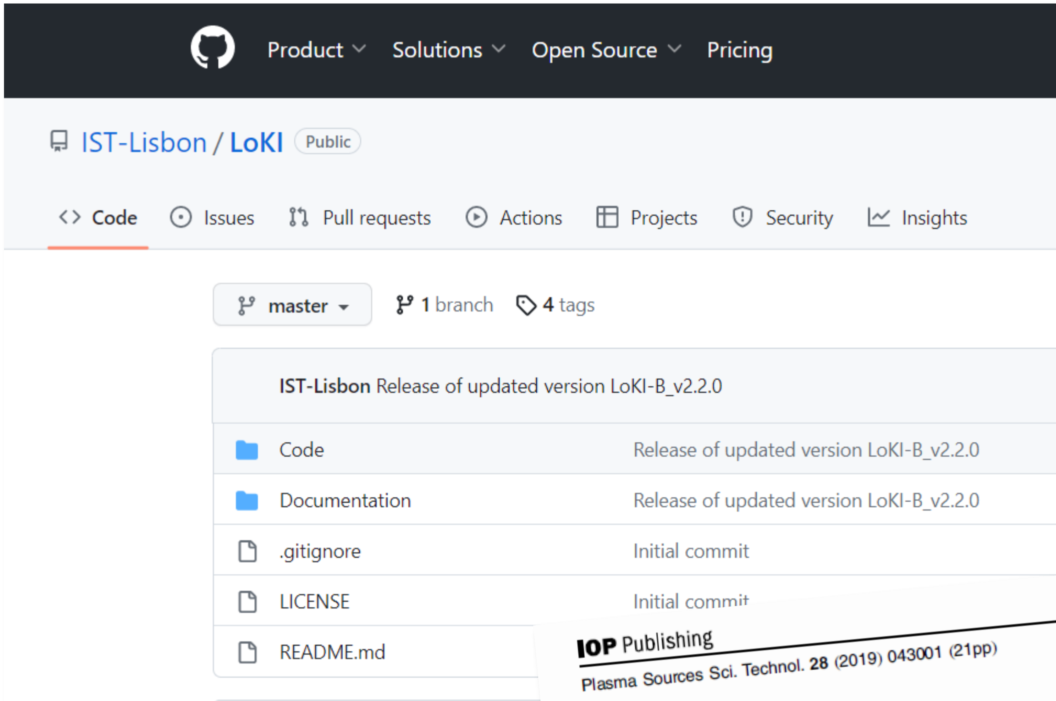
LisbOn KInetics

On-going studies

CO_2 - CO
O_2, N_2, N_2 - O_2
N_2 - H_2
CO_2 - N_2 - Ar
CO_2 - CH_4 / H_2O
He, He - O_2

LoKI development
sharing, publishing

https://github.com/IST-Lisbon/LoKI
https://nprime.tecnico.ulisboa.pt/loki
A Tejero *et al Plasma Sources Sci. Technol.* (2019)



LoKI

- to be released soon
- to be assigned a DOI

Plasma Sources Science and Technology
https://doi.org/10.1088/1361-6595/ab0537

IOP Publishing
Plasma Sources Sci. Technol. **28** (2019) 043001 (21pp)

Topical Review

The LisbOn KInetics Boltzmann solver

A Tejero-del-Caz[1], V Guerra[1], D Gonçalves[1], M Lino da Silva[1], L Marques[2], N Pinhão[1], C D Pintassilgo[1,3] and L L Alves[1]

[1] Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
[2] Centro de Física das Universidades do Minho e do Porto, Campus de Gualtar, Braga, Portugal
[3] Faculdade de Engenharia da Universidade do Porto, Porto, Portugal

Final remarks

Final remarks

The sharing of codes in LTPs (and elsewhere)

- could significantly improve the quality of computational predictions in LTPs
- could nurture and support a new generation of researchers developing computational algorithms and models

We have been trying to do so in the development of LoKI

The good practices and recommendations discussed here

- are well-known
- require a culture change from researchers, publishers and funding institutions, where openness is supported and sharing software is encouraged as part of the high-quality standards in scientific research (the path seems more consolidated for data)

The main conferences in the field

could be used as forum to design and carry out collective efforts for the verification and benchmarking of codes

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team

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