A standardization effort for low-temperature gas reactions

3rd DRD1 Collaboration Meeting, CERN
WG4

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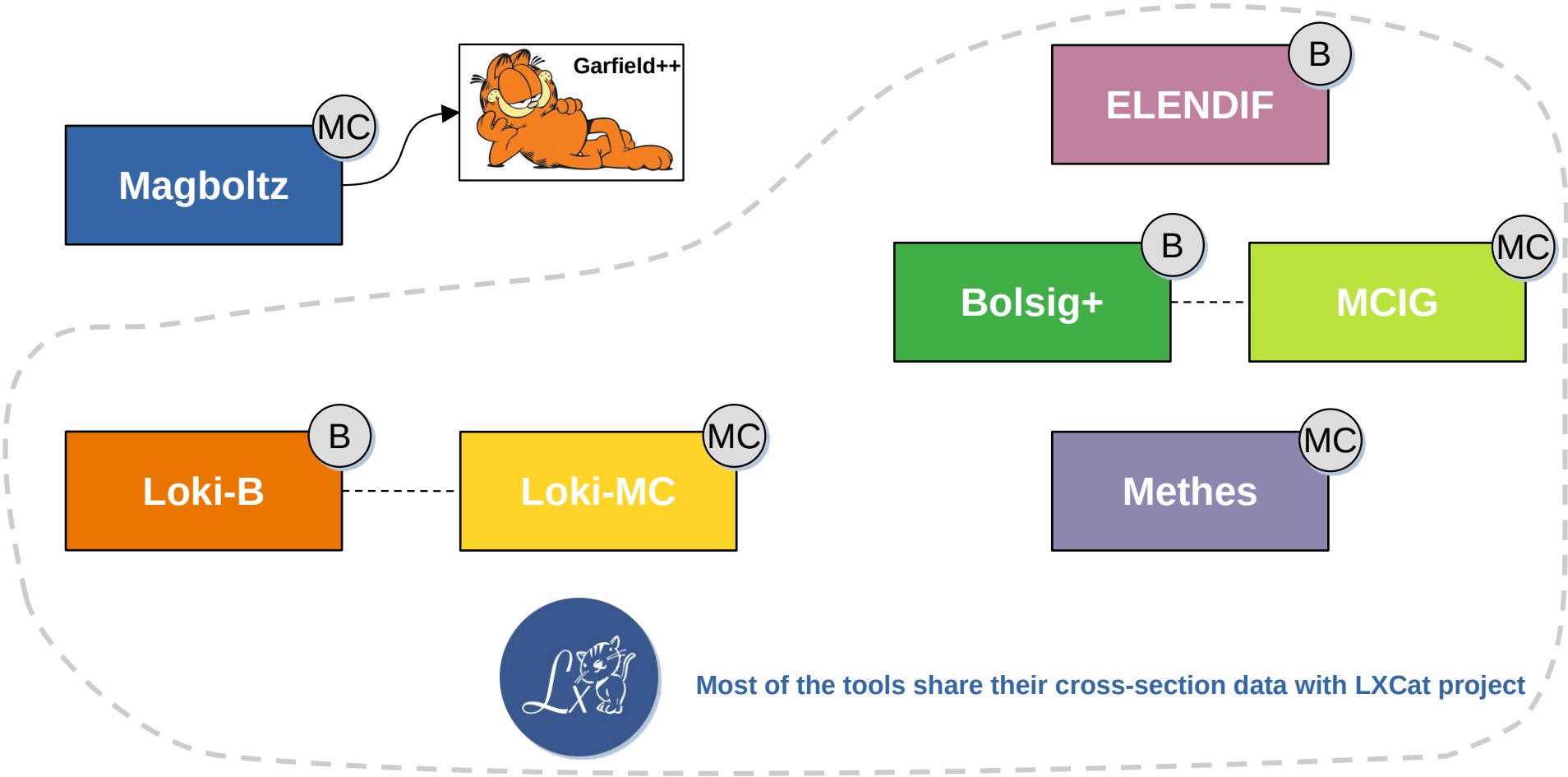
Dec 11, 2024

Summary

1. Current status of software interoperability
2. Common syntax proposal
   a) Reactions
   b) Molecules
   c) Excitation states
3. Practical examples

Status of notation interoperability

Most common software tools used for gaseous medium simulation



Status of notation interoperability

Bolsig+

Each simulations tools need to find a way to define the excited state definition using custom-defined comments in the cross-section input files.
These comments are not interoperable meaning that each cross-section database is only compatible with their respective tool.

...
Name of the target particle species. This name is a character string, freely chosen by the user, e.g. "Ar". Optionally for excitation processes, the name of the corresponding excited state can be specified on the same line, separated from the first name either by arrow "->" (dash + greater than) or by double-head arrow "<->" (less than + dash + greater than), e.g. "Ar -> Ar" and "Ar <-> Ar*", respectively. In the later case BOLSIG+ will automatically define the inverse superelastic process, constructing the superelastic cross-section by detailed balancing, and considering the indicated excited state as the target. In this case, the ratio of statistical weights must be input in the 3rd line (see below).*
...
For elastic and effective collisions, the ratio of the electron mass to the target particle mass. For excitation or ionization collisions, the electron energy loss (nominally the threshold energy) in eV. For attachment, the 3rd line is missing. In case of an excitation process where an excited state has been indicated on the 2nd line using double-head arrow "<->", the 3rd line must specify also ratio of the statistical weights of the final state to the initial state as the second parameter in 3rd line this is needed by BOLSIG+ to calculate the de-excitation cross-section. The statistical weight ratio, if given, will also be used by the automatic superelastics option in BOLSIG+. If this ratio is not provided then BOLSIG+ will assume it unity.
...

Common syntax proposal

Elastic scattering

```
e + H2O -> e + H2O
```

Generic excitation

```
e + O2 -> e + O2 (*)
```

Ionization

```
e + CO2 -> e + e + CO2^+
```

Dissociation

```
e + CH4 -> e + CH2 + H2
```

Dissociative attachment

```
e + CH4 -> CH2^- + H2
```

Complex molecules

```
e + i-C4H10 -> e + i-C4H10
```

```
e + CH3(CH2)4CH3 -> e + CH3(CH2)4CH3
```

Reversible reactions

```
e + O2 <-> e + O2 (*)
```

Ion bullet reactions

```
Ar^+ + H2 -> Ar^+ + H + H
```

Common syntax proposal

Reactions with multiple outcomes

```
e + CO2 -> e + CO2 (*) [75%] or e + e + CO2^+ [25%]
```

```
e + O2 -> e + O2 (*) [2/3] or e + O + O [1/3]
```

Reactions with intermediary steps

```
e + H2 -> e + H2 (*) -> e + H + H
```

Excitation states

Generic excitation state

Detailed excitation state:

each element is optional but the order is important

Vibrational states

Examples

V3

3rd level

2V1

2nd overtone of 1st level

2NV1

1st harmonic level
2nd overtone

V1[ST]

1st level stretching

(see next slide)

V(101)

1st sym. stretching
0th bending
1st asym. stretching

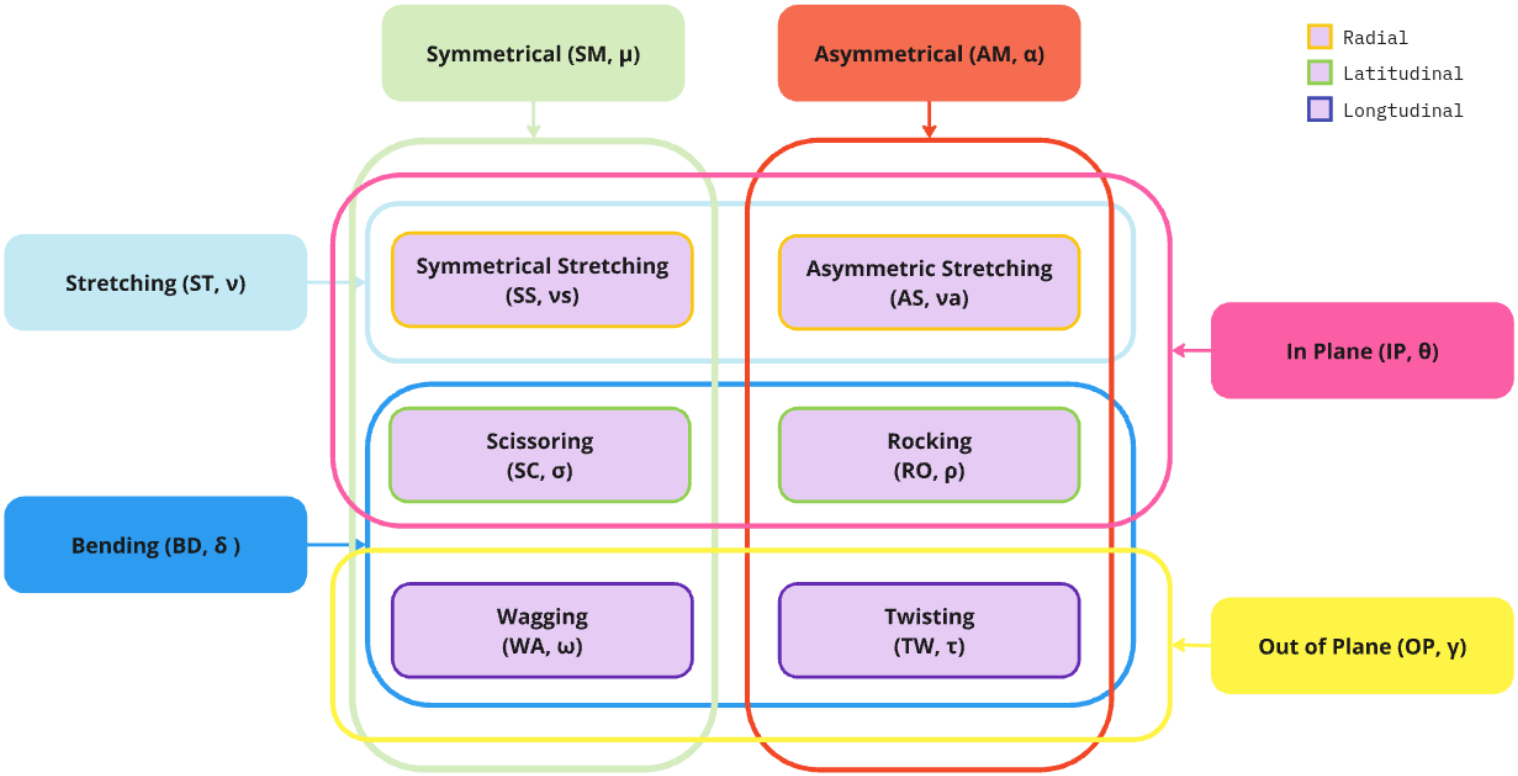
(linear molecules only)

Combination bands

V1+V2[ST]

V1-V2

Vibrational states



* Torsional = Deformation = Bending

Rotational states

Examples

J=1	J=2 K=1	J=2 Ka=1 Kc=1
Only one axis	Two axis: main axis and projection on the other one	Three axis: main one and projections on the other two
R(1)	R(21)	R(211)
(compact mode)	*(compact mode)*	*(compact mode)*

Electronic excitation

A lot of different coupling scheme:

Name	Description
LS	Russell-Saunders coupling
JJ	jj coupling
JL	jl coupling
RH	Racah coupling
PS	Paschen coupling

→ `X 5s2` or `X 1 3DEL1u+`

→ `(1,2)2`

→ `2p[3/2]2`

→ `(3DEL1) 2p[3/2]2`

→ `2p1`

Excitation ranges

- Often when reading cross-section tables, we find out that the tables does not represents a single physical process but a collection of different ones.
- Often these processes are represented as ranges of one parameter (bounded or unbounded).
- A proper syntax shall support natively the possibility to define ranges for the excitation states

`(2-H)V1`	`J=(2-5)`	`J=2 Ka=* Kc=1*`	`X 5s(1-3)`
Vib exc. from overtone 2 to ∞	Rot exc. from level 2 to 5	Rot exc. level 2, all projections	Ele exc. J between 1 and 3

What we have already

- A PEG syntax that is able to parse everything shown in this presentation

  This will allow anybody to implement the parsing of reaction in its own software.

  Repository: https://gitlab.com/micrenda/zmoles-peg

  (NB. repository is private, write us an email if you want to have access or collaborate with us)

- A reference implementation (Zmoles) that use the PEG syntax to produce a set of C++ classes representing reactions, molecules and excited stated

  This will allow anybody to integrate the parsing in its software if they use C++ or a language with C++ binding

  Repository: https://gitlab.com/micrenda/zmoles

  - *(NB. repository is public, but use the branch **devel** where the latest changes are integrated)*

- A syntax checker: to validate any given string if correctly representing a reaction

  Bonus: you get along syntax validation also charge, mass conservation checks and others

What we need

Help

We have limited experience with excitation states syntax and we may have overlook / misunderstood the used syntax.

Feedback

From real world experience:

- Are you missing some functionalities?
- Something is not well represented?
- Suggestions?

Thank you for your attention

For any follow up question do not hesitate to contact me at:

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