Improving interoperability for gaseous-detector simulation tools

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Content of the presentation

1)The three beasts and where to find them

2) What we are doing? Partial results ...

3) Conclusions

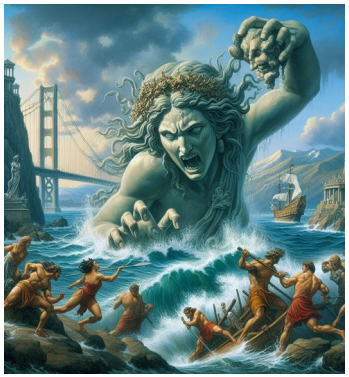
The three beasts and where to find them

Beast 1 – Magboltz is like a black-box

Magboltz is the most **widespread** and **reliable** solution available, and virtually all the existing gas physics experiments/simulations use and depend on it. It is **fast** and produces **correct results**.

Unfortunately, it is a monolithic solution, and there is no way to extract its power and learn from it. People tried to rewrite it in Python (PyBoltz), but the main issue is still there.

There is real progress only when the advantages of a new technology become for everyone (H. Ford)



Beast 2 - cross-section tables incompatibility

Each tool can work efficiently only with its own cross-section database. Using a different database requires painful manual work to categorize processes one by one, especially the ones containing **excitations**.

Examples: **Loki-MC** does works with **IST-Lisbon** database, **Bolsig** does work with **Siglo** database, etc.

It is like your **Ford** car works only with **Exon** gasoline. This does not make sense.

Beast 3 – Software-parsable processes and molecular states

There is no **concrete**, n**on-ambiguous**, software-readable syntax for describing gas-scattering processes (including excitation states). Each software program invents its wheel and adds its **magic comment** to its specific cross-section database!

What are we trying to do?

Our first idea to attack **Beast 1 – Magboltz is like a black-box** , was:

How difficult is it to extract the cross-section tables from Magboltz?

Steps:

1) Create an interface with **Magboltz** and read the cross-section tables

2) Re-sample the tables so we get a reasonable number of energy-points while maintaining all the interesting features of the cross-section tables

And finally:

3) Categorize the extracted tables

4) Validate the results using the extracted data into an **already validated** tool (e.g. Bolsig, Loki-MC, etc.) to see if we can get back the **drift-velocity** produced by **Magbolz**.

Steps 1 and 2 were really simple to perform, but the steps 3 and 4, were unexpectedly hard, and they stopped us.

Main problems:

- Softwares are supposed to work with their cross-section databases (**beast 2**)
- Using our database we need to add some information about the process, but we do not have a **language** to communicate/store this (**beast 3**).

What are we trying to do?

To win the **Beast 2 - cross-section tables incompatibility**, we believed we were the right persons for the job:

We have extensive experience converting LxCat databases into machine-readable formats, and we can use this expertise to create tools that convert LxCat databases (or any database in our ZCross XML format) into databases that can be used by the most common simulation tools (Bolsig, Loki-MC, etc.)

We were only half right: indeed, we can handle conversion quite easily and create perfect input files for any simulation tool.

However, we treated excitation states as "**take-as-is**" strings and did not try to parse and understand them (*to be honest, we are not the only ones who do this*).

Unfortunately, this information matters, and if you want precise results, you must be able to differentiate between, e.g., rotational, vibrational and electronic excitation states and calculate their population.

But how do we handle this? We did not have even a universal machine-readable syntax to describe that.

So, there is no choice but to attack **Beast 3 – Software-parsable processes and molecular states**.

What are we trying to do?

To win the **Beast 3 – Software-parsable processes and molecular states**, we prepared a syntax that can be read both from humans and machines.

We are still working hard on this, and we hope to be able to publish it in an article for the community's use.

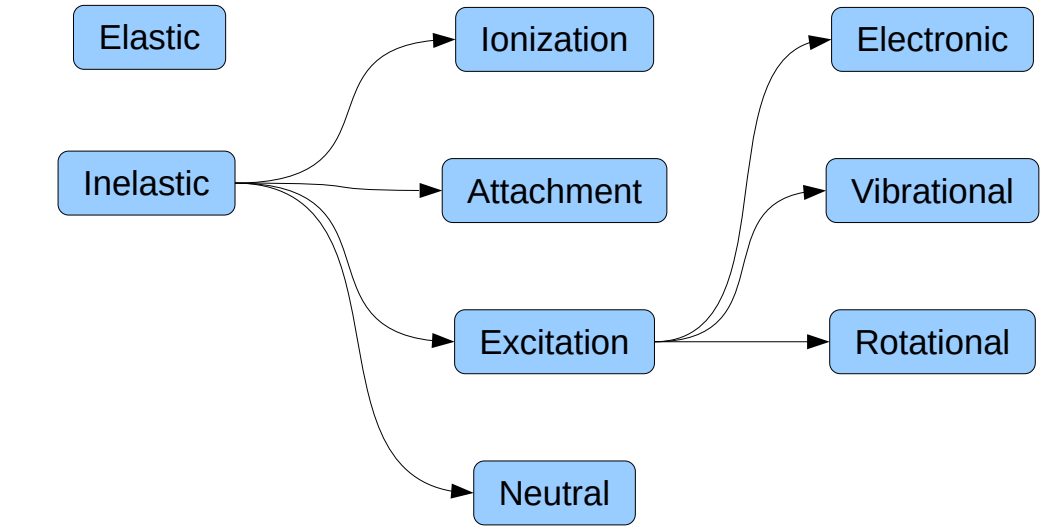
Main characteristics:

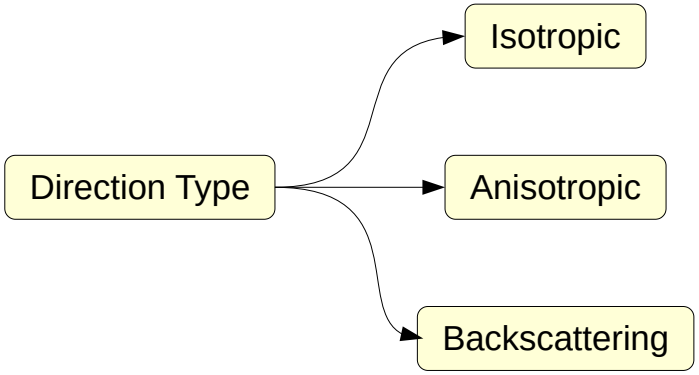
1) Both human and machine-readable
2) Well-defined and unambiguous
3) Try to cover all the cross-section processes existing in the field (we are trying, on the first instance, to be able to cover all Magboltz processes)
4) Reuse, whenever possible, existing conventions and symbols to make adoption easier.
5) Able to describe processes with different outcomes (aka different channels)

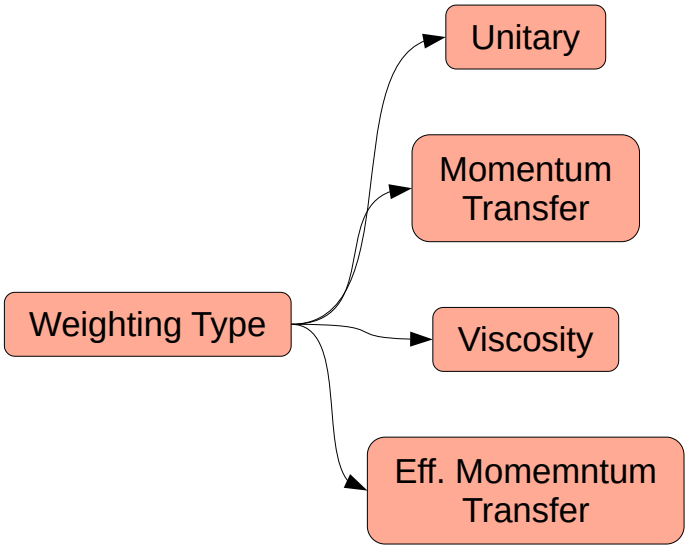
We are not only defining it theoretically, but we are also providing a reference implementation (aka a software who parse that syntax) to make sure that the syntax is coherent and can be parsed in real-life scenario.

What are we trying to do?

Process classification







Integral

Differential

Excitations have different coupling scheme that shall be supported

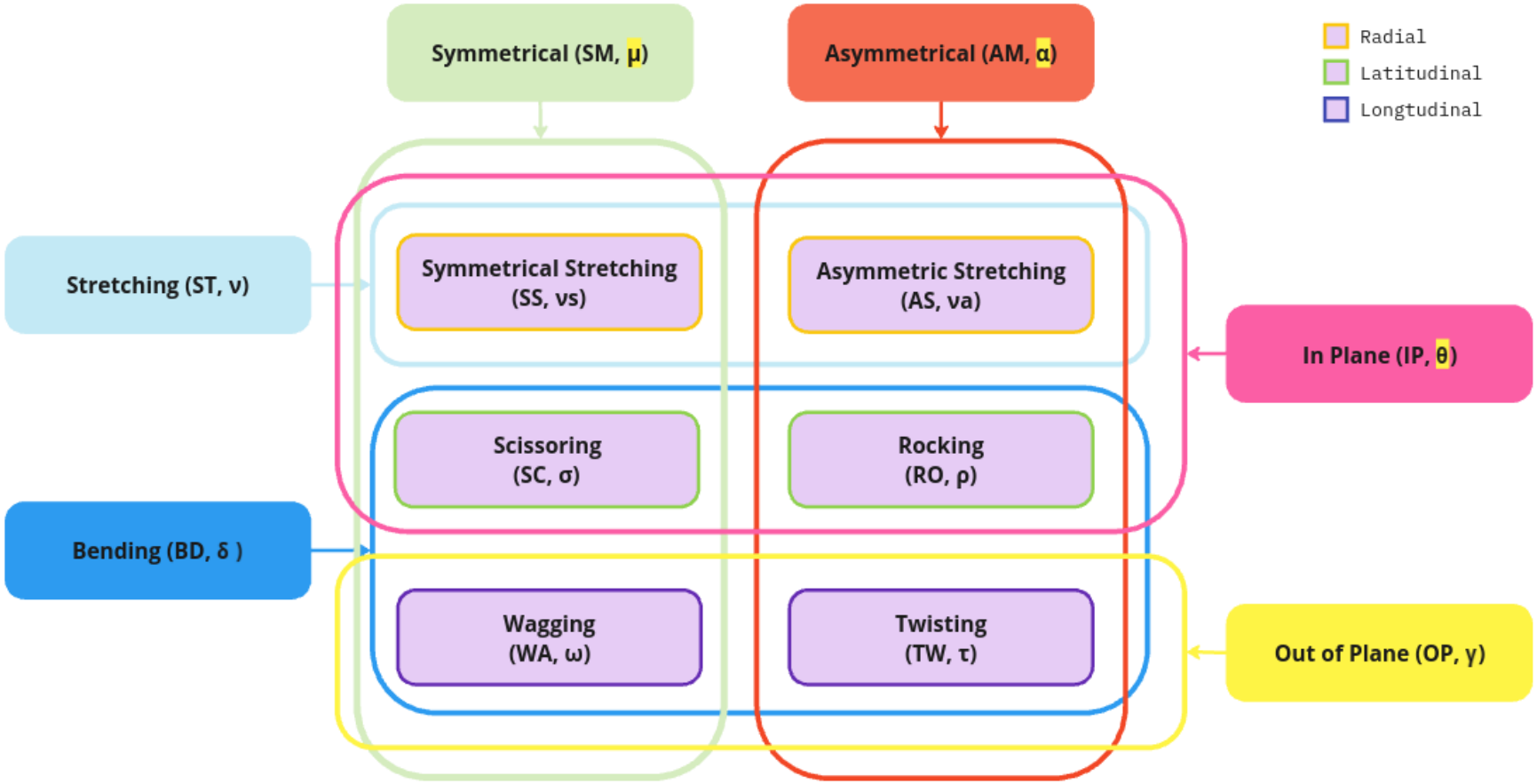
Electronic excitation

1) LS Coupling (Russell-Saunders Coupling)
2) jj Coupling
3) J_1J_2 Coupling
4) J_1L_2 Coupling
5) LS_1 Coupling
6) Racah notation
7) Parchen notation

What are we trying to do?

Vibrational mode

Vibrational modes are classified using the following diagram



* Torsional = Deformation = Bending

Our partial results

Cross-section tables from **Magboltz**

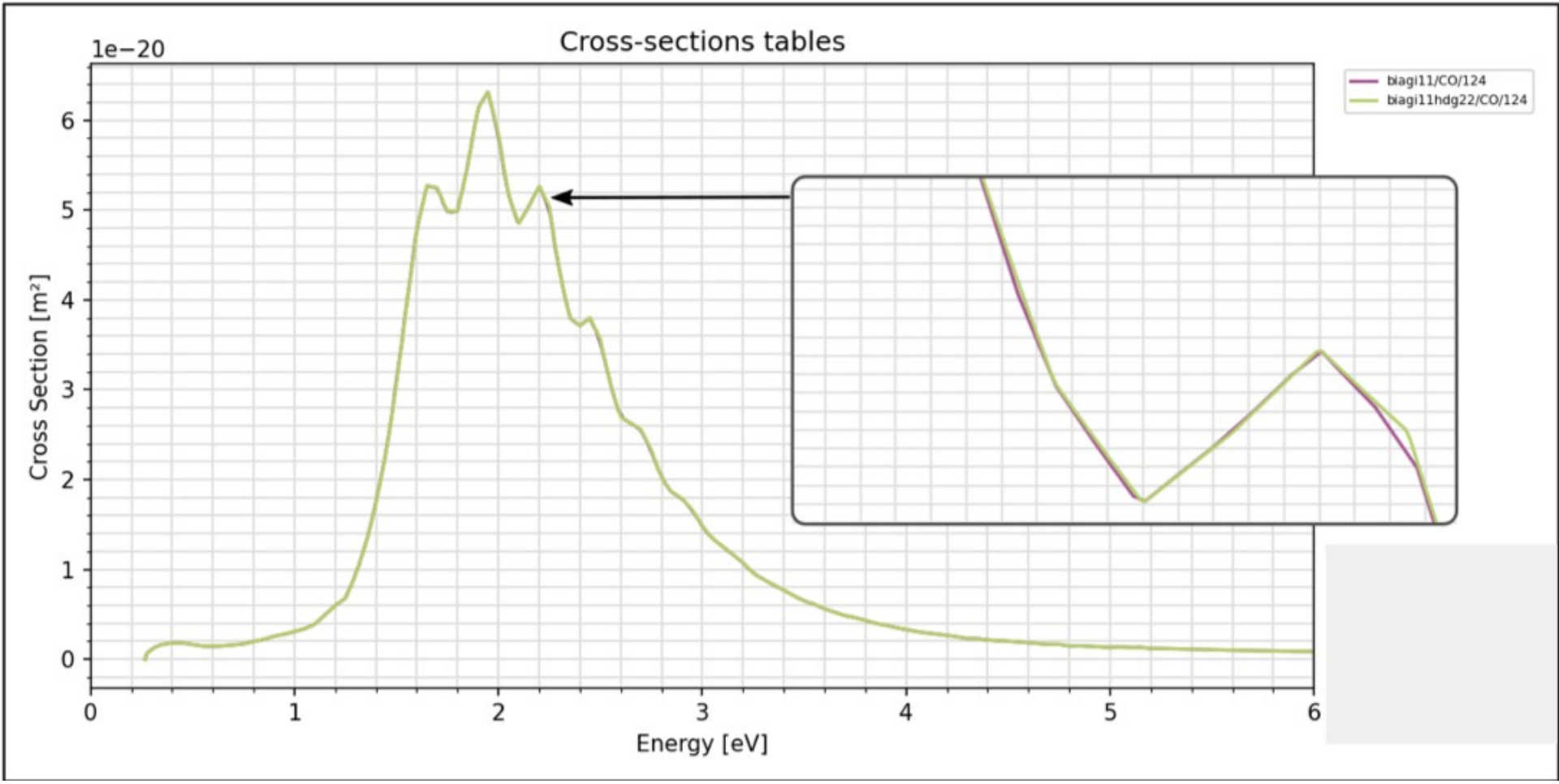
Extracted **3732** cross-section tables for **54** gases:

Elastic cross-sections:	**73**	(normal elastic + momentum transfer)
Inelastic cross-sections:	**3659**	(including super-elastic)
→ Ionizations:	**485**	
→ Excitations:	**2709**	
→ Attachments:	**86**	
→ Neutral dissociations:	**379**	

TODO:

Categorization of excitations (ele, vib, rot) with precisely defined final states

Our partial results



The HD table (biagi11/CO/124) has ~ 21.000 energy samples: not really usable for Monte-Carlo simulations (or other sims)
The optimized table has only 131 energy samples : way easier to manage !

Conclusions

We strongly believe these beasts must be overcome to bring fresh air to the gaseous community.

However, we feel we are the **wrong people** trying to fix the **right problem**: sometimes, we lack the right background (we are elementary particle physicists, and our experience with gas physics is quite limited).

As a result, we sometimes take the wrong path, spend too much time on subjects that are simple for others, or start with incorrect assumptions.

If someone wants to join us in this quest to hunt the beasts, please do not hesitate to contact us.

Thank you