Comments on Heavy-Particle Collision Data Assessment; General Discussion

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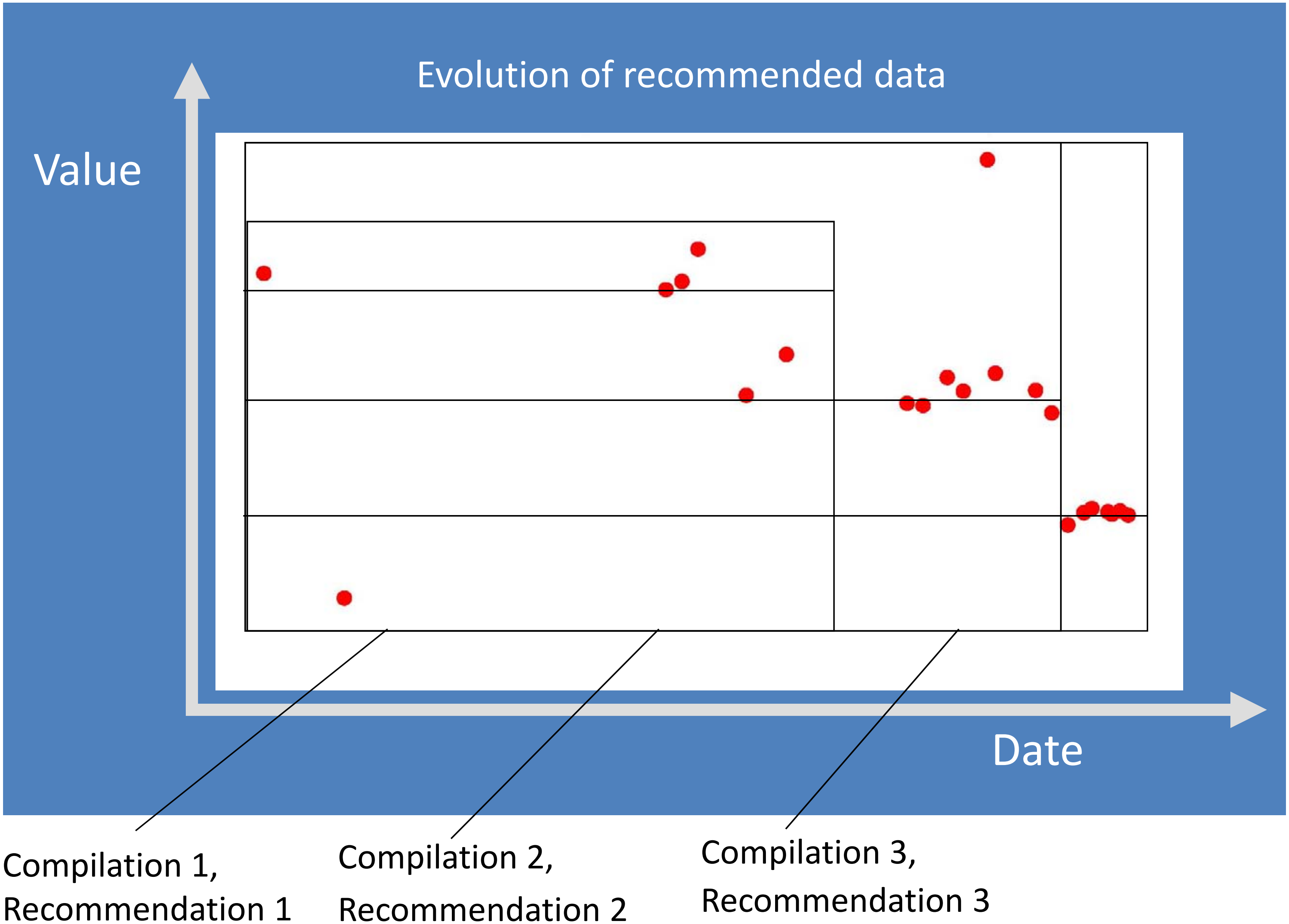
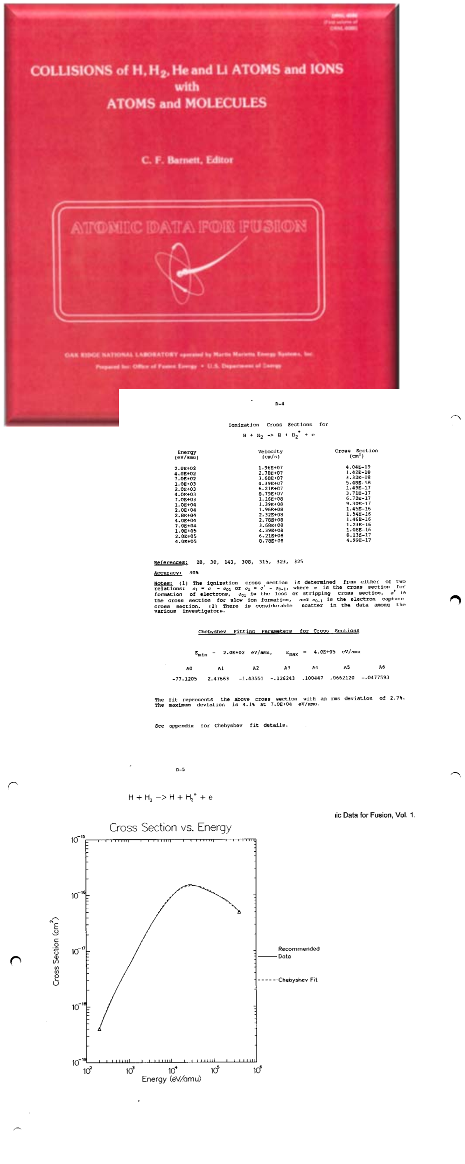
How has heavy-particle collision data been assessed and provided to the fusion research community over the years?

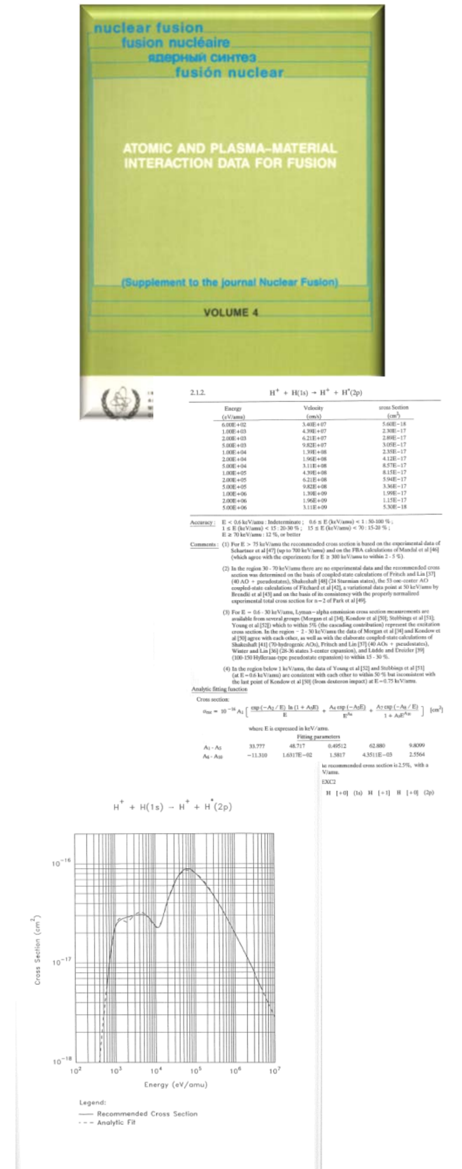
- Contrary to our widely held belief that all men and women are created with equal potential in life, not all atomic data are created with such equal potential and therefore a process has historically been adopted consisting of …
  - bibliographic database creation
  - data collection and compilation
  - data evaluation and recommendation



Evolution of recommended data
Value
Date
Compilation 1,
Recommendation 1
Compilation 2,
Recommendation 2
Compilation 3,
Recommendation 3

Data centers or other groups of experts …





With this foundation, evolution has occurred of both needs and capabilities to fulfill the needs

- Modelers in particular, but also experimentalists, have come to need more detailed data that is not easily provided by the historical process

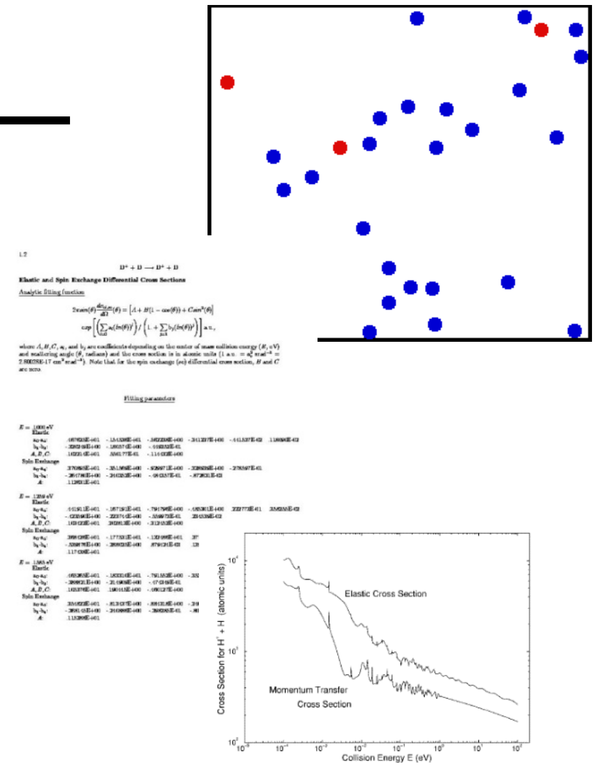
- Also, the field of heavy-particle collision physics continues evolve on its own

  - with fewer and fewer experimental activities as interests change to newer fields of study, and

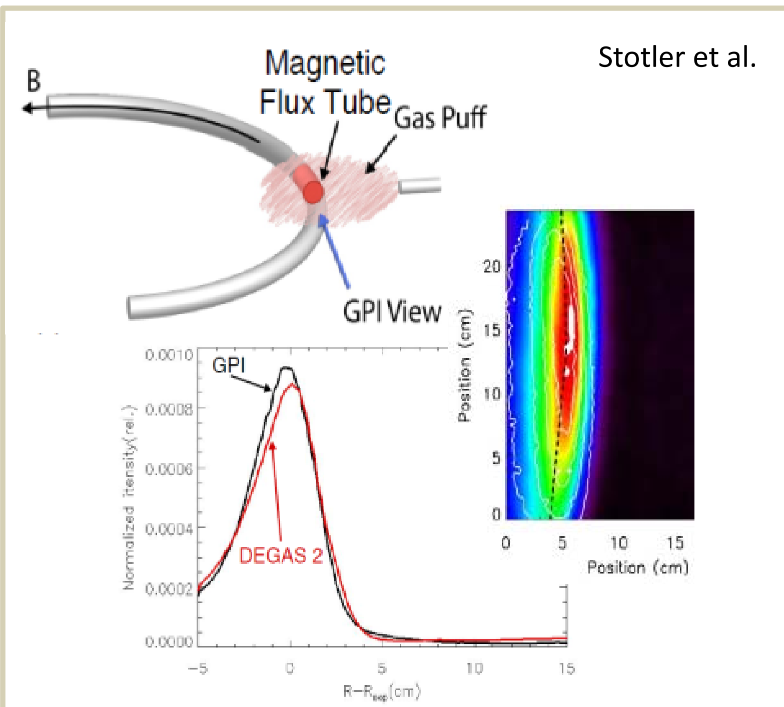
  - Theoretical work also diminishes in the number of practitioners staying in this area, but, crucially, also evolves to be able to provide *demonstrably convergent* results for both fundamental cases and broad ranges of needed data

- Heavy-particle collision example: Krstić and Schultz elastic and transport cross section database

Transport of ions in fusion & astrophysical plasmas



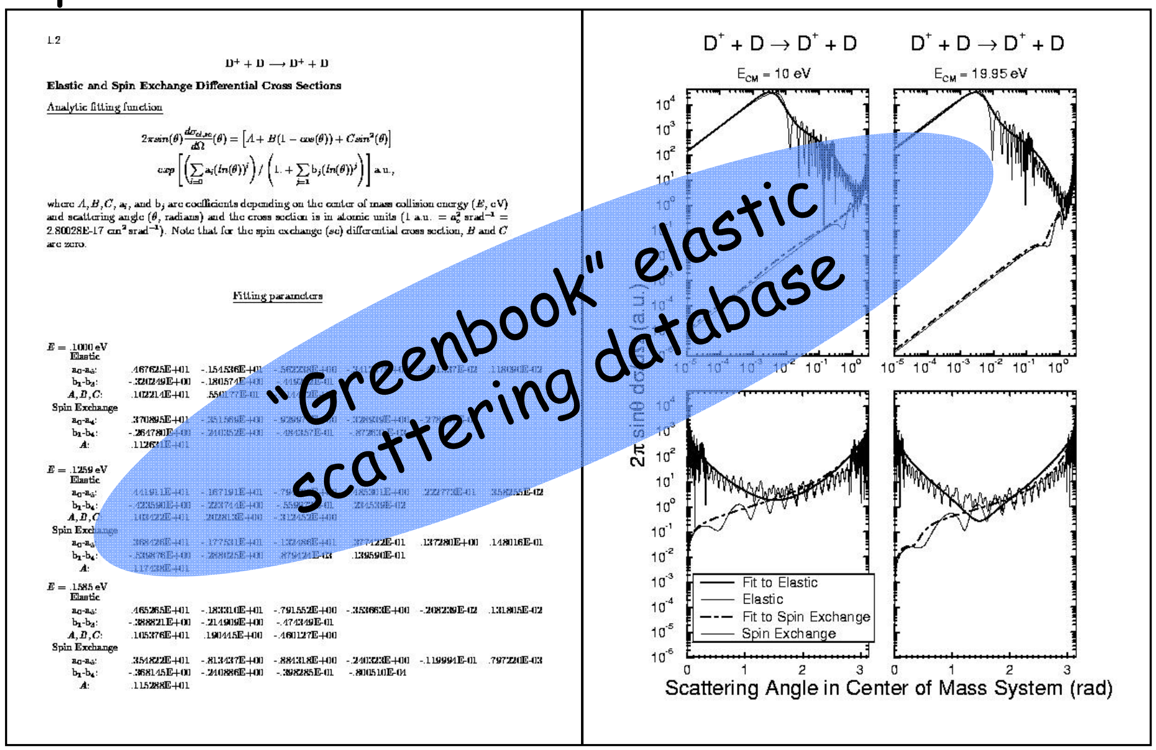
- Accurate and complete description of elastic scattering is crucial for modeling the transport of ions and neutrals in gases and plasmas and interpreting observed characteristics from experiments
- Calculations of such are among the first atomic scattering calculations ever done, yet there is a persistent need for ever more accurate and especially more comprehensive data (Krstić & Schultz)



- Simulations based on the elastic scattering database for gas puff imaging (GPI) of fusion plasmas elucidates the origins of plasma turbulence
- Stotler et al. have used the neutral transport code DEGAS 2, confirmed by measurements, to described emission from He, D_2 gas puffing

CFADC Elastic Database

- All hydrogen isotopic variants if (H^+, H) + (H, H_2, He)
- Needed to model plasma charge, momentum, energy, and particle transport – DEGAS 2 → CPES
- Fully quantal calculations of differential and integral elastic cross sections and transport moments
- Fitting formulae
- Scaling laws
- IAEA "Greenbook" Vol. 8
- Raw data on web
- 250 integral, 3000 differential cross sections



However, for readily understandable reasons, B2/Eirene for ITER design does not use the ORNL elastic database, as does DEGAS-2, but rather the classical elastic scattering data from Bachmann

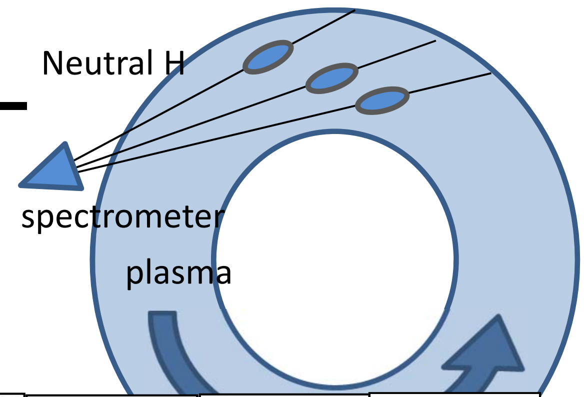
- Modelers and experimentalists will most likely use the most convenient available data, not replacing it with data judged to be more accurate or comprehensive due to the effort required to make the switch, possibly repeat extremely long series of simulations or experimental analyses, and their uncertainty about changing it without proof of the need for these “risks”

Given the need for more accurate and more comprehensive data, what approach should be taken to provide it?

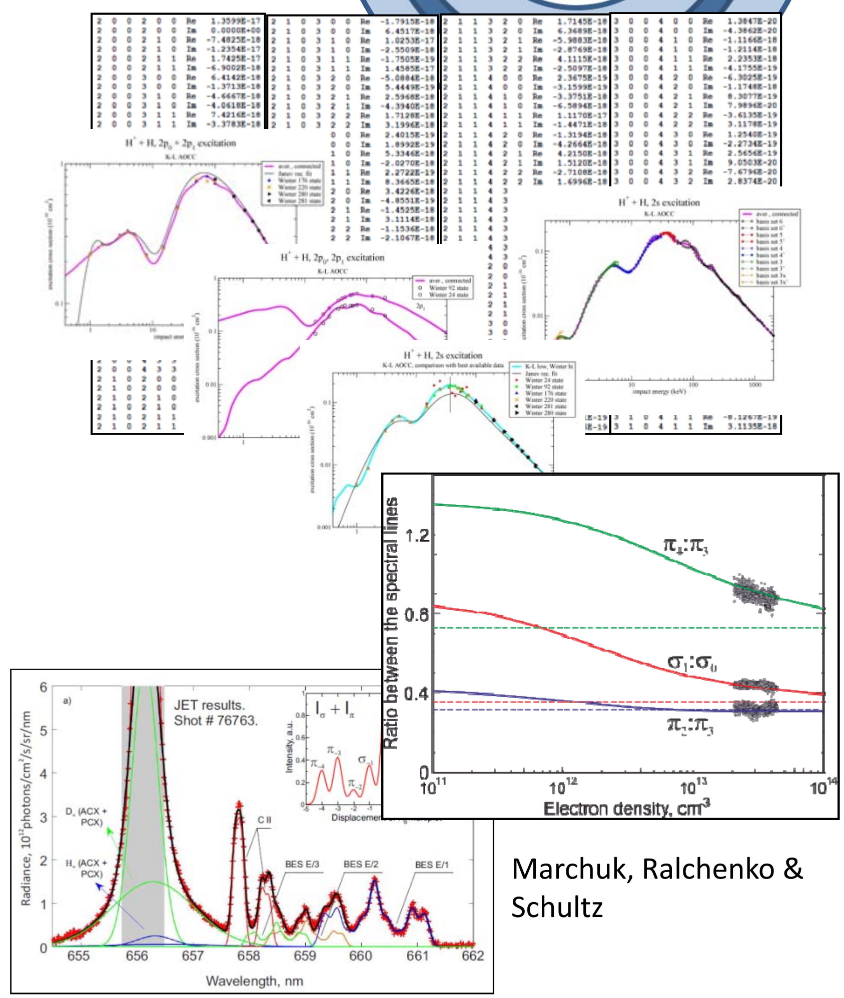
- Regarding all heavy-particle collision systems for which it is possible, demonstrably convergent theoretical methods should be used, tested if and when possible by existing experiments (either direct atomic collision experiments, or via plasma experiments)

- Example, ongoing work of Marchuk, Ralchenko, and Schultz on an excitation database used in beam emission spectroscopy

Plasma diagnostics based on excitation

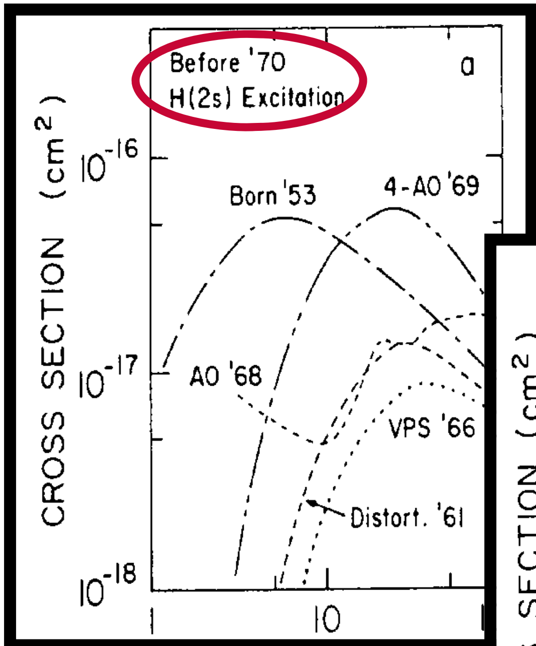


- Fusion plasma diagnostics such as beam emission spectroscopy and motional Stark effect spectroscopy depend on atomic data for charge transfer and excitation
- Plasma parameters such as field strength, temperature, density, and magnetic field orientation can be determined from these diagnostics
- Collisional-radiative models need not only cross sections for excitation to specific states but also density matrix elements, not previously available for a comprehensive, wide range of states and impact energies
- Modeling based on this data has been applied to neutral beam diagnostics for ITER and existing experiments, showing, for example, that typical statistical assumptions about state distributions in the plasma are not valid



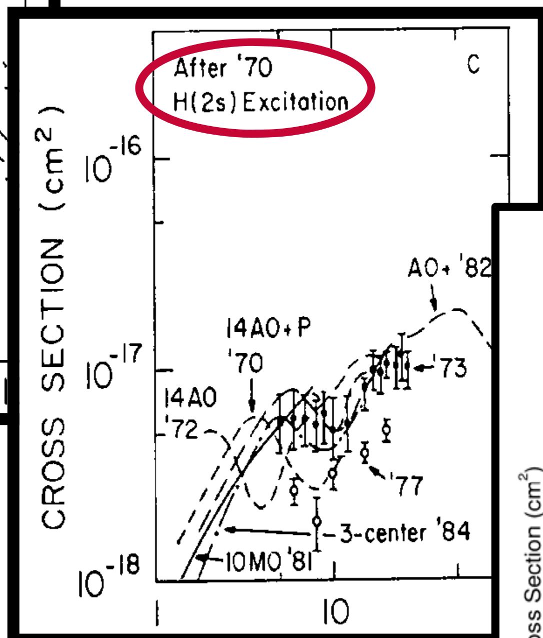
Marchuk, Ralchenko & Schultz

Evolution of knowledge of H^+ + H excitation



Energy (keV)

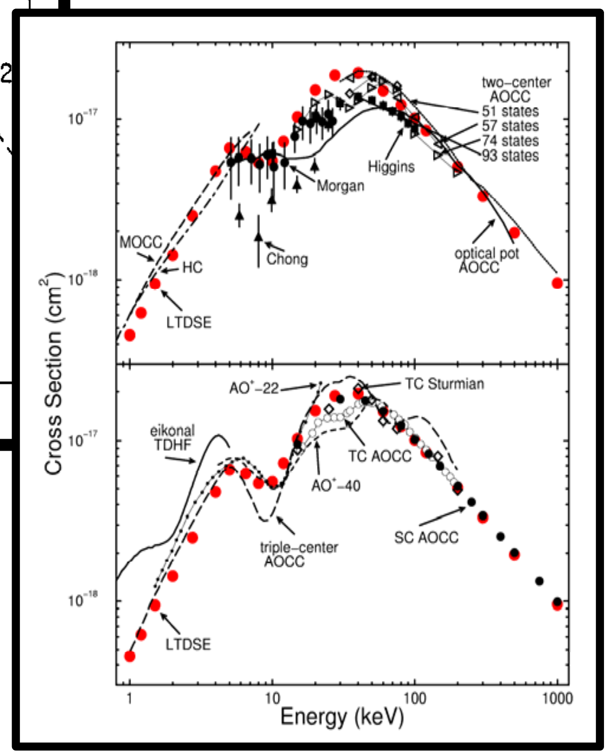
Kimura & Lane 1989



Energy (keV)

Drivers: gaseous and plasma physics needs; experimental advances; theoretical evolution towards direct, demonstrably convergent methods

Schultz et al. 1999



Late 1990's

For other data needs, it will simply not be possible in the near future to make such demonstrably convergent calculations

- The size and scope of some heavy-particle collision data needs, and the nature of the systems these pertain to, will continue to be out of reach for some time of demonstrably convergent calculations

Conclusions

- The need for both refined and new heavy-particle collision data for fusion (and other applications) persists, particularly for more accurate and more comprehensive data sets
- Owing to the evolution of the AMO and data center communities, the historical approach of data collection to recommendation cannot be sustained, nor do the most recent needs for comprehensive data sets fit with this model
- Therefore, the way forward is to update existing data sets for heavy particle collisions and produce new ones using demonstrably convergent methods, validated when possible by AMO experiments or plasma experiments
- We must realize too that there will persist needs for large datasets that cannot be created with such demonstrably convergent approaches
- Finally, there is the challenge to engender recognition of the special need for AMO data production, collection, evaluation, and dissemination for long term support, critical to other fields and requiring its own sustained community of experts

General Discussion: Heavy-particle collision data