NAUSICAA : Improved neutron cross sections for reactor physics

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Issues on thermal cross sections

Cross sections libraries use special data for thermal neutrons

- Called S(α,β) (analogous to Sqω)
- Experimental data are old and have a low accuracy
- Reliability is low for hydrogenous liquids

Significant impact on hydrogen-based neutron cold sources

- Strong effect on cold neutron production modelling
- Possible impact on keff for nuclear facilities (mainly those using heavy water)

The idea

Measurement of S(q,ω) could lead to a new evaluation of the S(α,β) with an improved accuracy !

We propose a new way to evaluate thermal neutron cross sections

Direct input of measurements into THERMR

Basis : neutron scattering laws

ω = energy transfer

q = wave-vector transfer

The idea

Neutron inelastic scattering experiments are carried out every day at the ILL

Measurement of structure factor S(q,ω) for liquids is possible

$$S(Q,\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \;\; e^{-i\,\omega\, t} \, \frac{1}{N} \sum_{\alpha,\beta=1}^{N} \left\langle e^{-i\,\mathbf{Q}\cdot\mathbf{R}_\alpha(0)} \, e^{i\,\mathbf{Q}\cdot\mathbf{R}_\beta(t)} \right\rangle$$

Double Differential Cross Section is directly linked to S(q,ω)

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \frac{k_1}{k_0} \, \tilde{S}(Q,\omega)$$

$$\tilde{S}(Q,\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \; e^{-i\omega t} \, \frac{1}{N} \sum_{\alpha,\beta} \left\langle \, b_\alpha^* \, b_\beta \;\; e^{-i\mathbf{Q}\cdot\mathbf{R}_\alpha(0)} e^{i\mathbf{Q}\cdot\mathbf{R}_\beta(t)} \right\rangle$$

The idea

$$\frac{d^2\sigma_T}{d\Omega dE'}(E \to E', \mu) = \frac{\sigma_b}{4\pi kT}\sqrt{\frac{E'}{E}}\; e^{-\beta/2}\; S(\alpha, \beta)$$

$$\frac{d^2\sigma_T}{d\Omega dE'}(E \to E', \mu) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E'}{E}}\, S_{exp}(q, \omega)$$

$$\beta = \frac{E'-E}{kT}$$

$$\alpha = \frac{E+E'-2\mu\sqrt{EE'}}{AkT}$$

$$S(\alpha, \beta) = kT\; e^{\beta/2} S_{exp}(q, \omega)$$

Project

Project objective : getting reliable S(α,β)

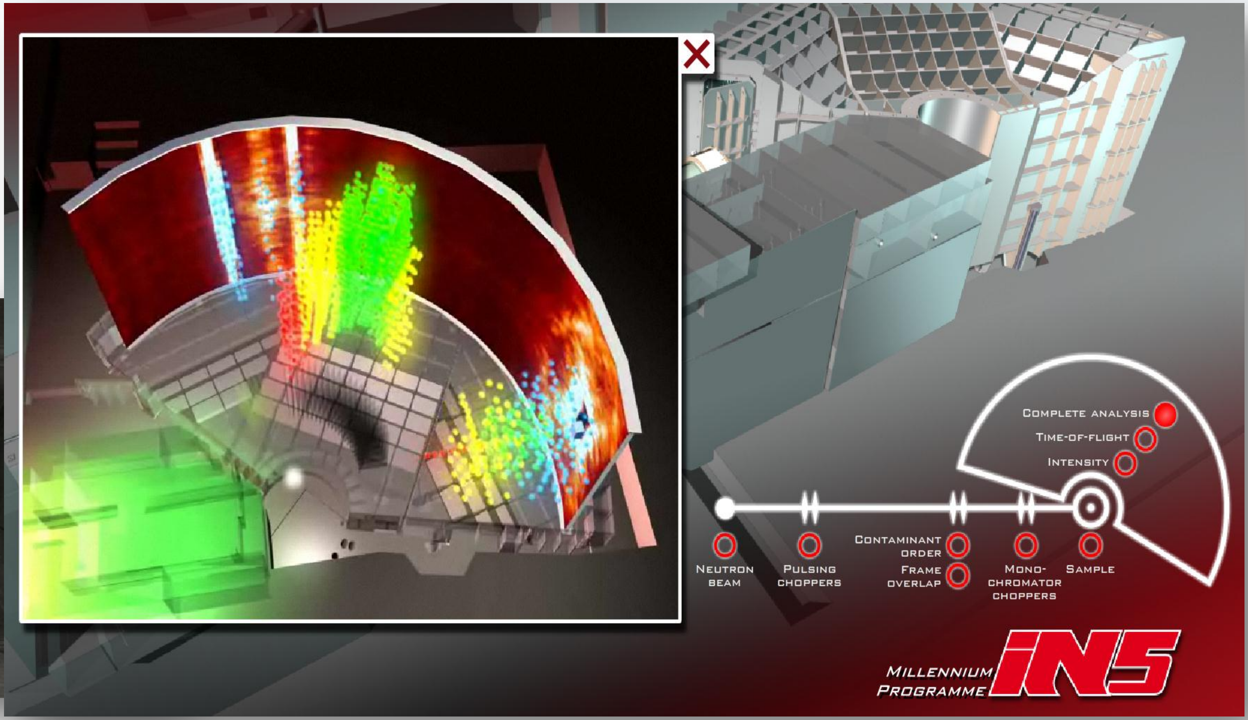
Project main steps

- Measurement of S(q,ω) for model systems (heavy and light water)
- Measurement of S(q,ω) for cryogenic liquids – CRISP project
- Transformation in .ace format for MCNP (thanks to NJOY code)
- Collaboration between the ILL and IRSN and University of Florence

Data processing

Get S(α,β) from experimental S(q,ω) and normalize them against experimental cross sections values.

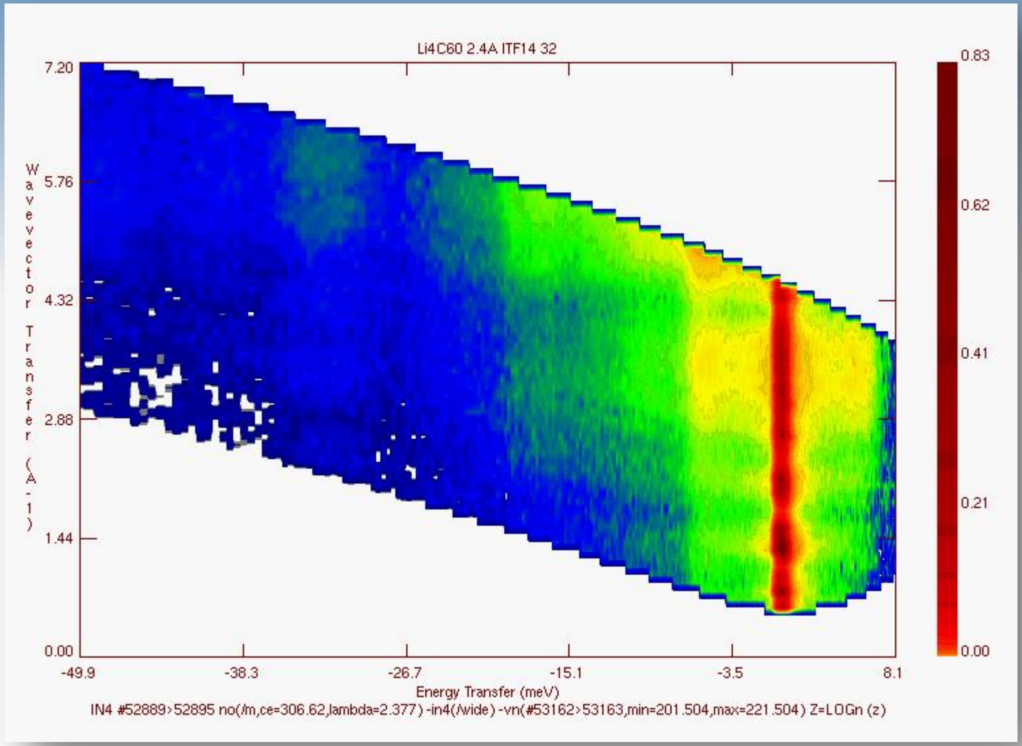
Measurements
on IN5 and IN4C
(ILL intruments)



Data processing

Measured (q,ω) domain limits incident energy to be < 50 meV

We have completed S(α,β) on a larger domain using Molecular Dynamics simulation.



Normalization : EXFOR for thermal neutrons

Data processing

These completed $S(\alpha,\beta)$ corresponds to the whole water molecule,

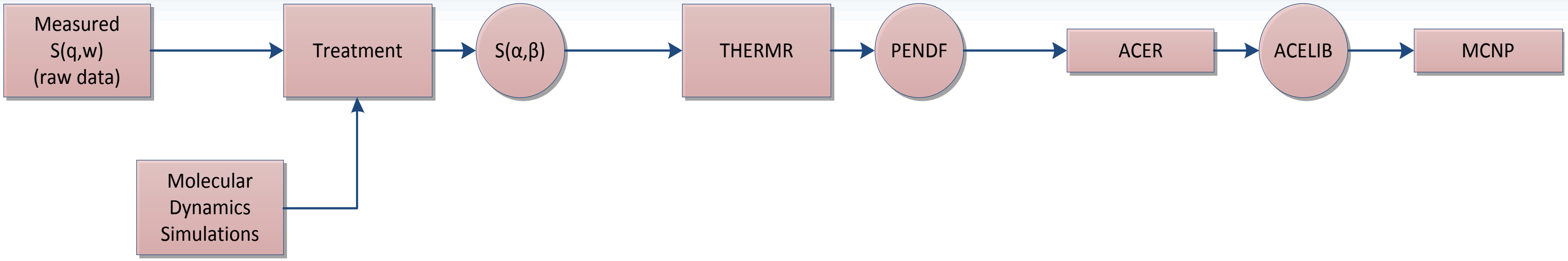
we transform them into $S(\alpha,\beta)$ for a single H or D by removing oxygen $S(\alpha,\beta)$ and dividing by 2

Then an ENDF file is created with this data and used as an input in NJOY – THERMR

NJOY – ACER gives us an ACE file

Process

We change the usual way to get nuclear data

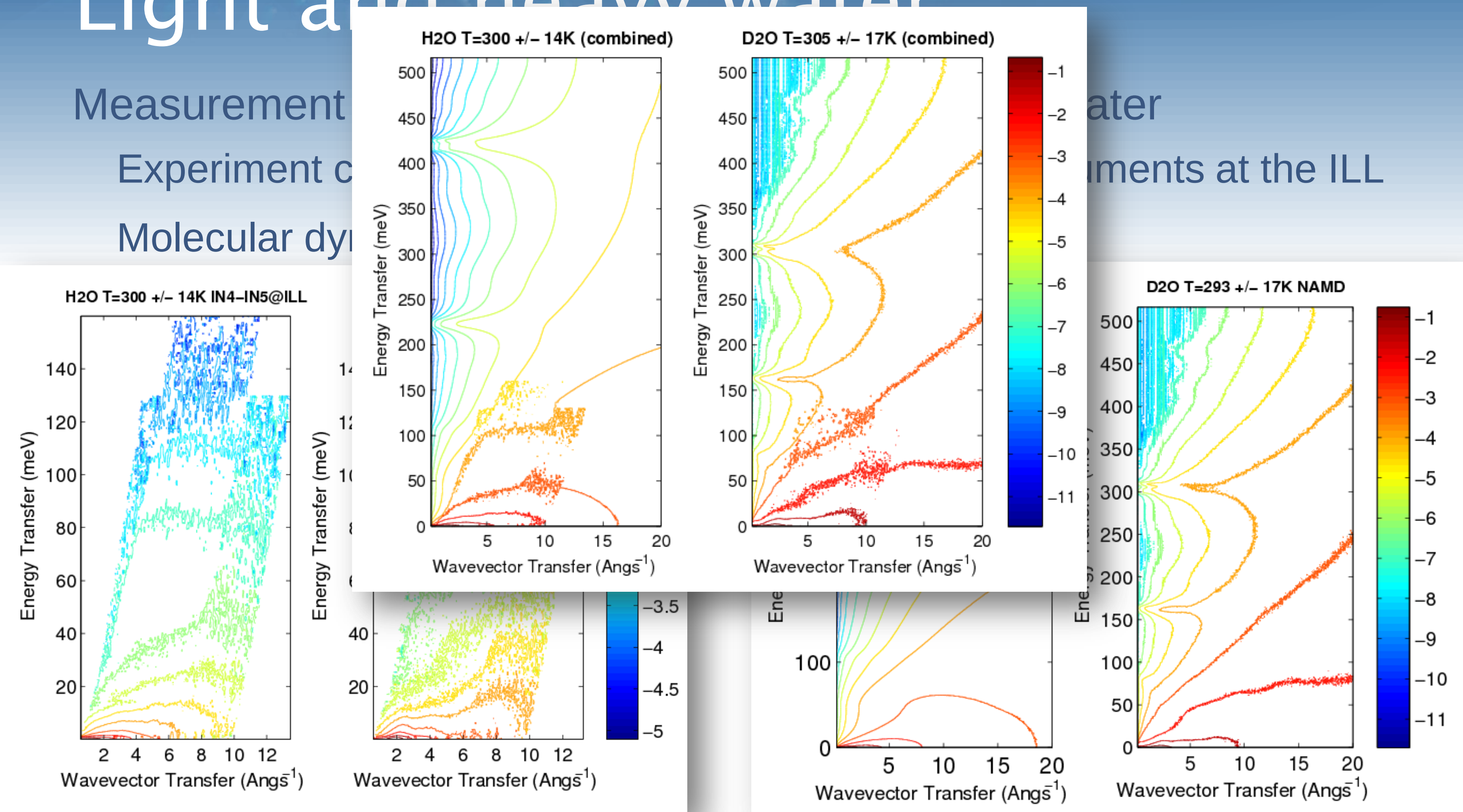


We go directly through THERMR

~~LEAPR~~

Light and heavy water

- Measurement ... ater
  - Experiment c ... uments at the ILL
  - Molecular dy...

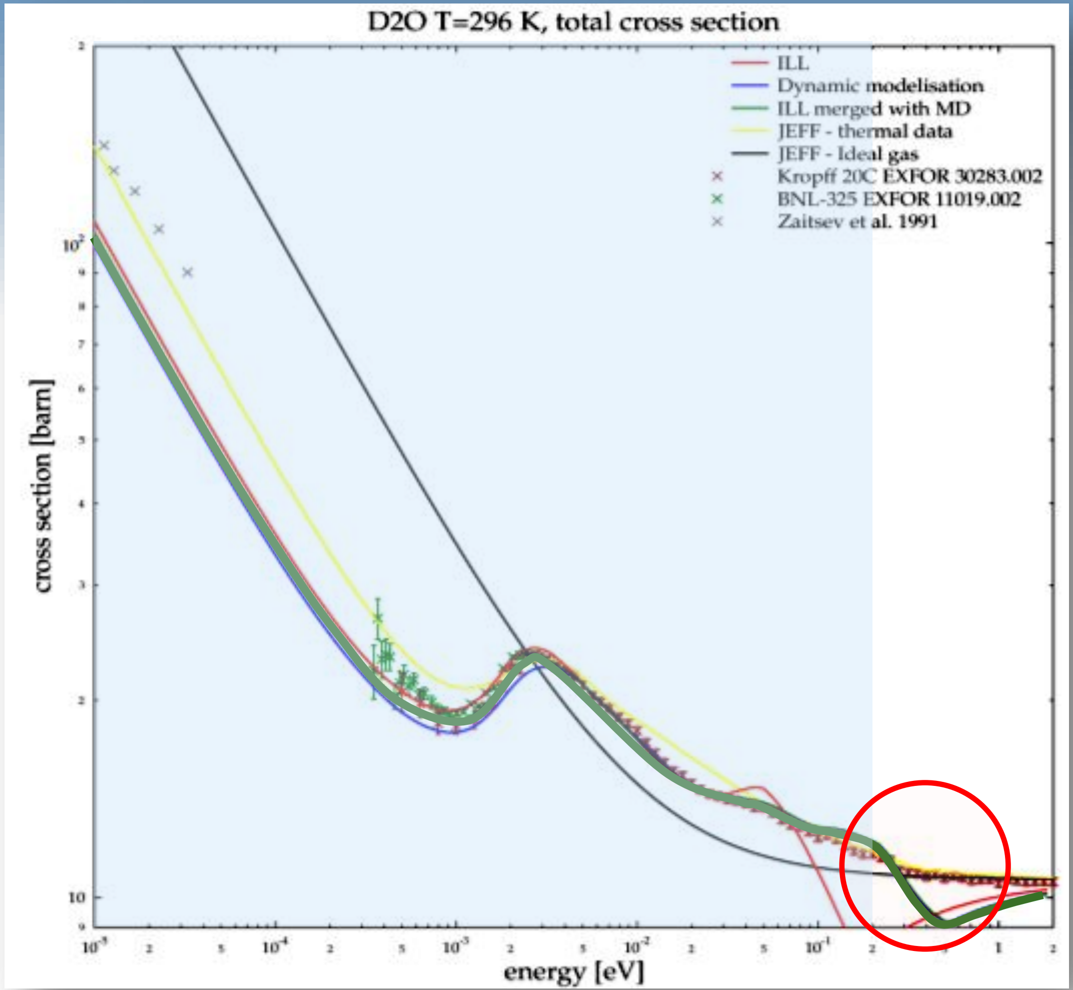


D2O cross section

Excellent result

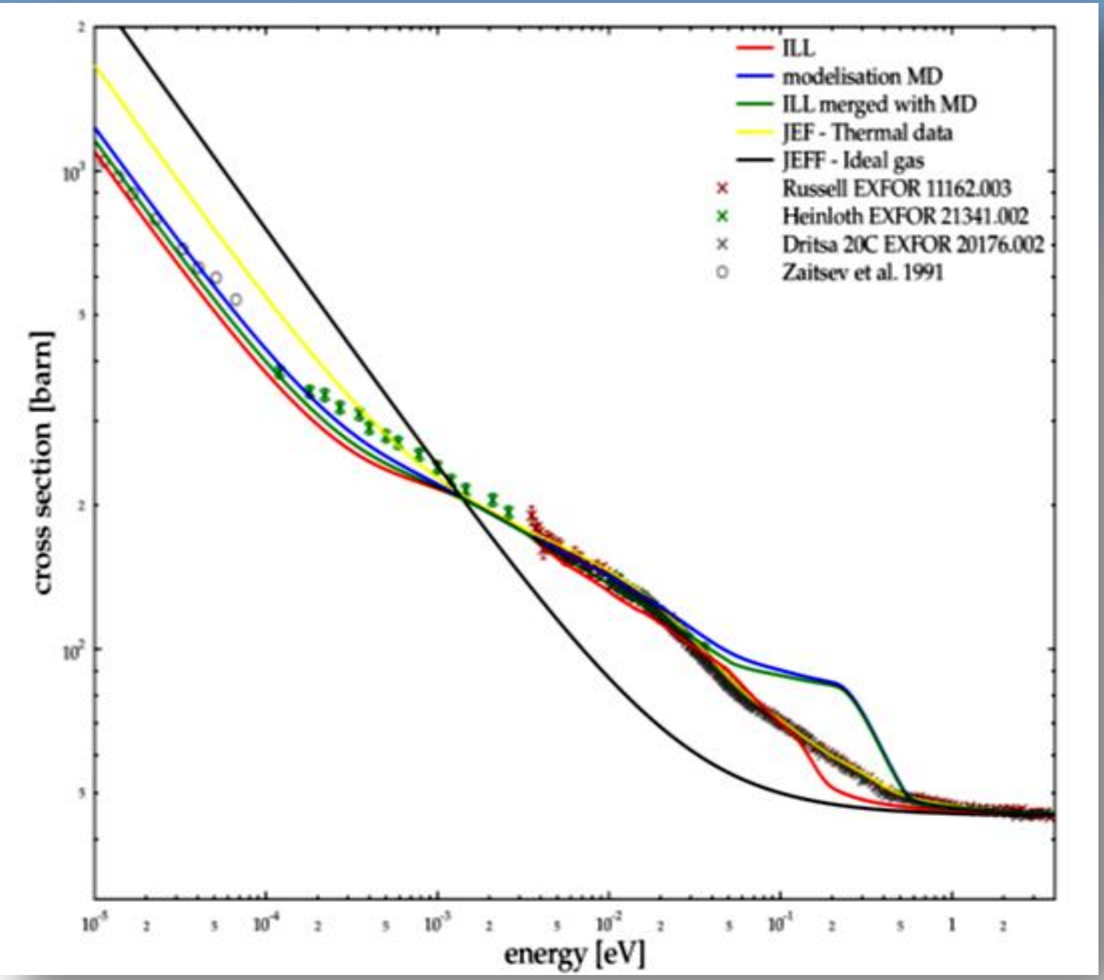
BUT : issue above 200meV

A steep decrease without any physical meaning



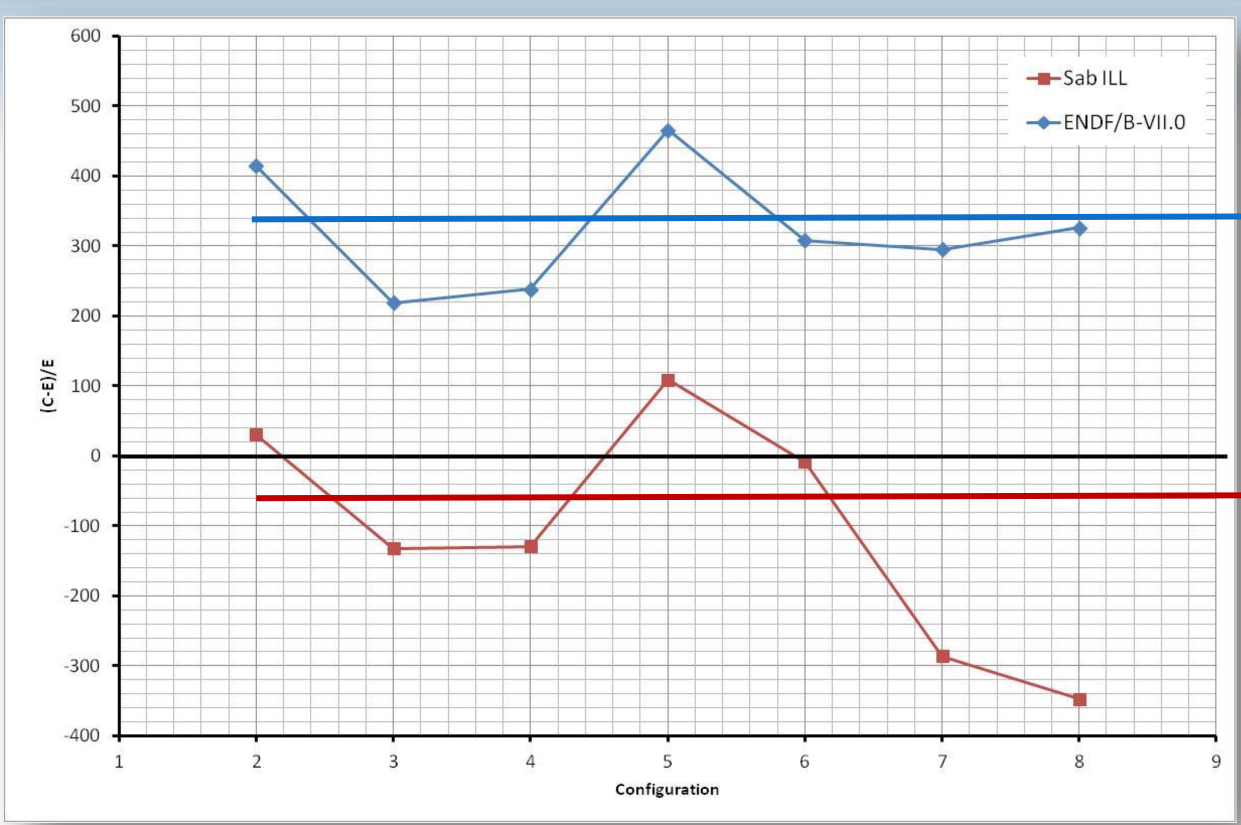
H2O cross section

Same case for H2O



Benchmark on RHF

Data were tested with success on the RHF MCNP model



Initial data

Bias : + 350pcm

ILL data

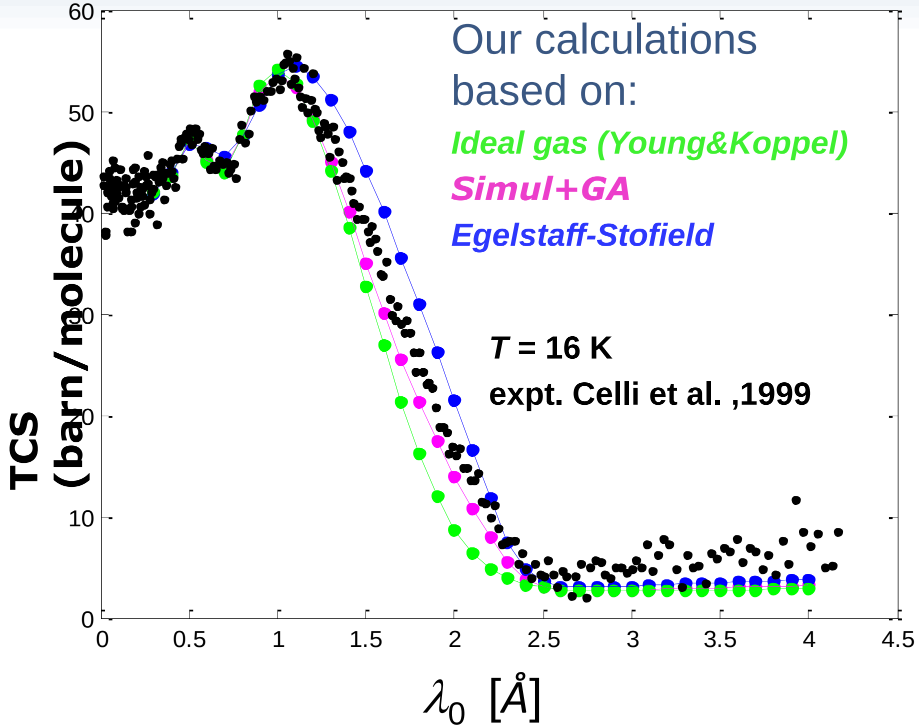
Much better spreading

Cryogenic liquids

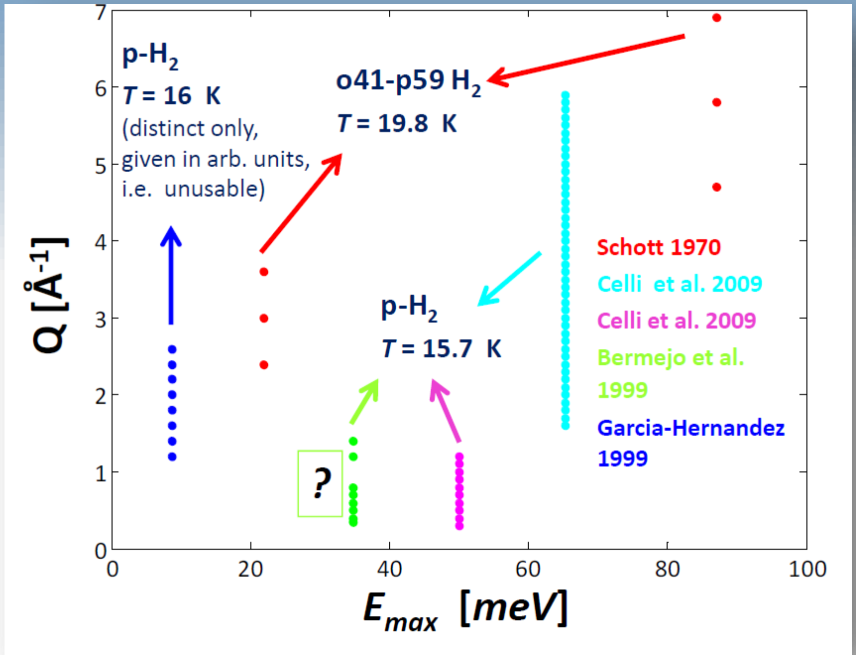
Double Differential Cross Section data on liquid H_2 are unexpectedly few and partly unreliable

Total cross section data on liquid H_2 need verification

Calculations can substitute experiments (avoiding difficult measurements on para-H_2 for example)

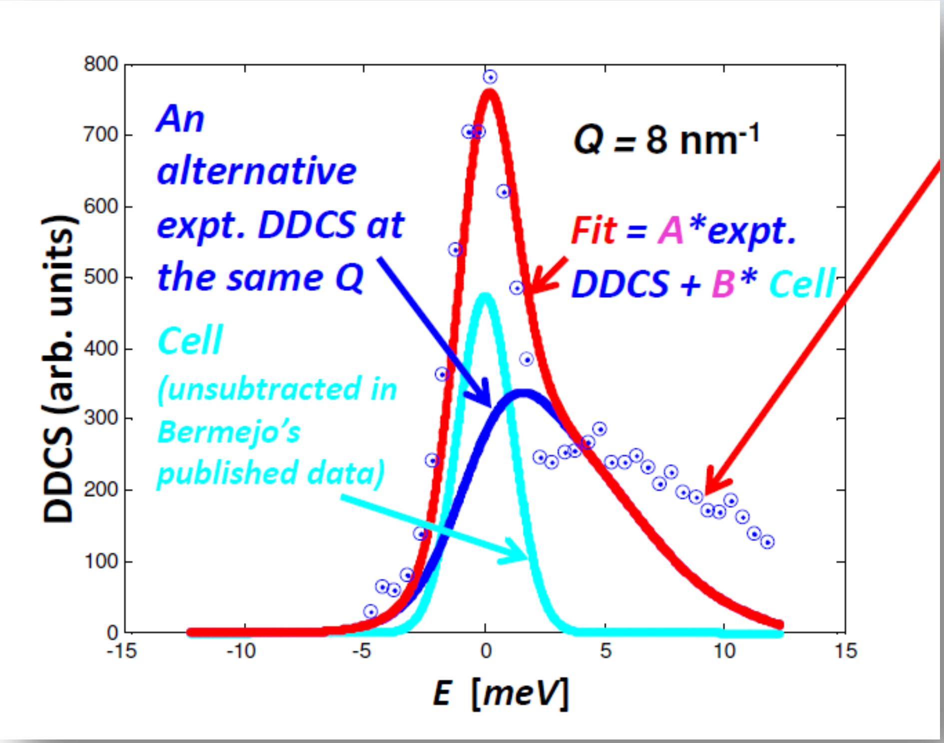


Cryogenic liquids



Few data available

When available : treatment is not clear or reliable

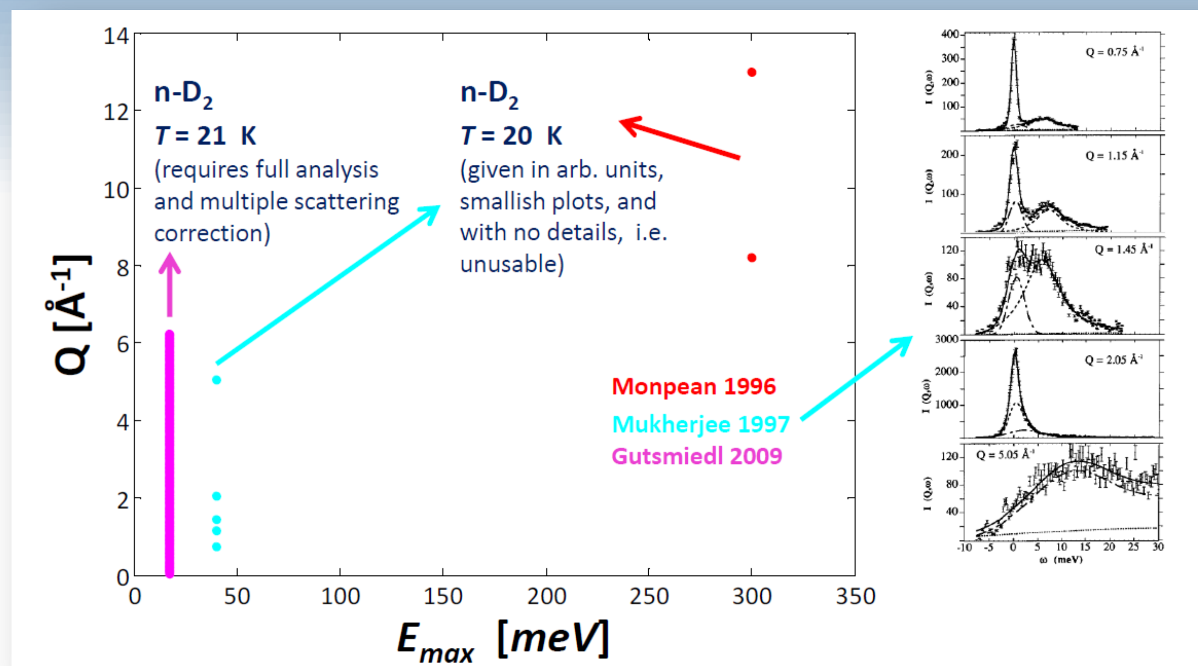


Cryogenic liquids

Situation with ortho-D_2 is even worse !

No data available for ortho-D_2

Data seem available for normal D_2 but in a very limited range



For both D_2 and H_2 : measurements and calculations are highly needed, especially at small q values (for all energies)

Conclusion of CRISP project

Measurement and implementation into MCNP was possible

Benchmark with first results was a success

Liquid hydrogen and deuterium : begun

UNEXPECTED : available data have a poor quality. Further measurements must be carried out

NA

Feasi

A lot

Propo

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Two main topics

Heavy / light water and data treatment optimization

- Experiments in several conditions of T & P
- MD simulations

Cryogenic Liquids (Hydrogen and Deuterium and...)

- Experiments (need high level of expertise)
- Quantum simulations (challenging)

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Solution : pool resources

Rely upon PhD students

Need of an international collaboration

We remain open

I'm inviting you to attend to a meeting at the ILL on July 1st and 2nd

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Thank you for your attention

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