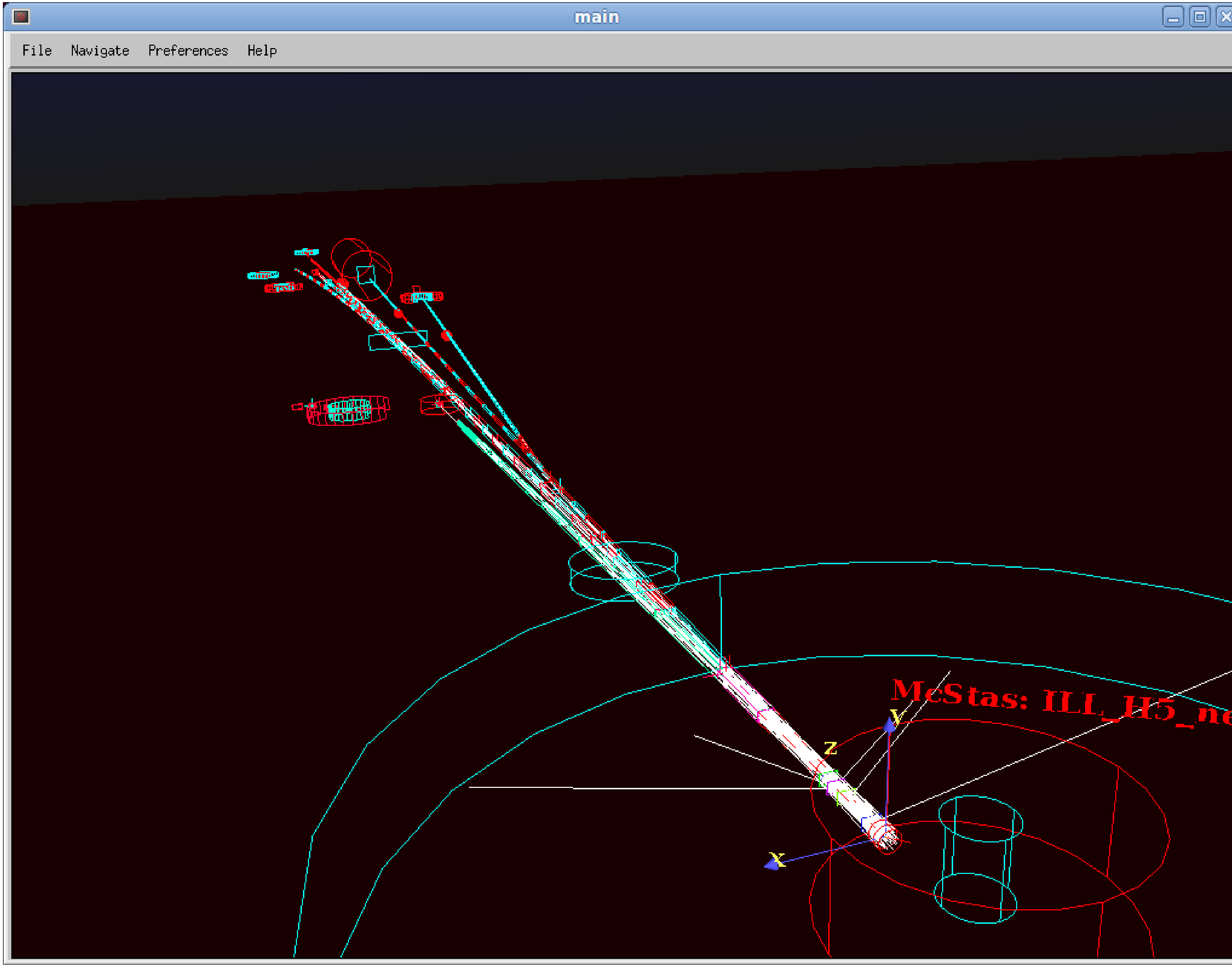
Advances on low energy moderator simulation using McStas: water, liq-^{4}He, liq-D_2

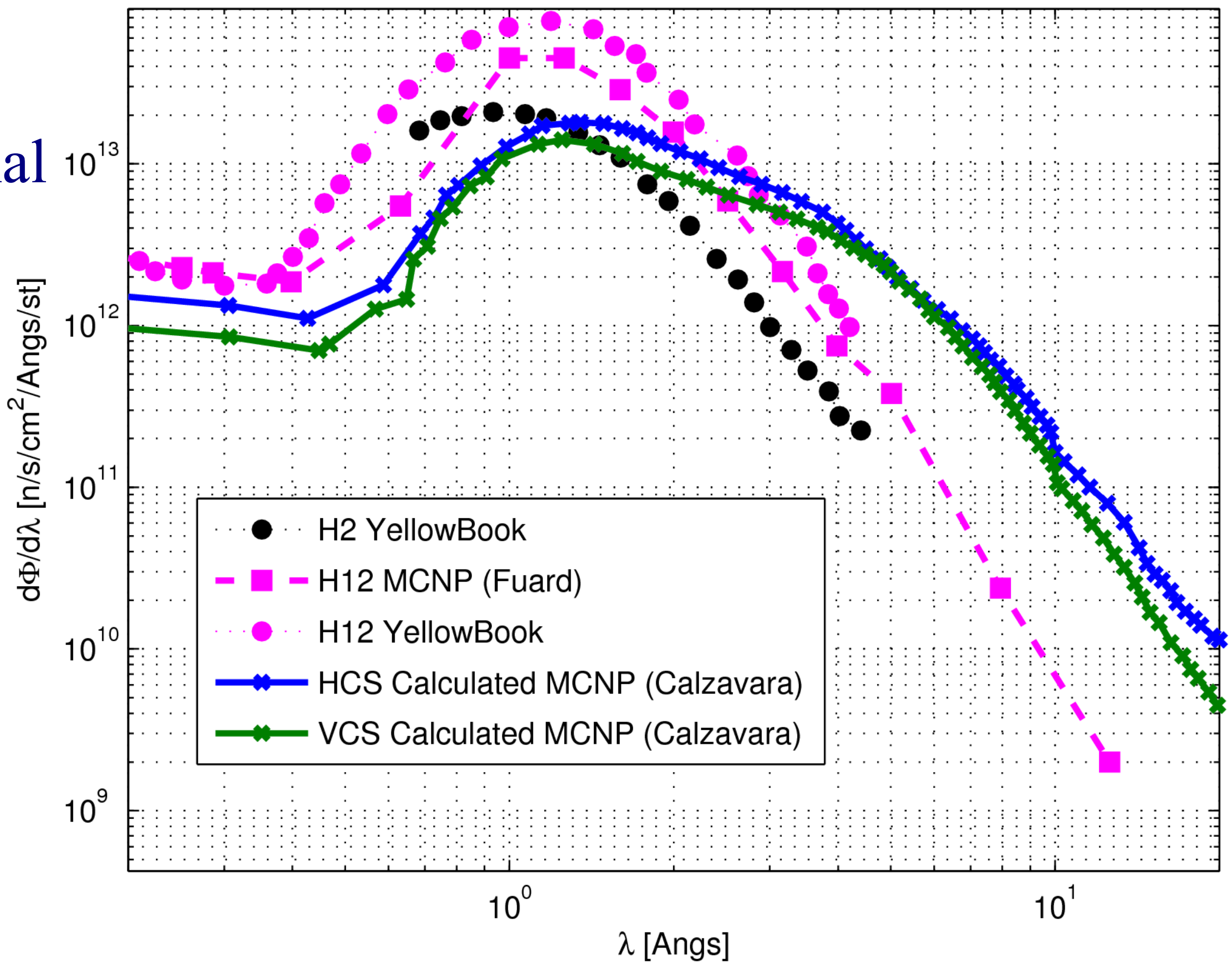
E. Farhi, O. Zimmer, Y. Calzavara, ILL


main
File Navigate Preferences Help
McStas: ILL_H5_ne
X
Y
Z

Starter dish: Brightness of the ILL

We benchmarked the ILL thermal and cold sources.

Thermal 8.10[13] n/s/cm²/st/Å
Cold: 2.10[13] n/s/cm²/st/Å

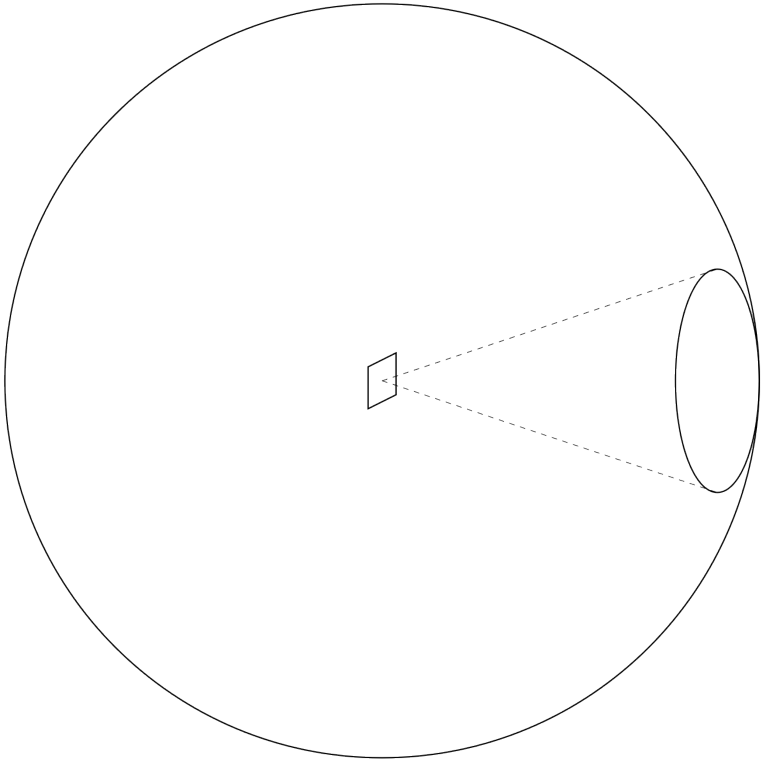


- Thermal source brilliance validated in agreement with the *YellowBook* data
- Cold sources are much **brighter** than reported in the *YB* by factor 3-10 vs *λ*
- Data and report published at <http://www.ill.eu/?id=11169>
- FRM2 and HZB data also available

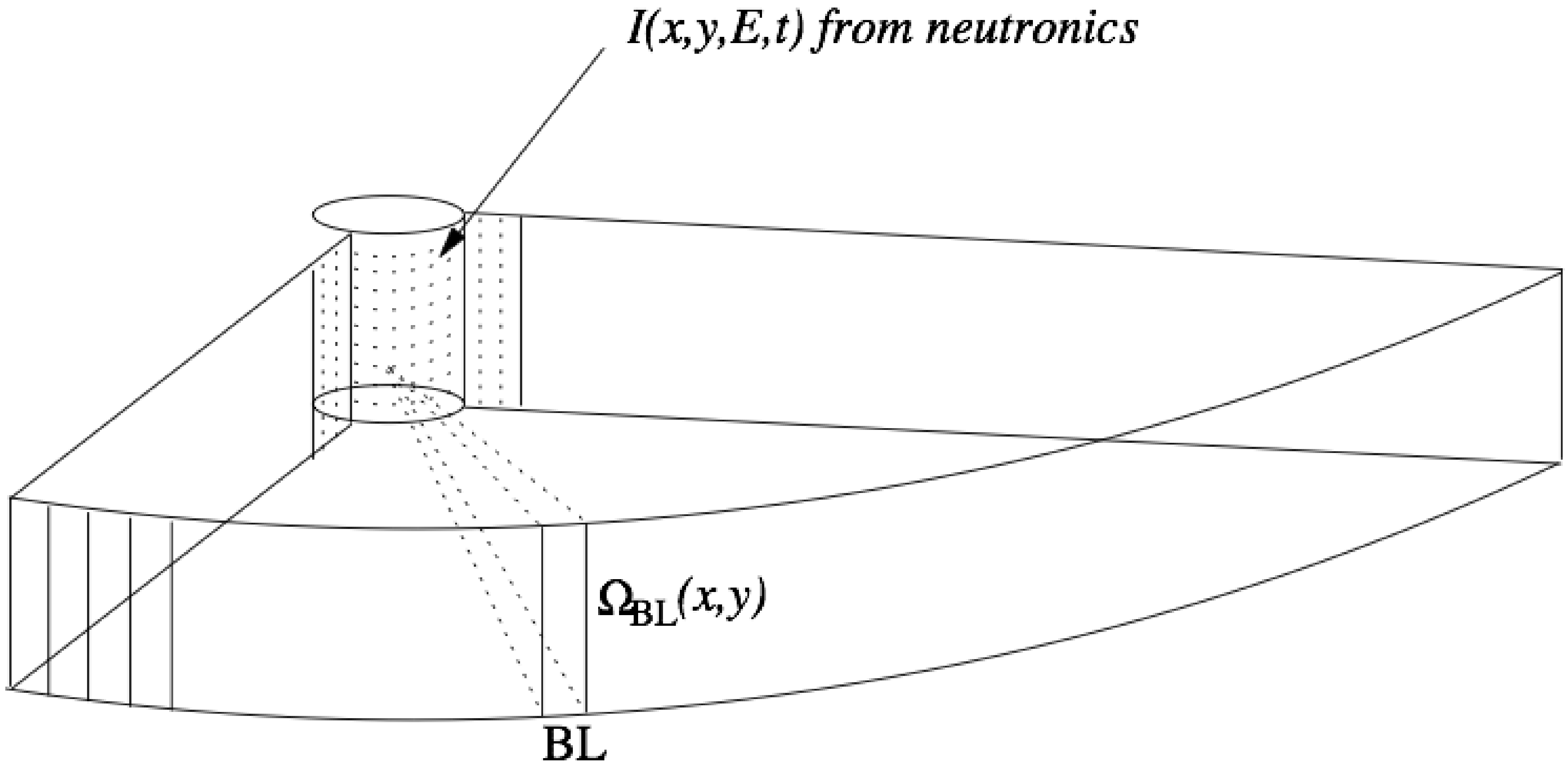
Source brilliance

- Reasonable unit to compare emittance of sources:

$$\mathfrak{B}\ [n/cm^2/s/ster/\text{Å}]$$



Moderators... (Where McStas starts)



$$I_{BL}(x,y,E,t) = \frac{\Omega_{BL}(x,y)}{4\pi} I(x,y,E,t)$$

The `Brilliance_monitor` Component

Special "Brilliance" monitor of FIXED size 1x1cm. If used in the right setting, will output "instantaneous" and "mean" brilliances in units of Neutrons/cm^2/ster/AA/s. Conditions for proper units:

- Use a with a source of area 1x1cm
- The source must illuminate/focus to an area of 1x1cm a 1m distance
- Parametrise the Brilliance_monitor with the frequency of the source
- To not change the source TOF distribution, place the Brilliance monitor close to the source!

with a source of area 1x1cm illuminating/focusing to an area of 1x1cm a 1m distance, this monitor will output "instantaneous" and "mean" brilliances in units of Neutrons/cm^2/ster/AA/s

Identification

- **Author:** Peter Willendrup, derived from TOF_lambda_monitor.comp
- **Origin:** DTU Physics
- **Date:** May 23, 2012
- **Version:** 1.1

Description

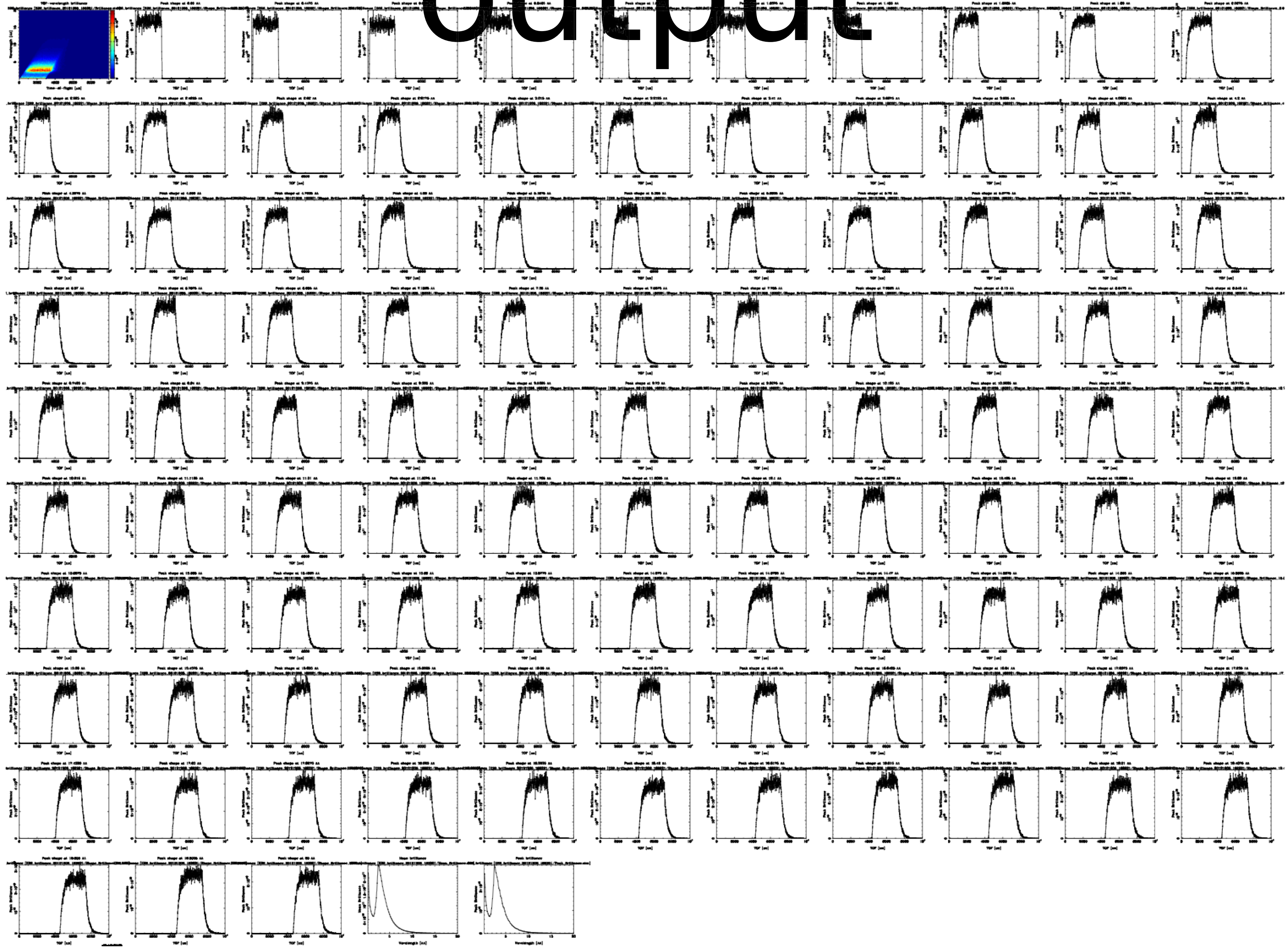
```
Here is an example of the use of the component. Note how the mentioned Unit conditions are implemented in instrument code.

COMPONENT Source = ESS_moderator_long(
   l_low = lambdamin, l_high = lambdamax, dist = 1, xw = 0.01, yh = 0.01,
   freq = 14, T=50, tau=287e-6, tau1=0, tau2=20e-6,
   n=20, n2=5, d=0.00286, chi2=0.9, I0=6.9e11, I2=27.6e10,
   branch1=0, branch2=0.5, twopulses=0, size=0.01)
 AT (0, 0, 0) RELATIVE Origin

COMPONENT BRIL = Brilliance_monitor(nlam=196,nt=401,filename="bril.sim",
        t_0=0,t_1=4000,lambda_0=lambdamin,
        lambda_1=lambdamax, Freq=14)
AT (0,0,0.000001) RELATIVE Source
```

Input parameters

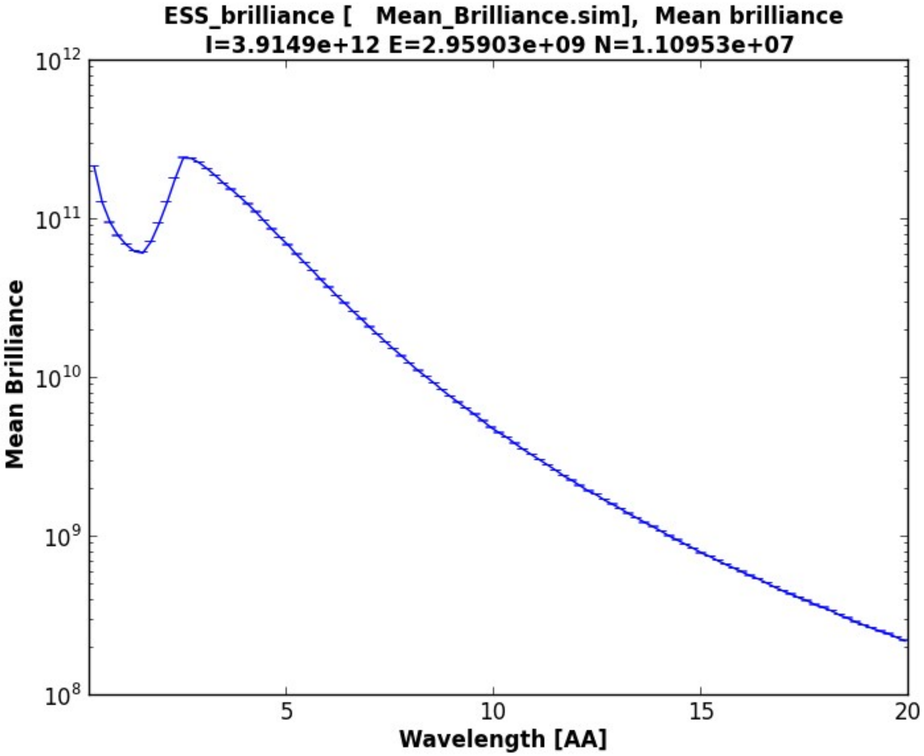
Parameters in **boldface** are required; the others are optional.

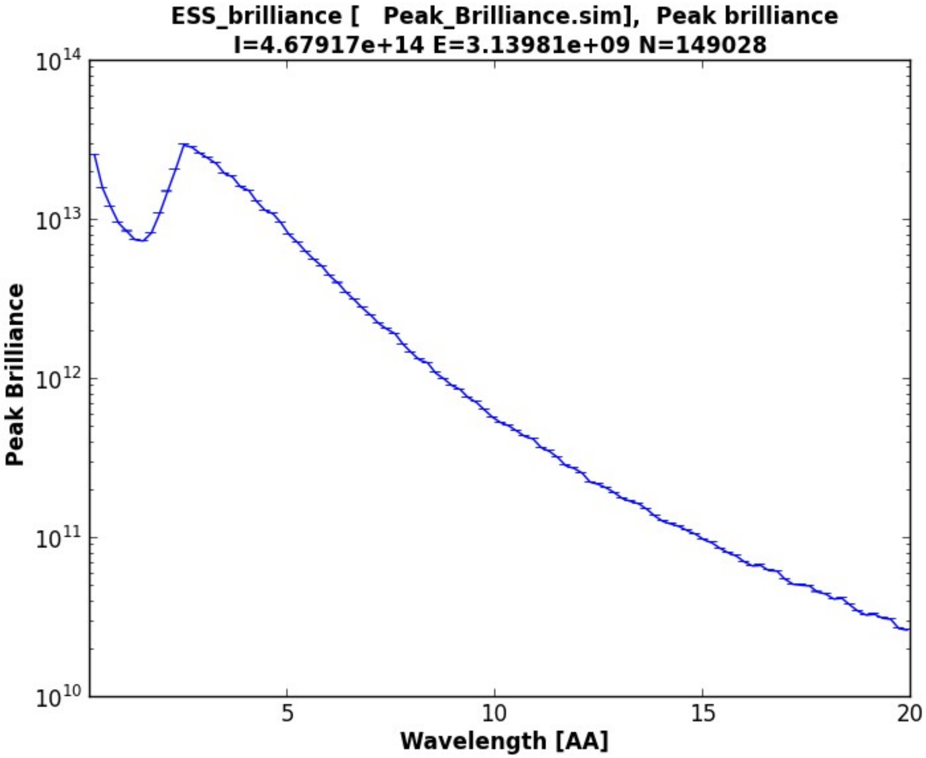
Name	Unit	Description	Default
nlam	1	Number of bins in wavelength	101
nt	1	Number of bins in TOF	1001
filename	string	Defines filenames for the detector images. Stored as: Peak_<filename> and Mean_<filename>	
t_0	us	Minimum time	0
t_1	us	Maximum time	20000
lambda_0	AA	Minimum wavelength detected	0
lambda_1	AA	Maximum wavelength detected	20
restore_neutron	1	If set, the monitor does not influence the neutron state	0
Freq	Hz	Source frequency. Use freq=1 for reactor source	

Brilliance_monitor output



Easy way to get brilliance curves





Using McStas for neutron moderation simulation

The moderation process implies a series of slow-down processes:

- Elastic collision with large momentum transfer – Compton scattering (q → Inf, high energy neutrons)
- Elastic scattering with lower momentum transfers ($q \leq$ few 10 $Å^{-1}$)
- Inelastic scattering on material dynamics ($Ei \leq$ few 100 meV)

Usual materials used for slowing down neutrons:

- Hydrogenated materials – water to get thermal neutrons (pre-moderator)
- Mesitylene (10-100K) – to get warm neutrons
- Liquid D2 and H2 – to get cold neutrons, using the rotational lines (e.g. 7-14meV)
- Solid D2 – same as above but heat extraction is less efficient (no flow)
- Liquid 4He – to get ultra cold neutrons from ~9Å neutrons (post-moderator)

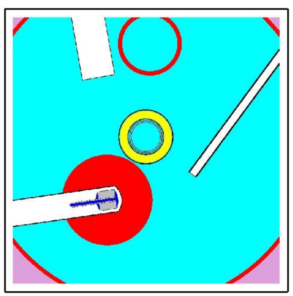
Instrument: Source: Generating neutron events

Neutron events may be currently generated from:

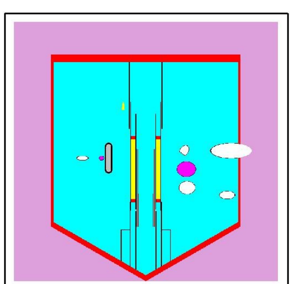
- A black body (Maxwellian distributions)
- Measured flux/divergence distributions
- MCNP and Tripoli (nuclear reactor simulation codes) event files

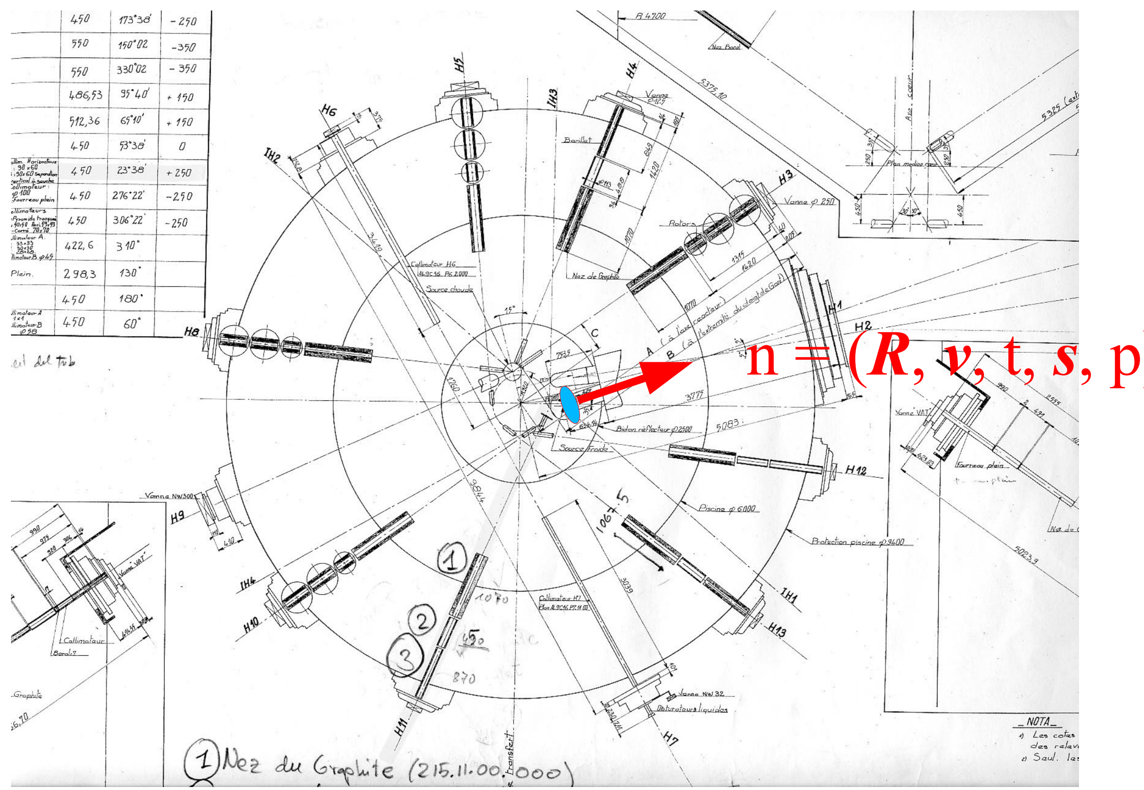
Other neutron generators are in principle easy to write (e.g. from GEANT4, FLUKA, ...)

top



side





So what's wrong with it ?

Available material neutron scattering cross sections for in ENDF:

liq-D2, lid-H2, H2O, D2O, liq-CH4, sol-CH4
ZrH_x, Graphite, Be, BeO
(that's all folks)

Weaknesses:

- Hardly produce Bragg peaks.
- Rely on analytical models at low energies.
- Mostly assumed to be incoherent-like.
- Very few temperatures available for each material.
- Data files often given for few discrete scattering angles (!!) – this is ok when averaging on many scattering events in a large volume, but not accurate.

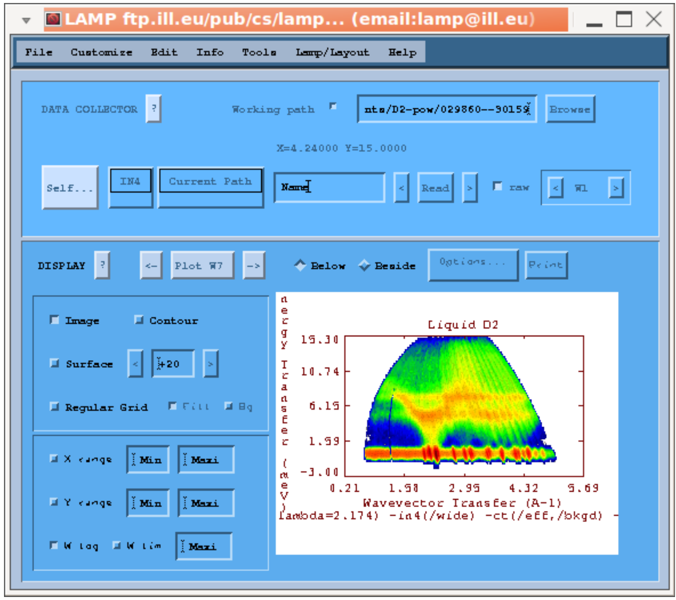
Improving these aspects also benefits to the neutron scattering community by setting new demand on material simulation accuracy in our MC codes.

Going further: getting new data for materials

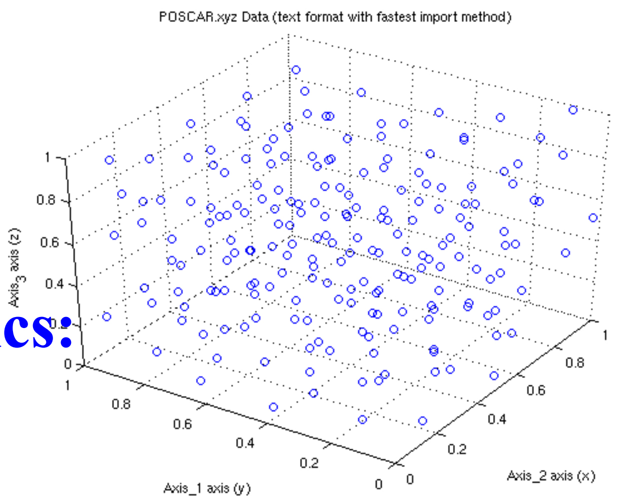
From experiments:

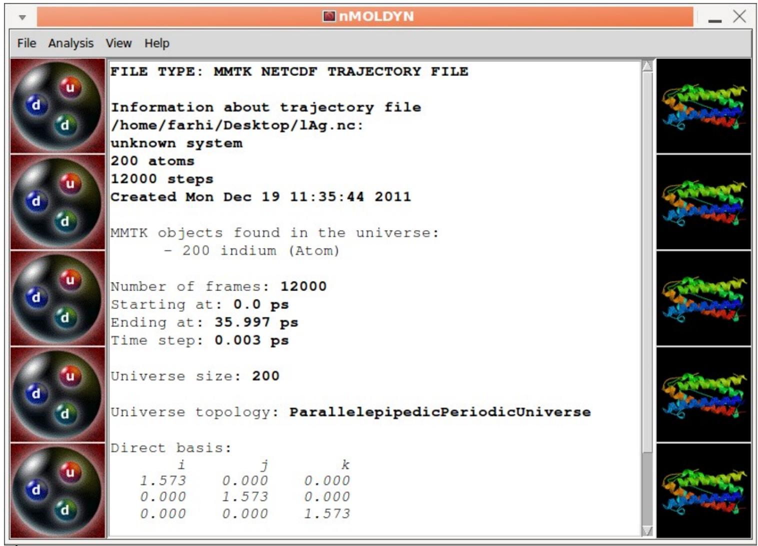
- Data mine or send new proposals
- Reduce data: normalize, subtract empty cell,
- Transform to *S(q,w)*

I use **LAMP** for this.



From molecular dynamics:





- Perform MD simulations
- Import trajectories
- Compute coherent and incoherent scattering *S(q,w)*

Mostly for high temperature materials – low temperatures are often quantum...

I use **VASP**, then **nMoldyn** for this. May use Material Studio.

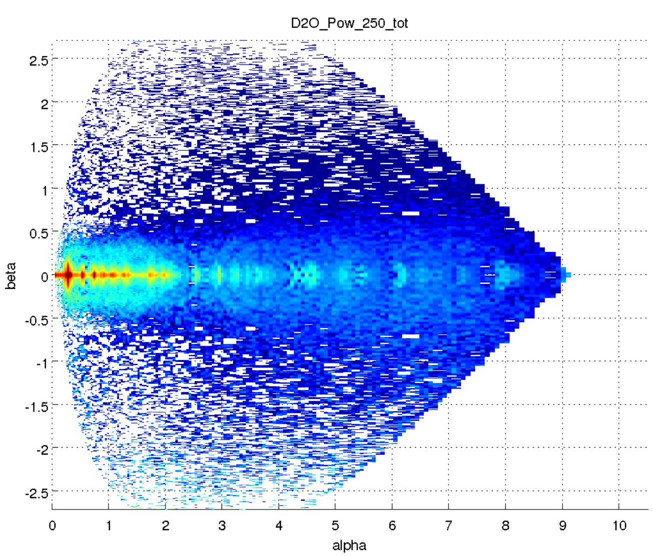
Water

Measurement on IN4 Farhi/Calzavara/Haeck

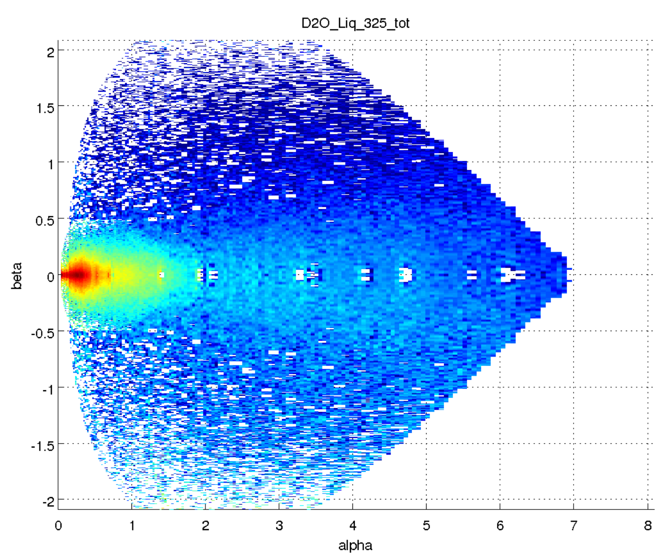
Exp 1-10-9: IN5 13-15 Sept 2010: H2O and D2O T=2-300 K; lambda=2,5,10 Angs

Use LAMP to generate S(q,w). Use iFit to convert to S(a,b).
Use NJOY to convert to ACE.

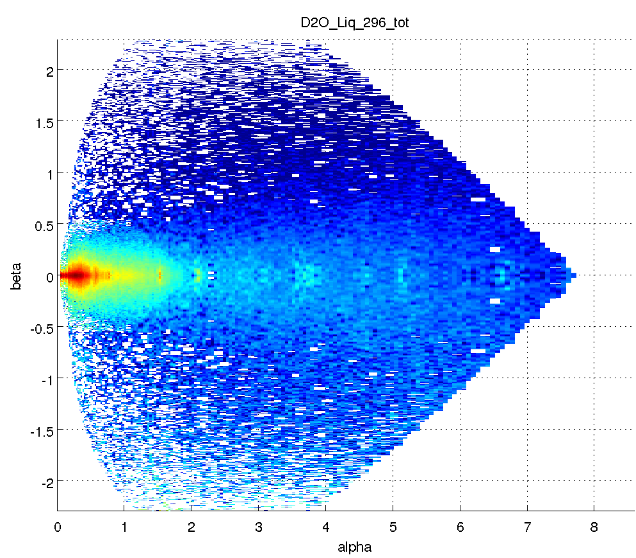
$$\alpha = \frac{E' + E - 2\sqrt{E'E}\cos\theta}{A\,kT} = \frac{\hbar^2\kappa^2}{2M\,kT} \qquad \beta = \frac{E' - E}{kT} = \frac{\varepsilon}{kT} \qquad S(\alpha,\beta) \sim S(q,\omega).\,q.M.(k_B T)^2$$



250K powder

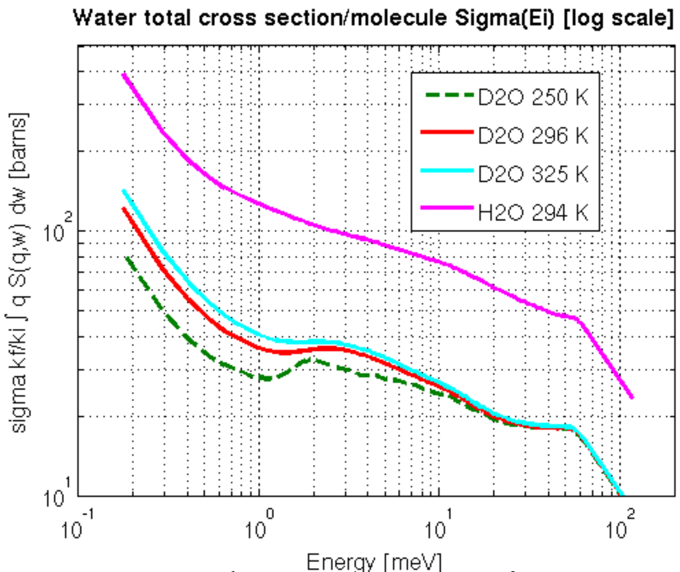


296K liquid

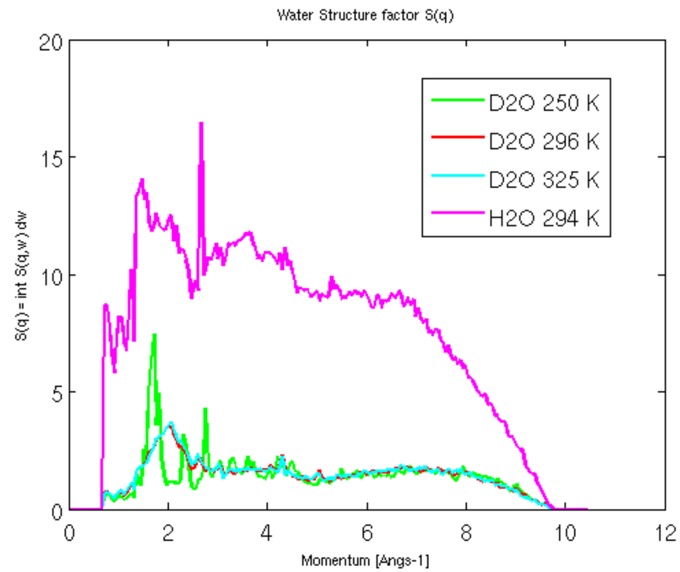


325K liquid

Water: comparing with existing data

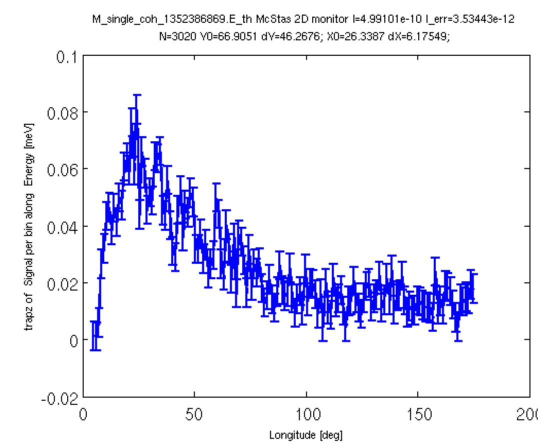


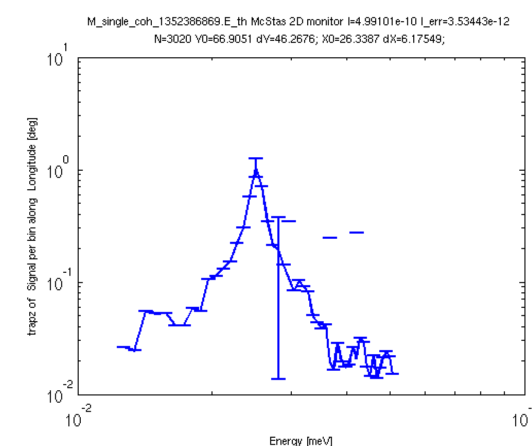
Total cross section



Structure factor

We have good data. Will definitively improve data bases and moderator models.





INTERNATIONAL ATOMIC ENERGY AGENCY

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I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

Thermal Neutron Scattering Data

for the Moderator Materials

NEUTRONS FOR SCIENCE

Computing for Science

Tools used for this study

Upgraded Isotropic_Sqw component:

- More accurate total cross section computation *σ(Ei)*
- Computes many physical parameters from *S(q,w)*
- Compressibility, sound velocity, $\langle u^2 \rangle$, elastic modulus, diffusion coefficient, collective excitation frequency w^2, gDOS, …
- Can handle both classical and quantum limit *S(q,w)* and symmetrize energy range, with Bose factor

iFit for handling the data

- Transformation $S(q,w) \rightarrow S(\alpha,\beta)$
- Plotting

A bit of theory for neutron-sample interaction

See Egelstaff or H. Fischer, *Rev. Prog. Phys*. **69** (2006) 233

Neutronist's Mantra

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma}{4\pi}\frac{k_f}{k_i} N S(q,\omega)$$

Holy Book (Squires)

Effective cross section for scattered intensity

$$\hat{\sigma} = \iint \frac{d^2\sigma}{d\Omega dE_f} d\Omega dE_f$$

V.F. Sears. Adv. Phys., 24, 1, 1975.

We like to play games in (q,ω) space

$$\frac{d\Omega}{d\theta} = -2\pi sin\theta$$

$$\frac{dq}{d\theta} = -\frac{k_i k_f sin\theta}{q}$$

Effective cross section in (q,ω) space

$$\hat{\sigma} = \sigma \iint \frac{S(q,\omega) q}{2k_i^2} dq d\omega$$

Probability to interact

$$p = e^{-\rho \hat{\sigma} x}$$

Scattering distribution

S(q,ω)

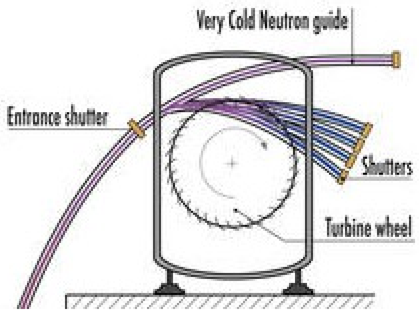
with importance sampling to scatter preferably where *S* is large

Generating UCN from cold neutrons

Cold neutrons are generated from moderation in e.g. *l*-H or *l*-D.

Ultra Cold Neutrons, produced from cold neutrons, used for fundamental physics (cosmology). Require high UCN density.

Currently max density at the ILL 30 cm^{-3} using a turbine (Doppler effect).



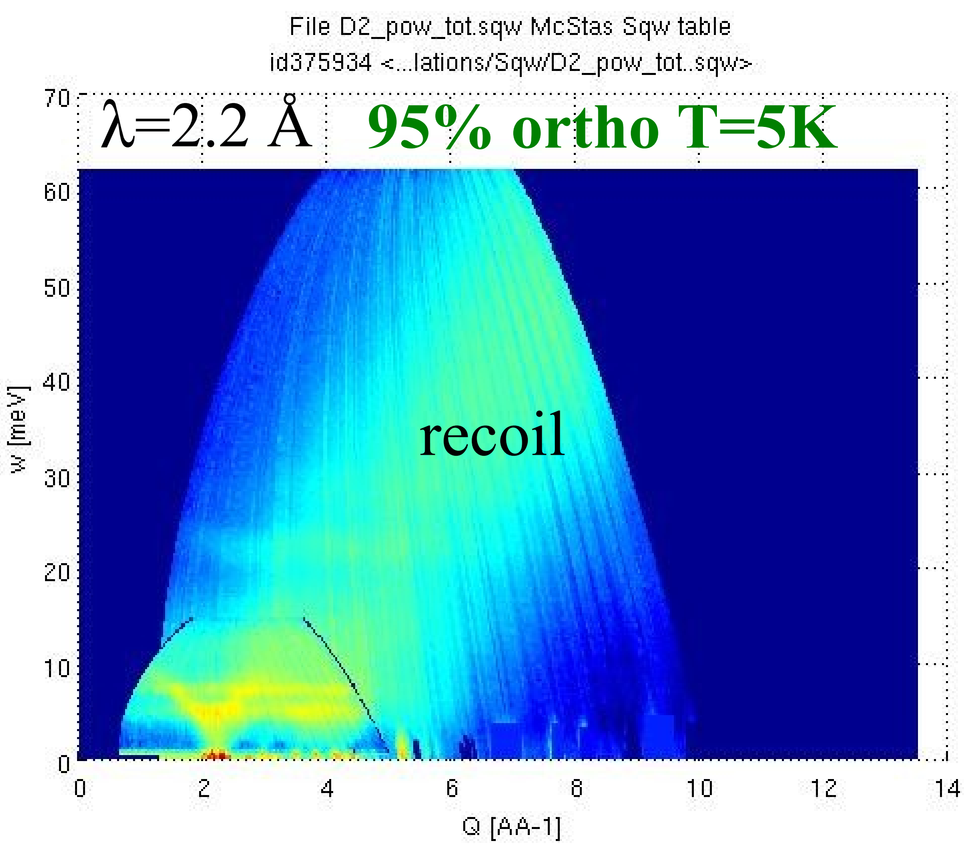
Idea : extract energy from cold neutrons using phonons at low temperature. Neutron can not regain energy because T is very low (<< phonon energy).

Materials : solid-D2, ^{4}He are promising

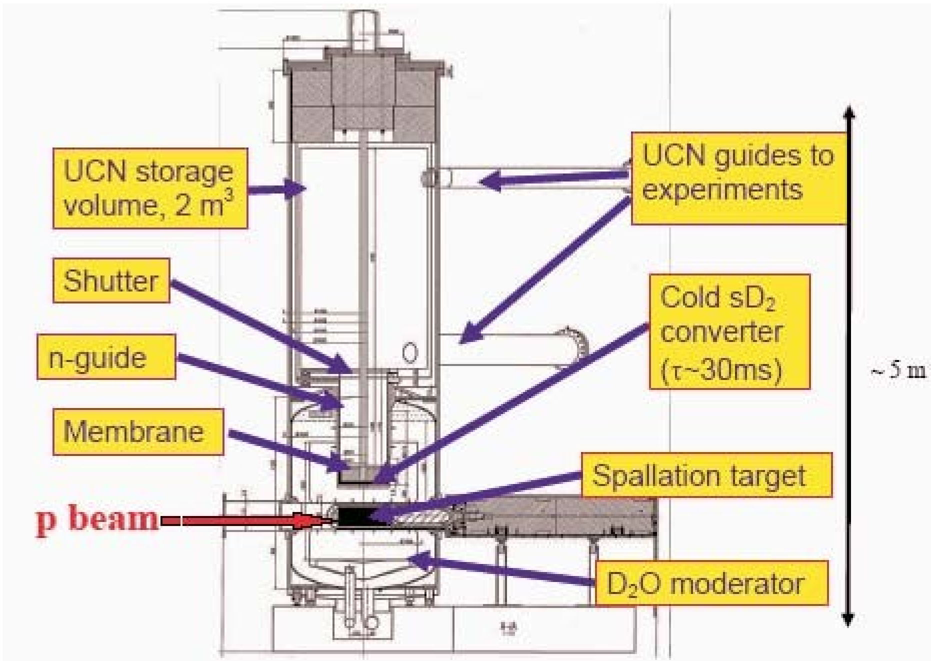
solid-D_2: production of UCNs

solid Deuterium as converter (o-D2):

- temperature: 5 K
- para-D2 content < 1%
- absorption cross section $\sigma_{abs} = 0.0005$b
- incoherent (2b) and coh (5b).
- Distribution of inelastic processes.



Used e.g. at PSI for the nEDM.



Data from Gutsmiedl (2007).

1 hour@**IN4**

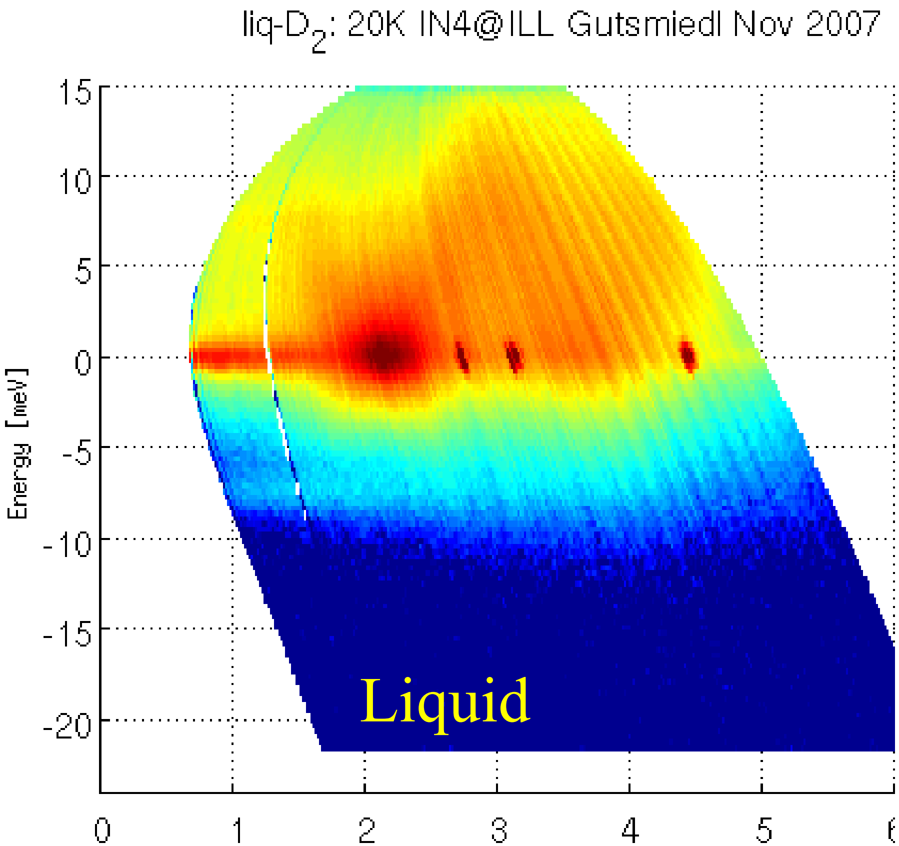
- A. Frei, E. Gutsmiedl, et al. *EPL*, **92** (2010) 62001
- Granada, *EPL* **86** (2009) 66007

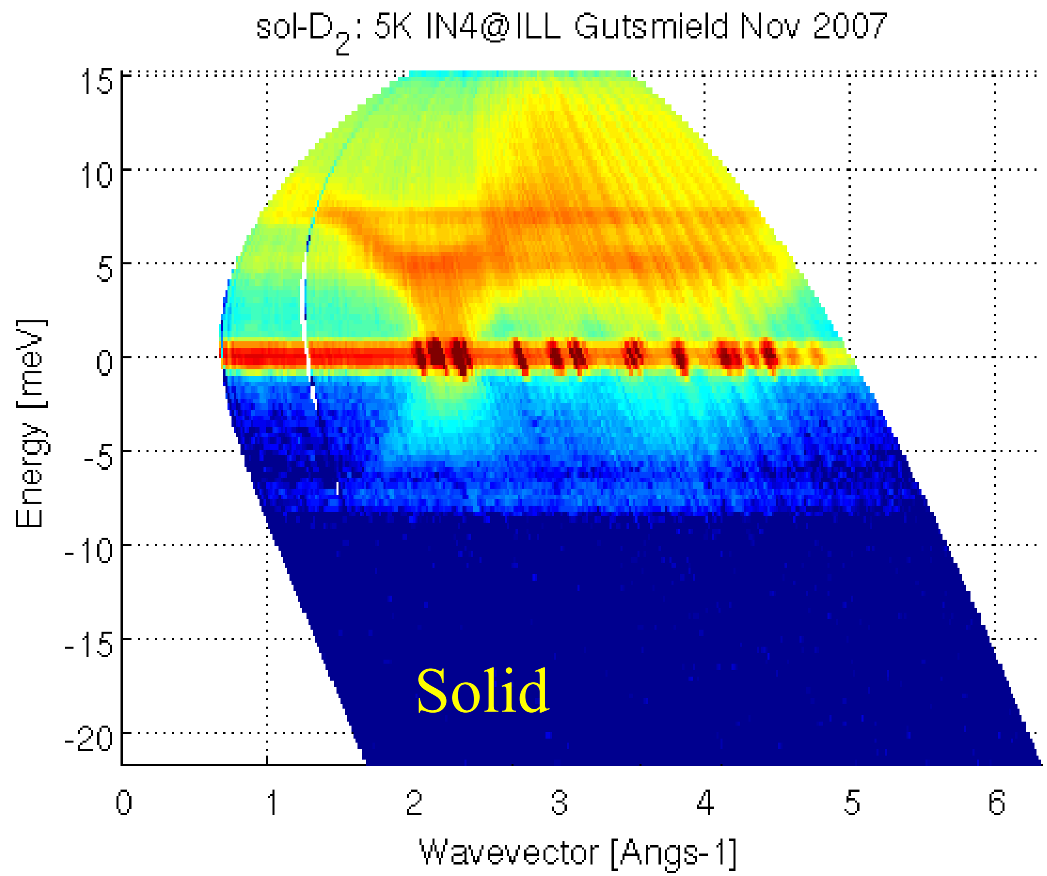
May be converted to ***S(α,β)***

to complement MCNP kernels

Also for l-D_2

Deuterium



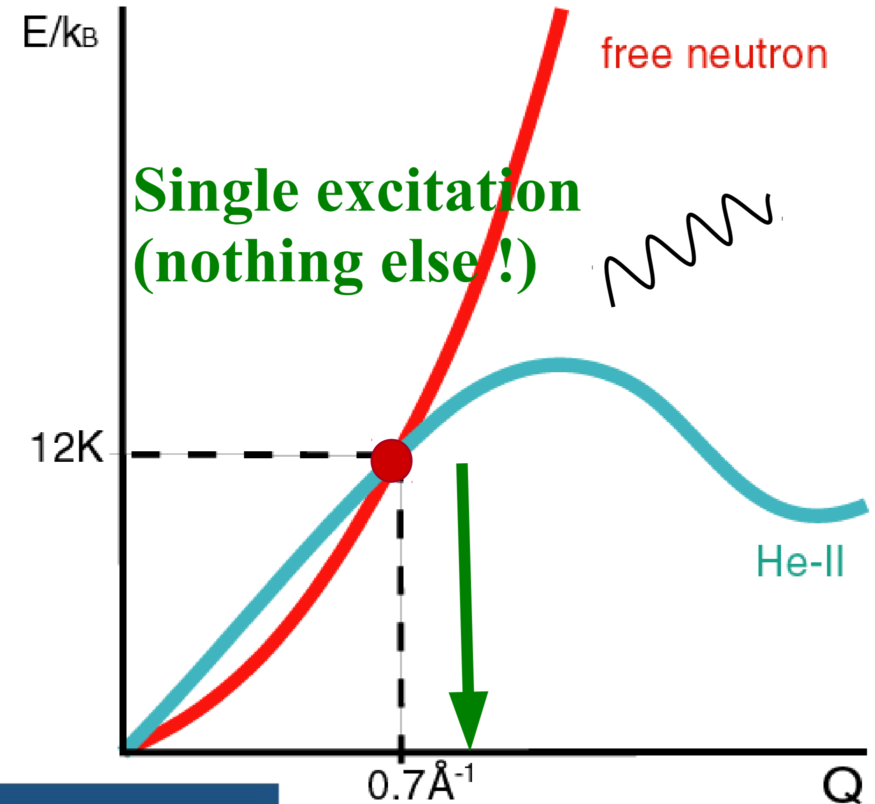


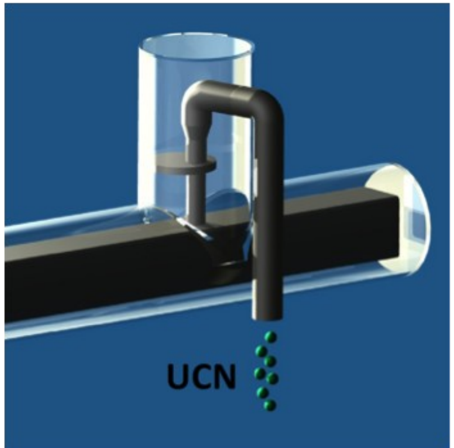
We shall use the same methodology as for water, and produce $S(\alpha,\beta)$ ACE files for MCNP.

liq-^{4}He: production of UCNs

Team : O. Zimmer, J. Bossy, T. Soldner, J. Ollivier, *et al.*
Idea from Pendlebury and Golub in 1970's, validated in 2002.

- Crosses at λ=8.9 Å for free (cold) n. Neutron loses all energy by phonon emission → UCN.
- Reverse suppressed by Boltzmann factor, l-^{4}He is at 0.5K, no 12K phonons.
- Extraction using open UCN converter demonstrated Y. Masuda et al., PRL (2002) 284801-1.
- Use large volume for maximum production and storage.





liq-^{4}He: simulation of the UCN: set-up

McStas

- We assemble a ^{4}He cylinder ϕ=6.6 cm 20 cm long (McStas).
- Send cold neutrons (velocity selector $d\lambda/\lambda$=+/-8 or 14%)
- Record escaping neutrons with ω < 250neV
- Model assembly : 1 hour (1 man) ; Computing time 1h (8 cores)

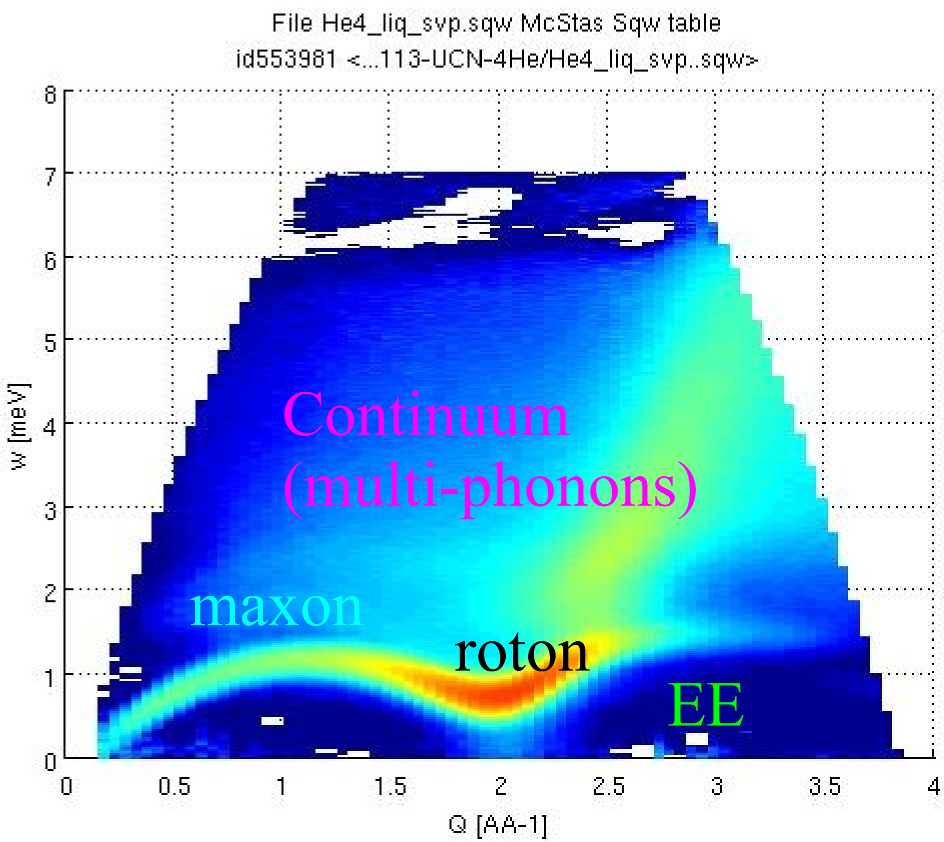
Liquid 4He

σ_{abs} = 0.00747 b (good)

σ_{coh} = 1.34 b

σ_{inc} = 0 b (perfect)

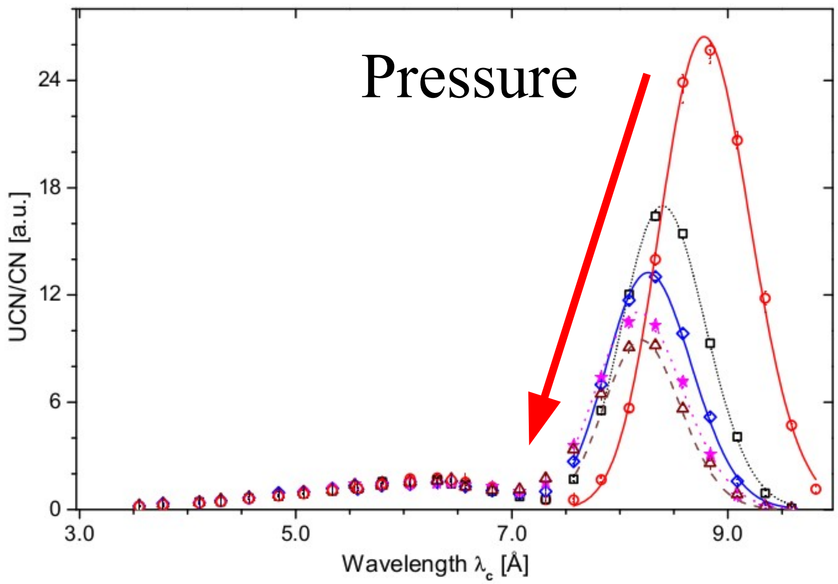
Excellent for long storage times and large volumes.



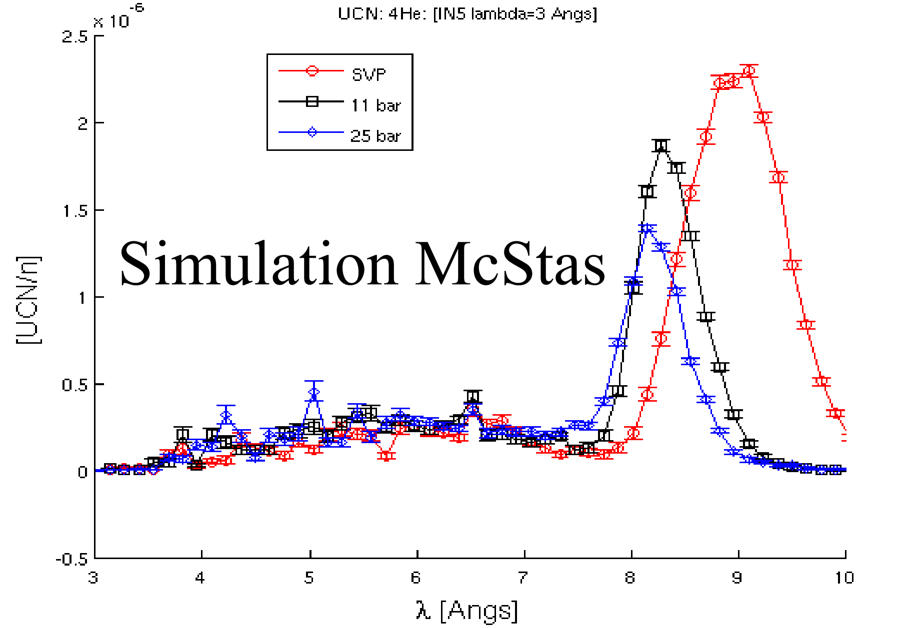
S(q,ω) data from J. Bossy and J. Ollivier. 2.5 hours@IN5. λ=3 Å

Also have IN5 λ=5 Å + IN6 λ=4 Å

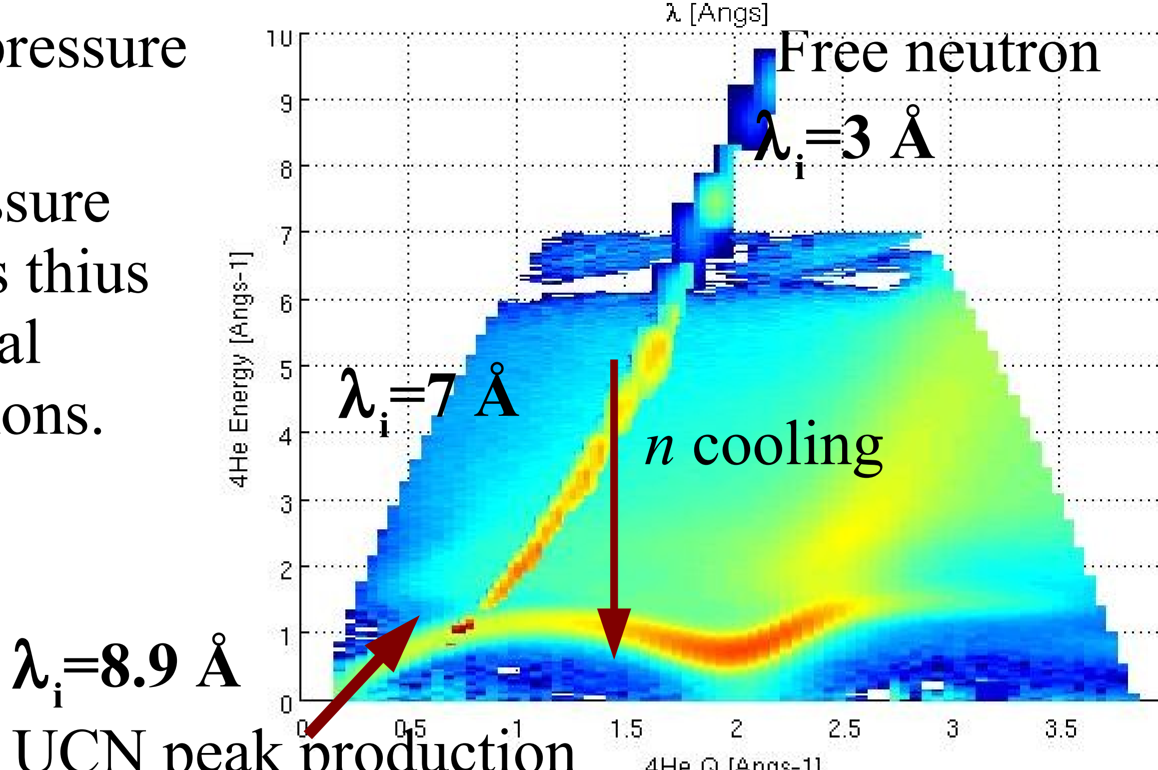
liq-^{4}He: simulation results



Measurement H113@ILL vs pressure



Increasing the density with pressure does not bring more neutrons as thius is compensated by a smaller total cross section from steeper phonons.



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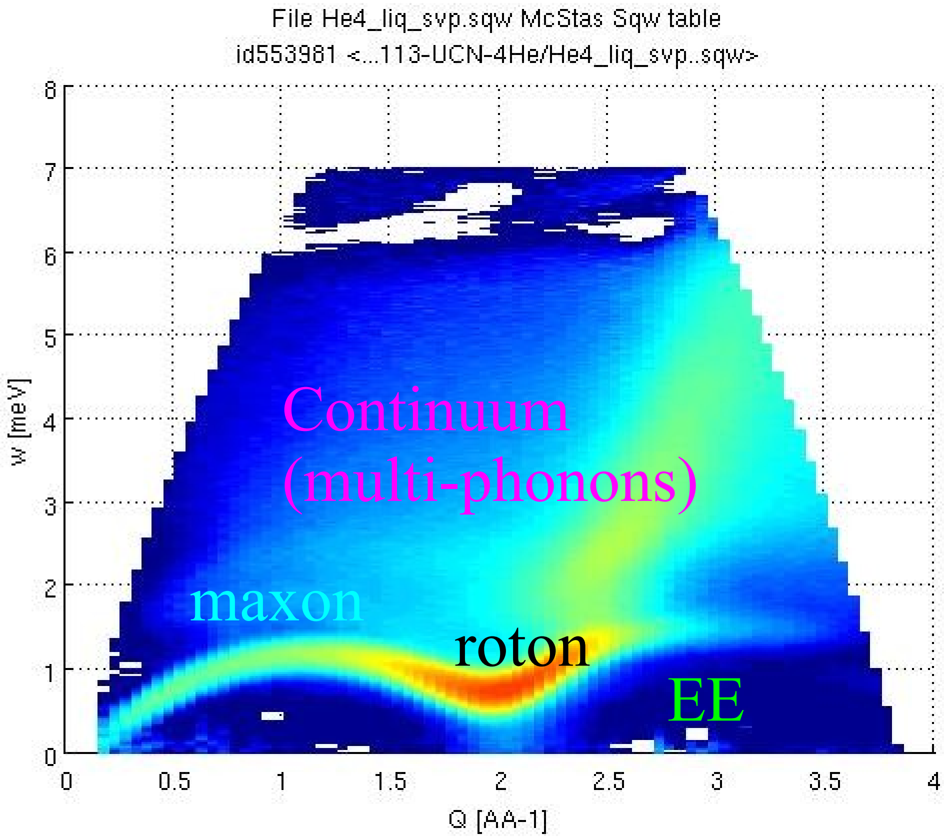

S(q,ω) data from J. Bossy and J. Ollivier. 2.5 hours@IN5. λ=3 Å

Also have IN5 λ=5 Å + IN6 λ=4 Å

liq-⁴He: simulation of the UCN: set-up

McStas

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- Send cold neutrons (velocity selector $d\lambda/\lambda$=+/-8 or 14%)
- Record escaping neutrons with ω < 250neV
- Model assembly : 1 hour (1 man) ; Computing time 1h (8 cores)

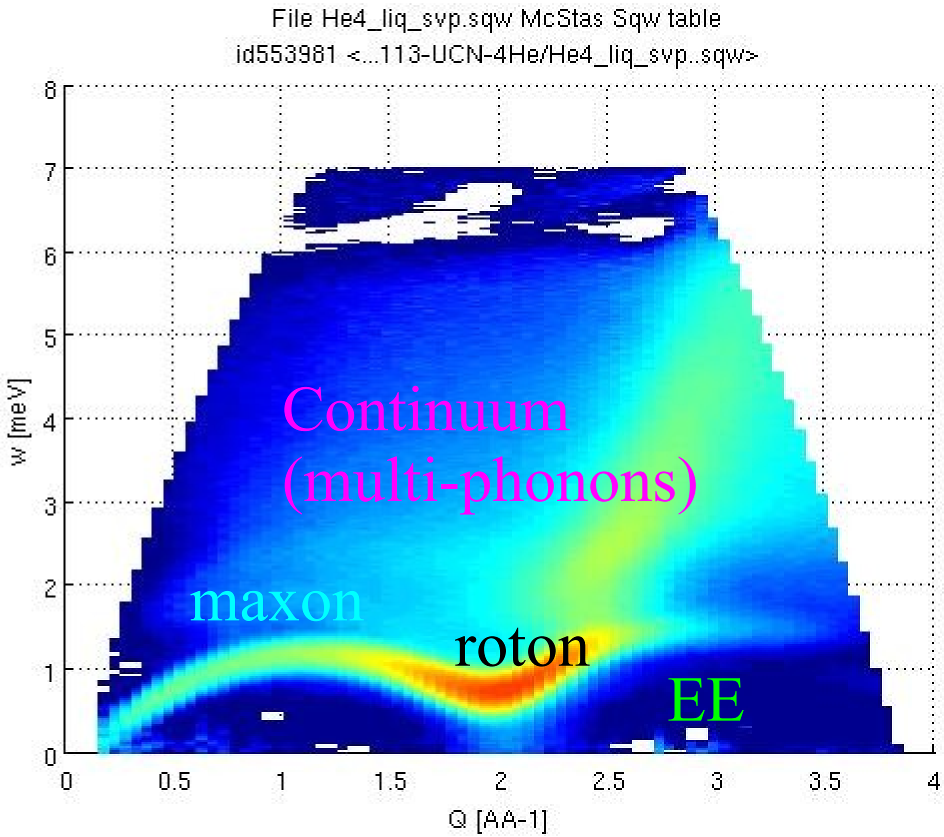
Liquid 4He

σ_{abs} = 0.00747 b (good)

σ_{coh} = 1.34 b

σ_{inc} = 0 b (perfect)

Excellent for long storage times and large volumes.



S(q,ω) data from J. Bossy and J. Ollivier. 2.5 hours@IN5. λ=3 Å

Also have IN5 λ=5 Å + IN6 λ=4 Å

And that will make a day (for today at least).