European Spallation Source (ESS):
a quantum leap in research opportunities

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Neutrons show "…. where the atoms are and what the atoms do"

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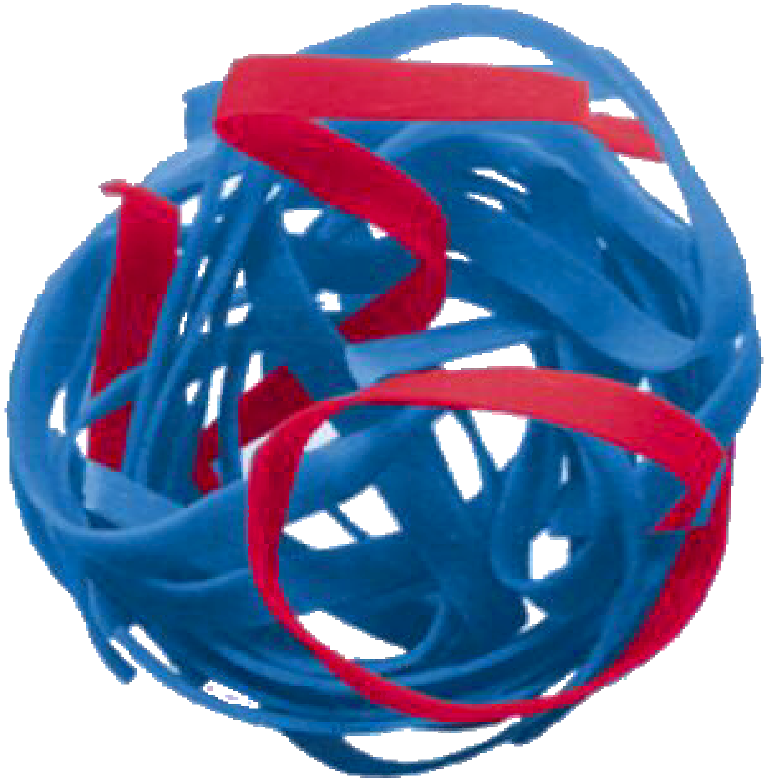
Direct atomic scale information **in space:**
elastic scattering (diffraction, diffuse and small angle scattering, …)
and **in space and time:**
inelastic neutron scattering

Neutrons are not the only probe to provide this kind of information, but they are the only ones to provide some of it.

The combination of several techniques allows us to eventually get the full picture (not even NMR can do everything alone!)

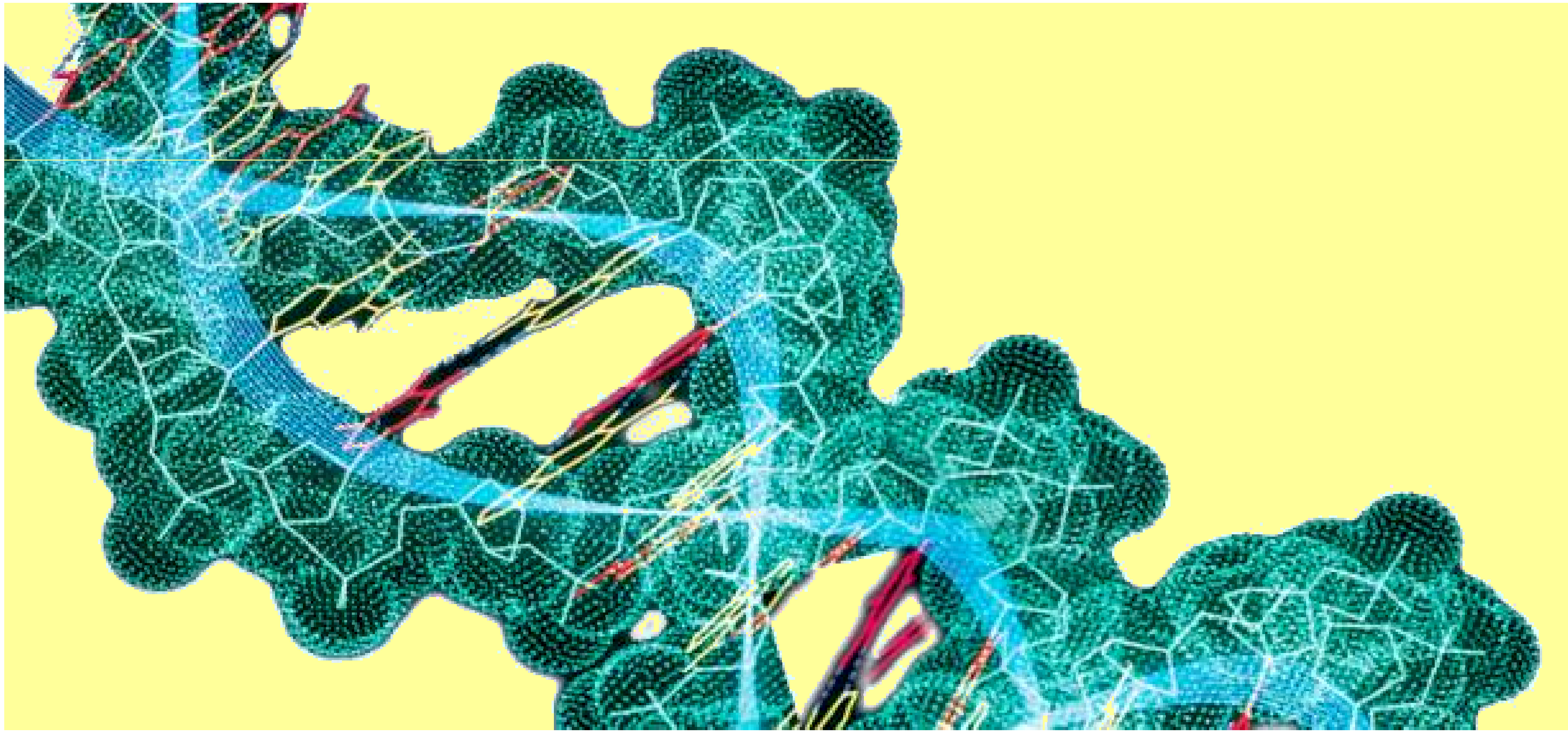
Some of these techniques only available at large scale facilities

Neutrons see the nuclei



Only neutrons enable isotopic labeling.

Neutrons see light as well as heavy atoms

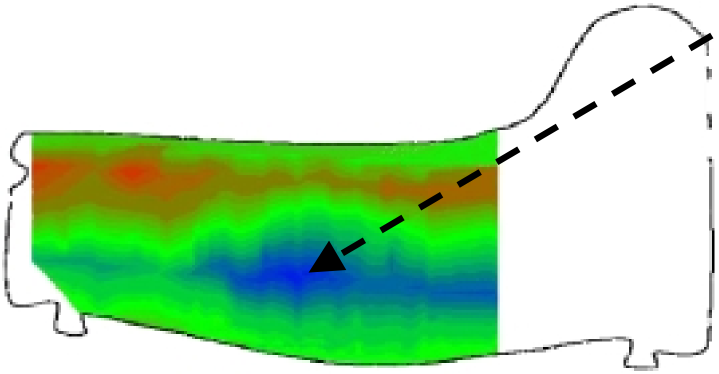


Only neutrons see H-bonds and catalytic H positions.

Neutrons see deep inside heavy (metal) parts

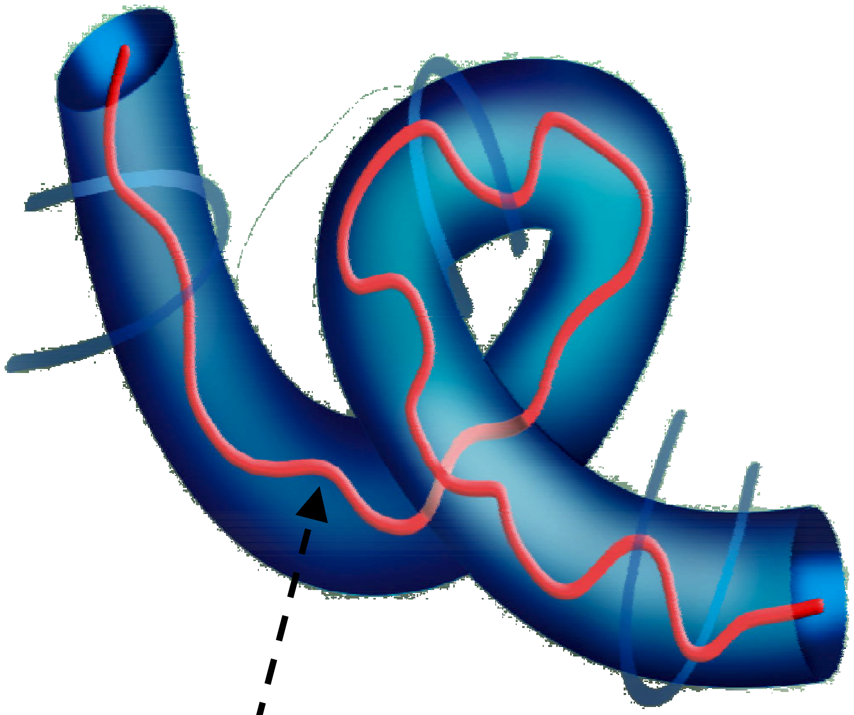
ICE accident (Eschede) :

- Tensile stress caused wheel failure
- Numerical simulations failed to predict, no experimental control done before accident

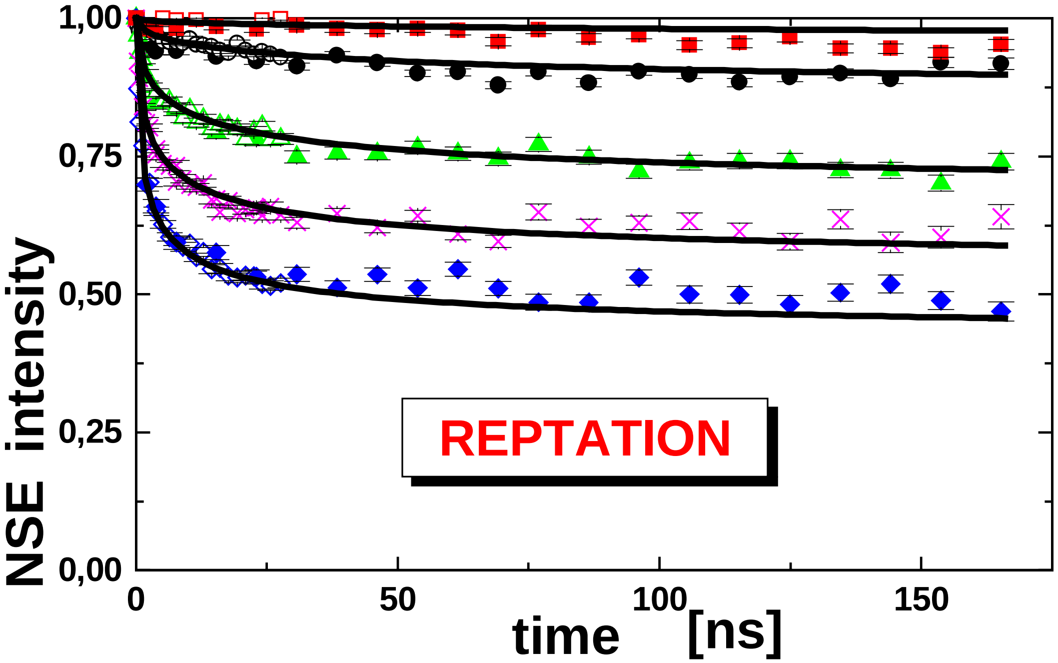


M. Grosse, U. Sthur, M. Ceretti, L. Köszegi, Journal of Neutron Research **9**, 489-493 (2001)

Neutrons see motion in nanoscale space-time domain: 1 - 10 nm, 0.1 - 100 ns



de Gennes reptation



In actual practice by now:

"…. where the atoms are and what the atoms do in single crystals"

Periodicity and symmetry helps in many ways to obtain atom by atom information in full details

Next challenge:

"…. where the atoms are and what the atoms do in non-crystalline matter"

… in order to understand and control soft matter, biological functionality, ….

This will be a central part of the ESS adventure

Inelastic signal:

$S(Q,\omega) \propto Q^2$ at small Q's

In single crystals: $Q = q + \tau_{hkl}$

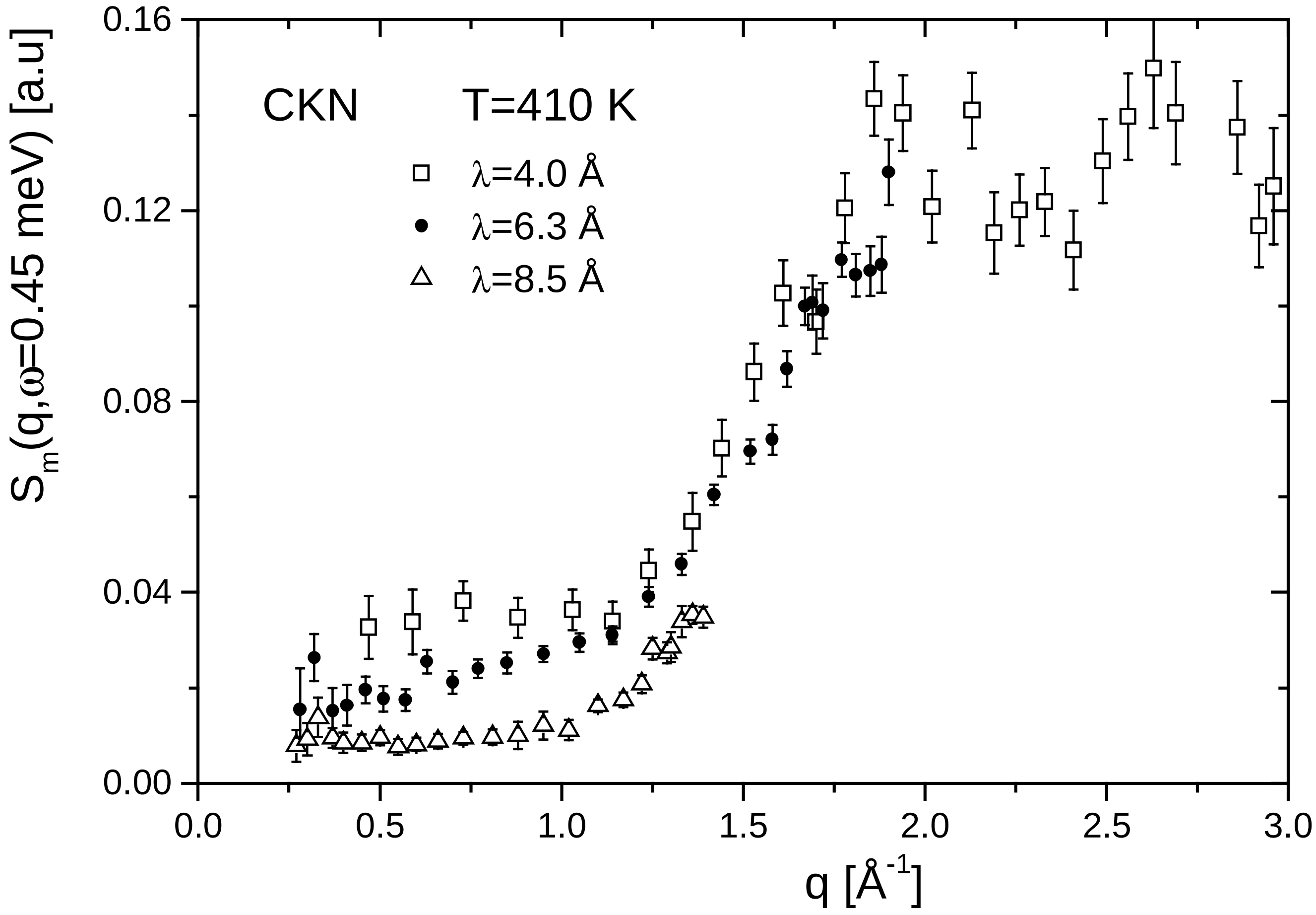
For non-crystalline matter:

a) small signal: need lot more particles

b) theoretical interpretation much more complex: need more powerful tools

What the atoms do?

Space - time behaviour G(r,t) ⬌ S(q,ω)

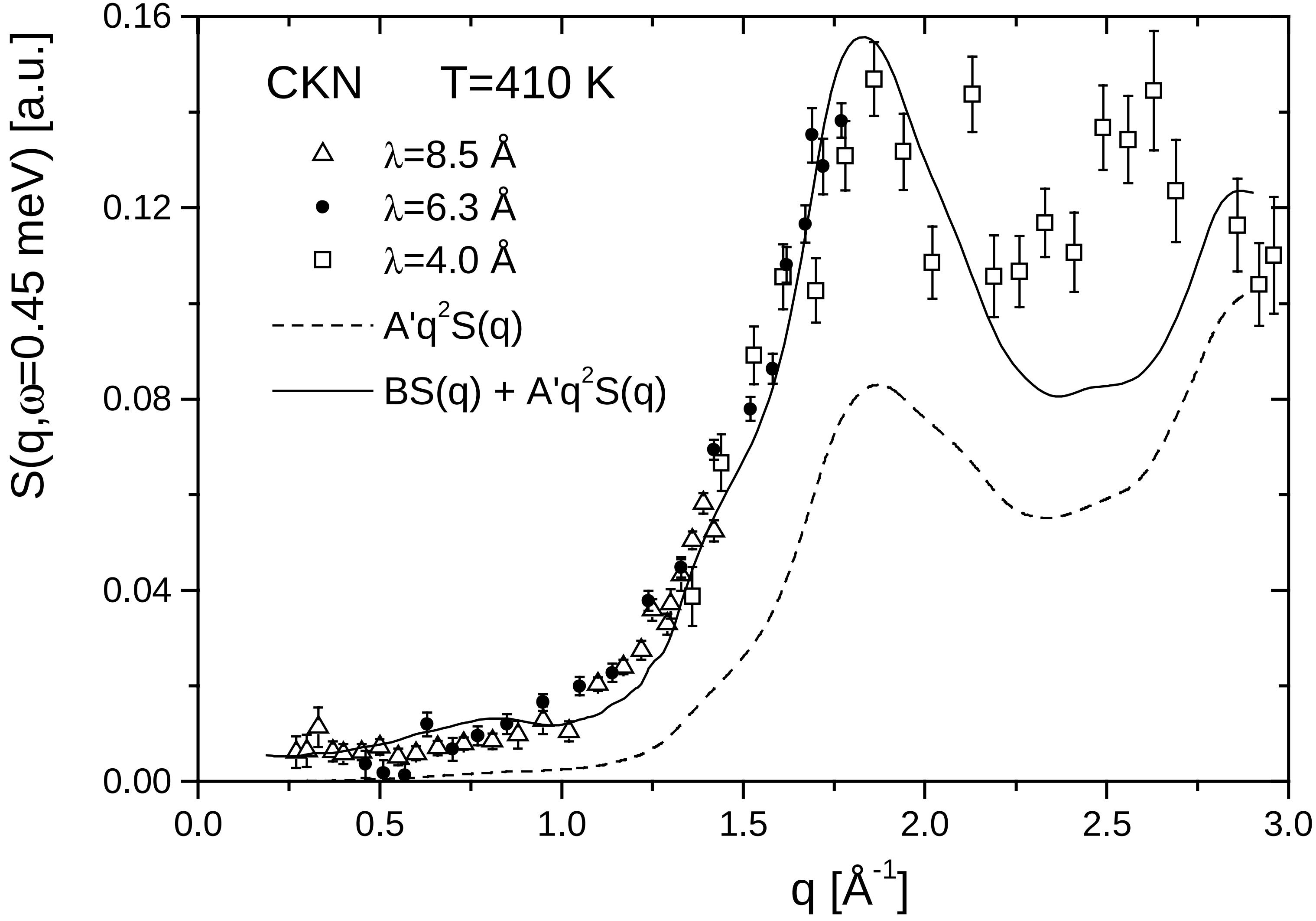


Ca-K-N0$_3$

supercooled liquid

Small signal - high background (multiple scattering)

Picosecond process: complex q dependence (spatially coordinated atomic motion)



X-ray scattering (synchrotron radiation):

recent progress in inelastic scattering (triple axis spectroscopy, nuclear resonance spectr.)

but **basically limited resolution and/or intensity**

10^{10} photons/meV/s in full beam at ESRF (same as ILL)

resolution:

by crystals ~ 1 meV ↔ 10^{-12} s (cf. neV - meV by neutrons)

by nuclear resonance ~ 5 neV, i.e. < 10^4 ph/s (cf. 10^7 n/s by Neutron Spin Echo at ILL)

Limited progress expected from > keV Free Electron Lasers (FEL)

State of the art:

Continuous (reactor) and pulsed (spallation) sources are complementary

Pulsed operation: more *efficient* use of the neutrons produced

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Continuous (reactor) and pulsed (spallation) sources are complementary

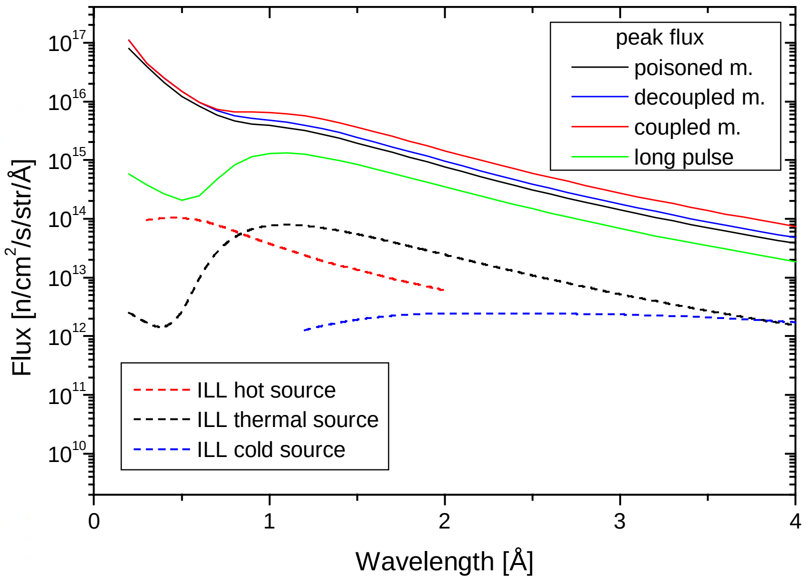
Pulsed operation: more *efficient* use of the neutrons produced

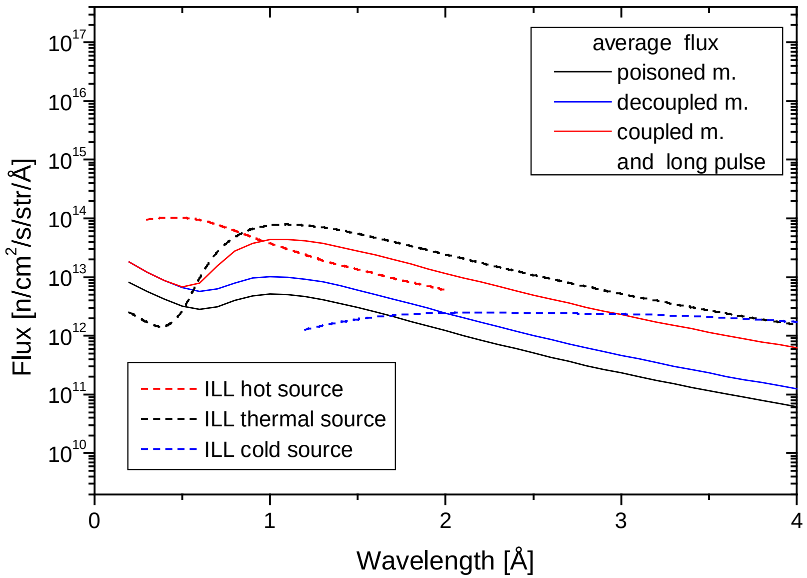
ESS goal: combine enhanced source performance with novel, improved instrumentation *into a quantum leap in experimental capabilities*

Unique neutron source performance

(reference estimate based on existing sources and studies)

In comparison: progress since 1950's: factor 4



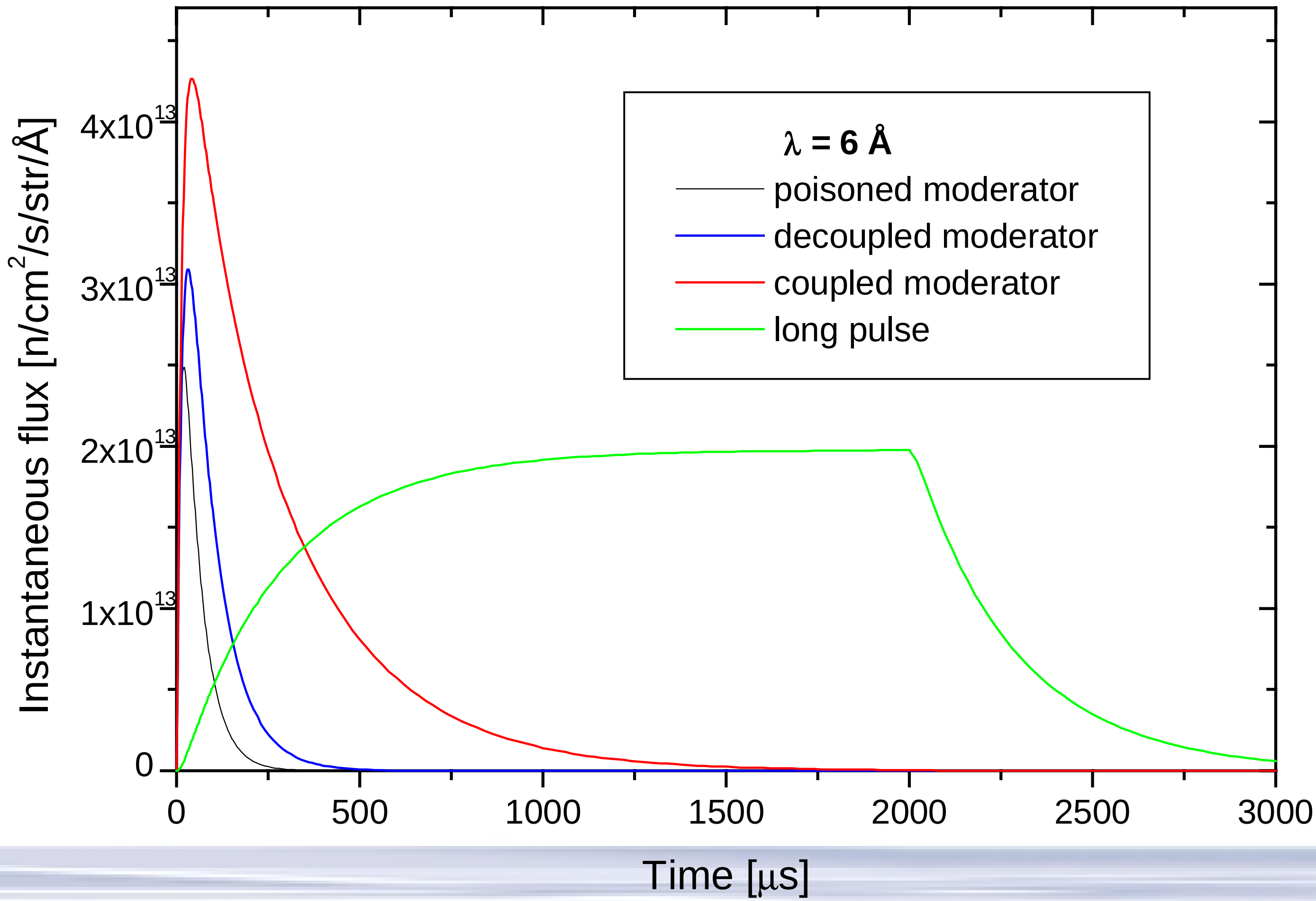


Peak instanteneous source brightness of ESS will be ~2 orders of magnitude higher than that of ILL and ISIS.

Time averaged brightness of coupled moderators at ESS will be comparable to that of ILL.

Choices for pulse lengths/intensity:

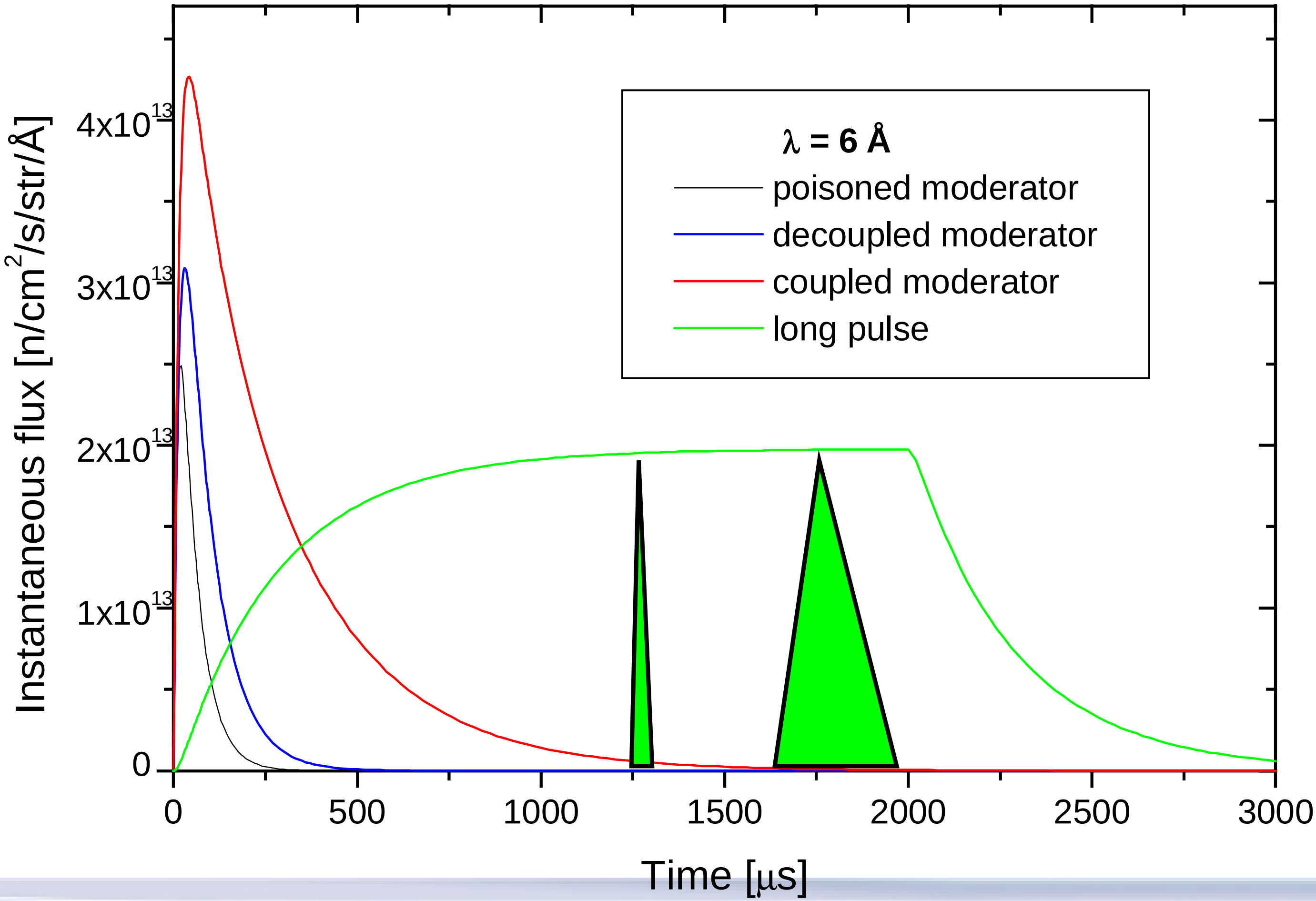
- better neutron moderation - more neutrons per proton - longer neutron pulses
- more protons per pulse: <u>long pulses</u> New!



Examples of new instrumental approaches

Adjustable pulse lengths:

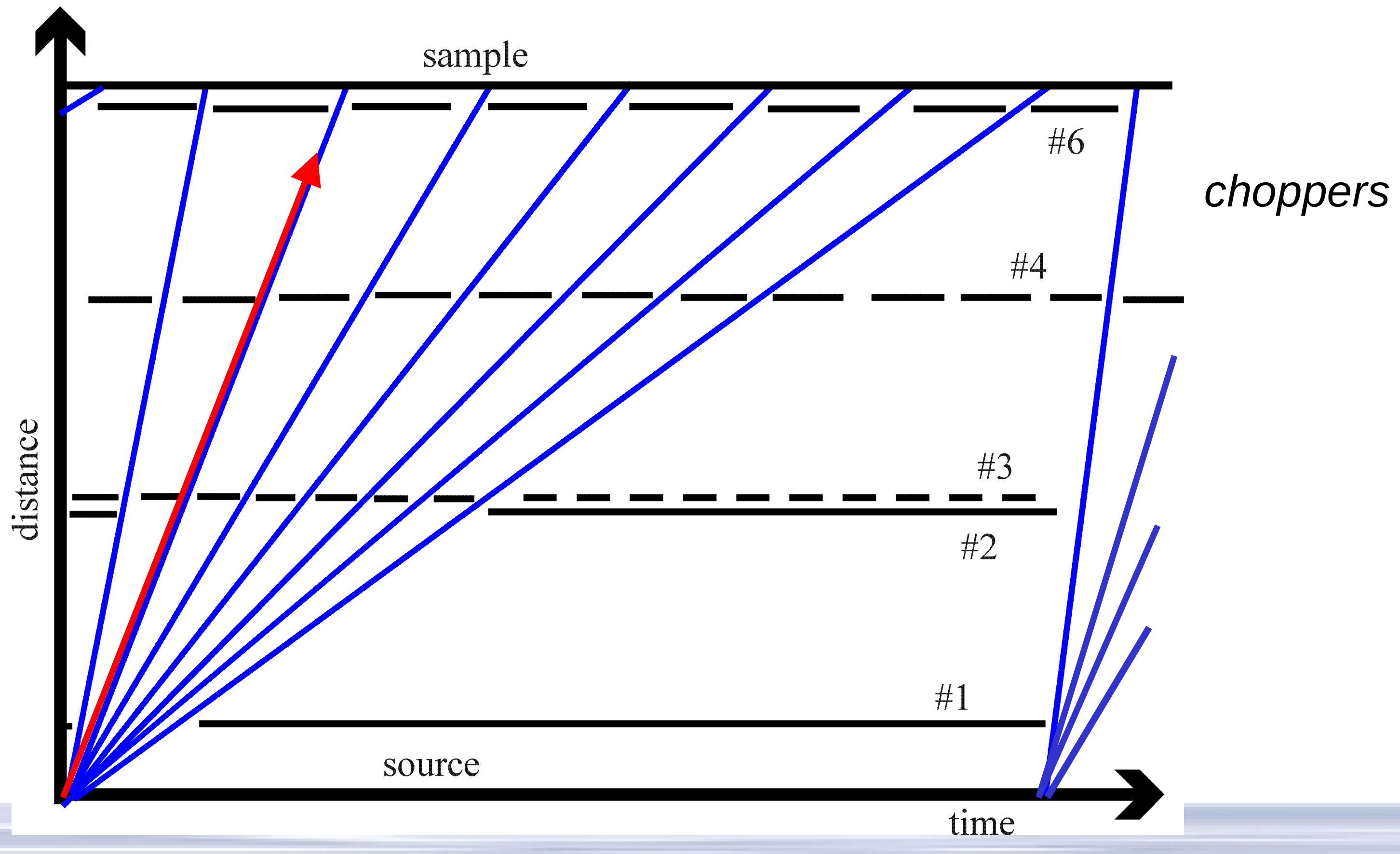
mechanical choppers can produce the shortest pulses for unprecedented resolution for neutrons: 10^{-5} (equal to synchrotron)



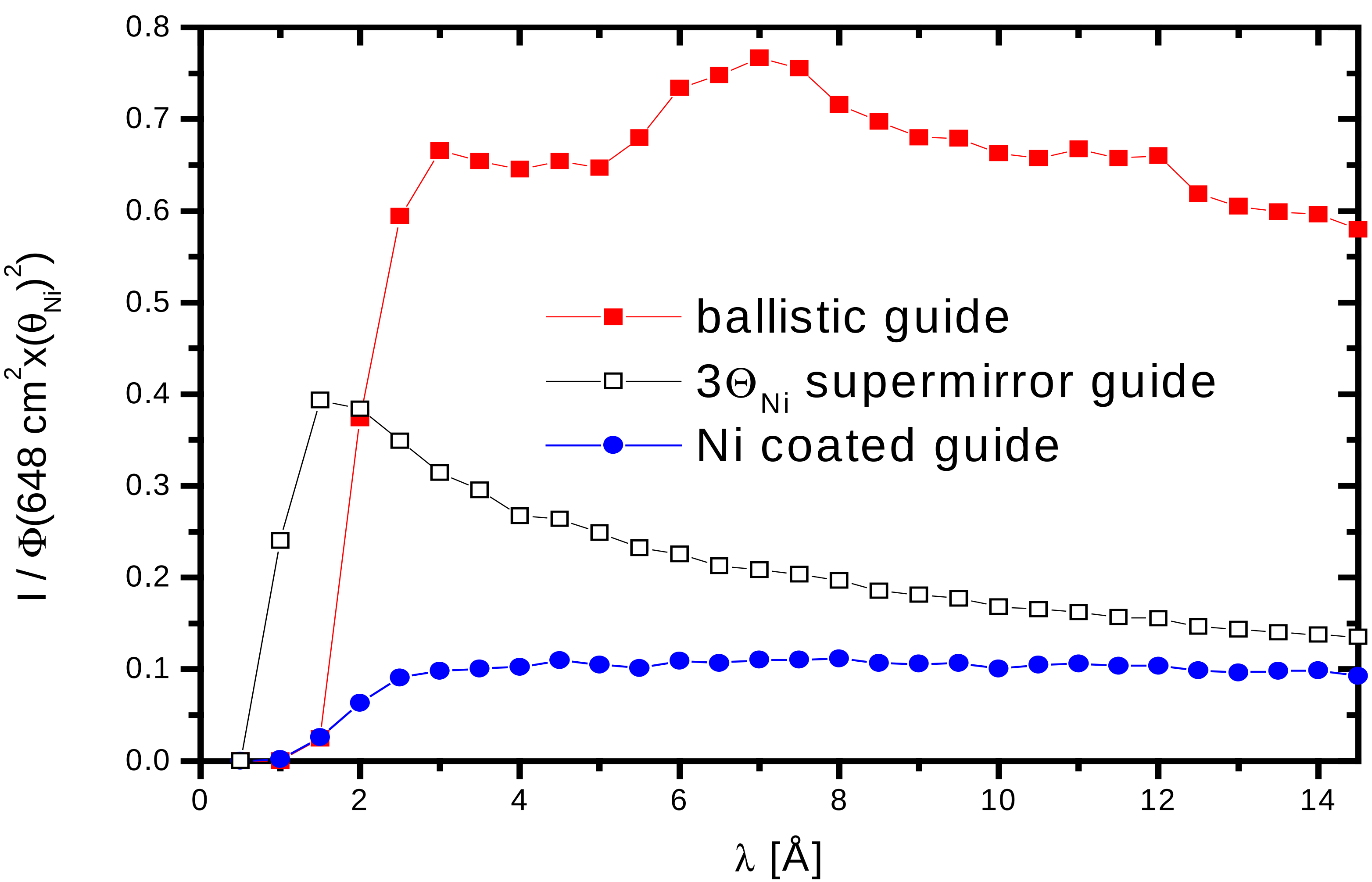
Inelastic scattering:

analysis of velocity after scattering on sample only requires 2 - 10 ms: ideal pulse repetition 100 - 500 Hz

Repetition Rate Multiplication: several pulses on sample from each source pulse (prototype in the making at LANSCE)



Largely enhanced beam delivery by advanced supermirror optics (e.g. for distances > 200 m)



Simulation results for the prototype in the making at LANSCE

Expected performance of generic instruments for ESS

compared to best *existing instruments* at ILL (blue numbers) or ISIS (black numbers)

Instrument	50 Hz 5MW	16.7 Hz 5MW	Source gain	Instr. improv.	Total gain
High energy chopper	•		30	1	30
Thermal chopper	•		30	8	240
Cold chopper	•	o	40	40	1600
Variable, cold chopper	o	•	30	40	800
Backscattering 0.8 μeV	•		25	2	50
Backscattering 17 μeV	•		150	4	600
Melecular sp. (TOSCA)	•		50	2	100
Electron eV spect.	•		30	10	300
High resolution NSE		•	10	10	100
Wide angle NSE		•	9	33.3	300
Triple axis		•	1	2-(5)	2-(5)

Up to 3 orders of magnitude total gains compared to existing instruments

Expected performance of generic instruments for ESS

Instrument	50 Hz 5MW	16.7 Hz 5MW	Source gain	Instr. improv.	Total gain
High resolution single X	•		>>10	>1	>>10
Chemical single X	•		>>10	>1	>>10
High resolution protein	•		>20	>1	>20
Low resolution protein	•		3-5	1	3-5
Single peak (Cryopad)	•	•	0.3-3	1	0.3.-3
High resolution powder	•	•	50	3	150
High Q powder	•		60	2	120
Magnetic powder	•	o	60	1	60
High res. reflectometer	•	o	20	2	40
High intensity reflect.	o	•	15	2.6	40
Liquids diffractometer	•		20	1	20
High intensity SANS		•	8	12.5	100
High resolution SANS	•		150	2	300
Engineering diffractometer	•		30	3	90
Diffuse scattering (D7)	o	•	15	20	300
Fundamental physics	•	•	1	NA	NA
Average (geometrical)			>19	>2.4	>47

Source gain: leading factor

ESS Instrumentation Task Group

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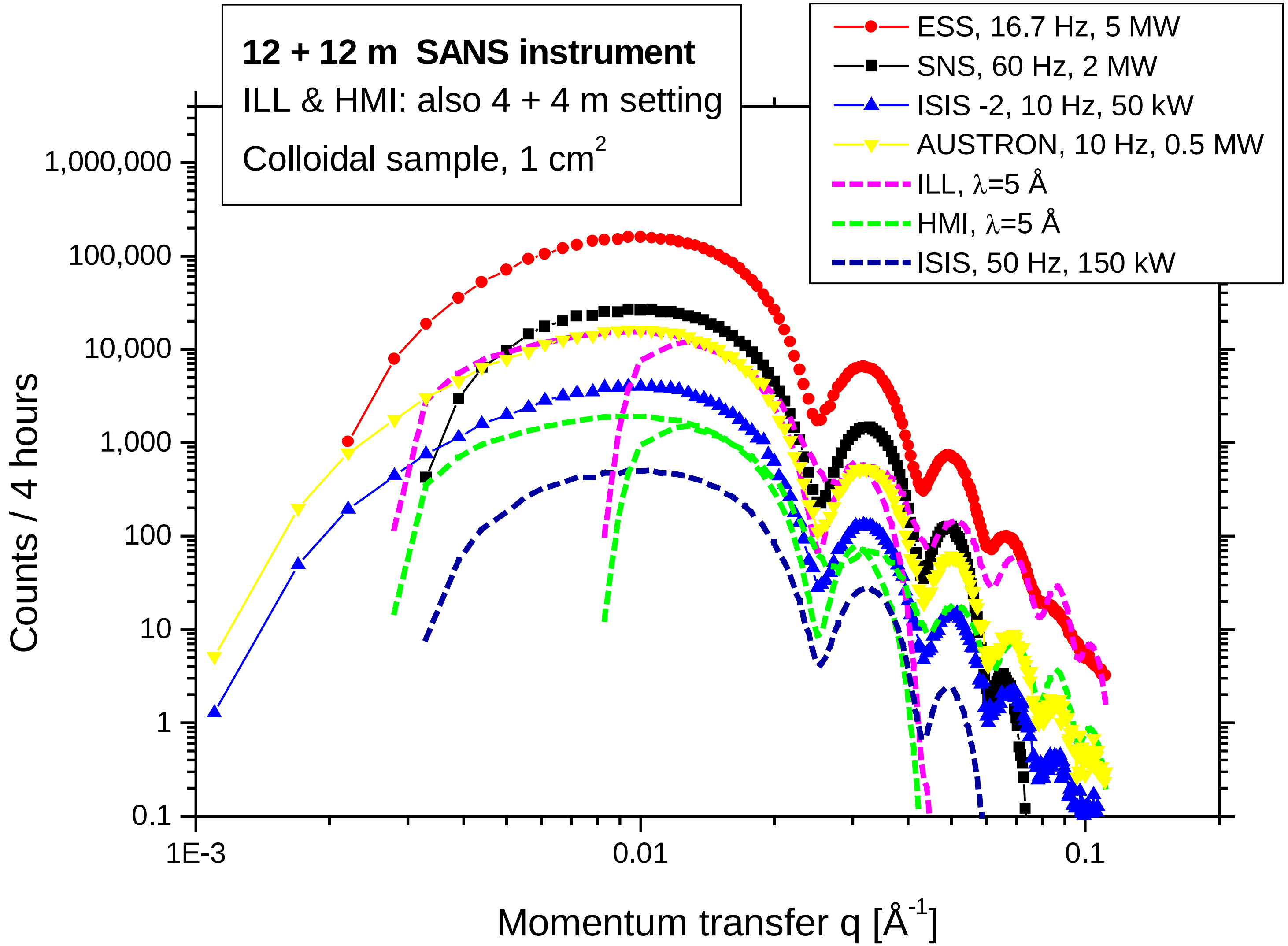
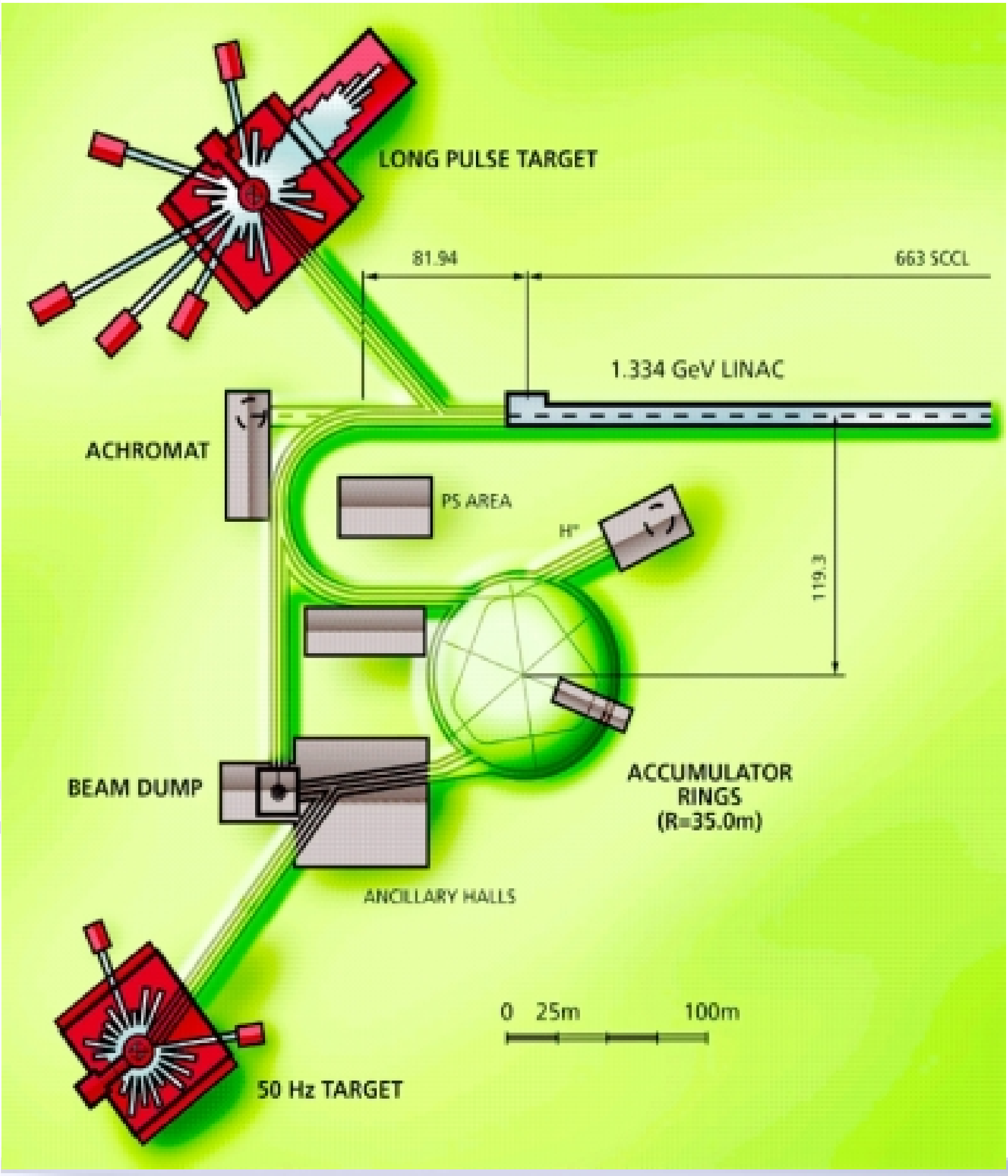
ESS (5 + 5 MW power): beam performance way beyond current facilities and projects





ESS

new level of performance compared both to current or projected **pulsed** **and** **continous** sources

Comparison of projected progress in experimental capabilities to explore nanoscale dynamics (1-100 nm, 10^{-12} - 10^{-6} s)

ESS (LPTS) (large sample)	X-ray FEL

a) Beam intensity on sample for inelastic scattering:

1.7×10^{11} 1/s/meV	$\sim 10^{11}$ 1/s/meV

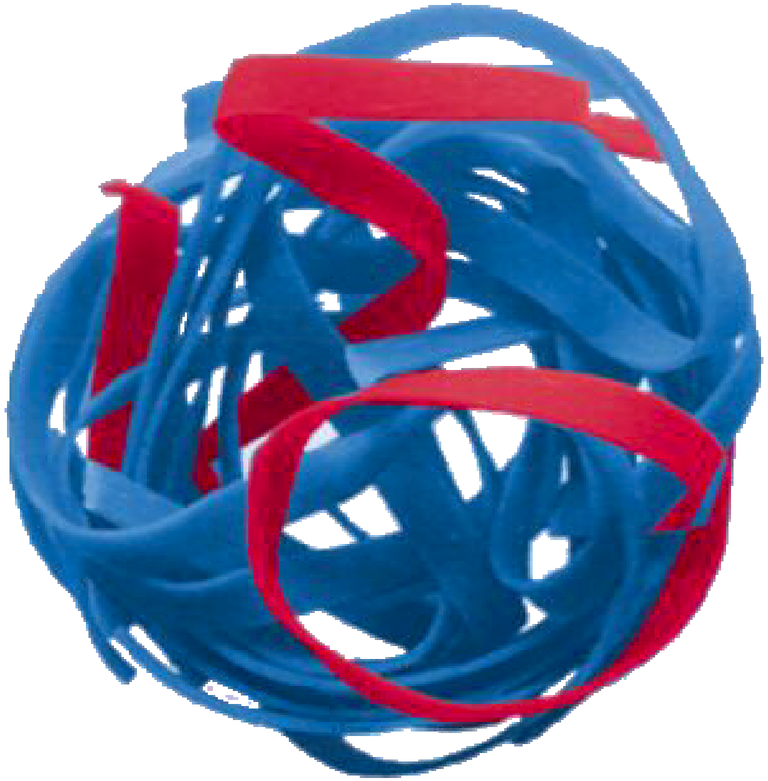
b) Beam intensity on sample for 5 neV resolution

$1\text{-}2 \times 10^{8}$ 1/s	$\sim 10^{6}$ 1/s

c) Gain over existing capabilities (data collection rate)

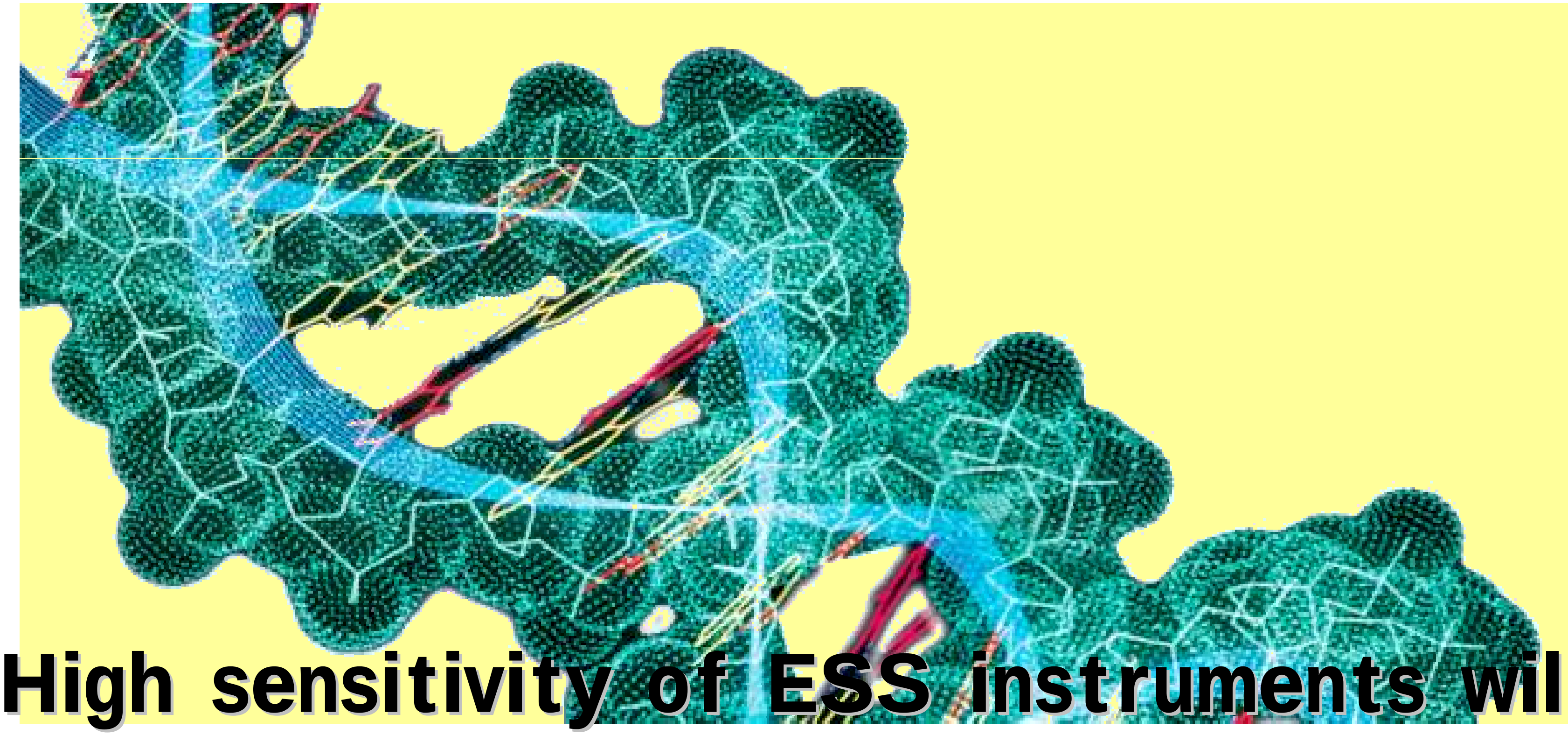
100 - 1000 x	100 x

Neutrons see the nuclei



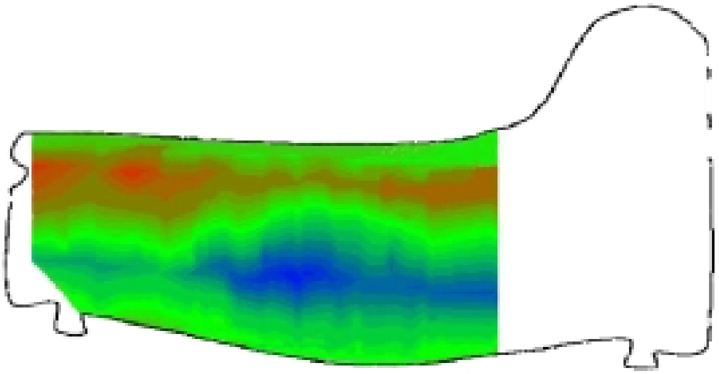
ESS will allow us to look at the function/motion of labelled groups

Neutrons see light as well as heavy atoms



High sensitivity of ESS instruments will be required to provide exact position/localization of thousands of H atoms

Neutrons see deep inside heavy (metal) parts



ESS will make possible
- to examine much larger safety critical parts
- to meet needs for fast answers in engineering
- to reduce reliance on simulations without experimental checks

ICE train wheel failure:

Current neutron data help to search for cause by

- indication of danger in 1D strain data
- inaccuracy of computer simulation results

Proof of risk would require 3D strain data→stress:

much higher neutron flux needed

Today´s high level decision-making paradigm:

"safe" = absence of knowledge of danger

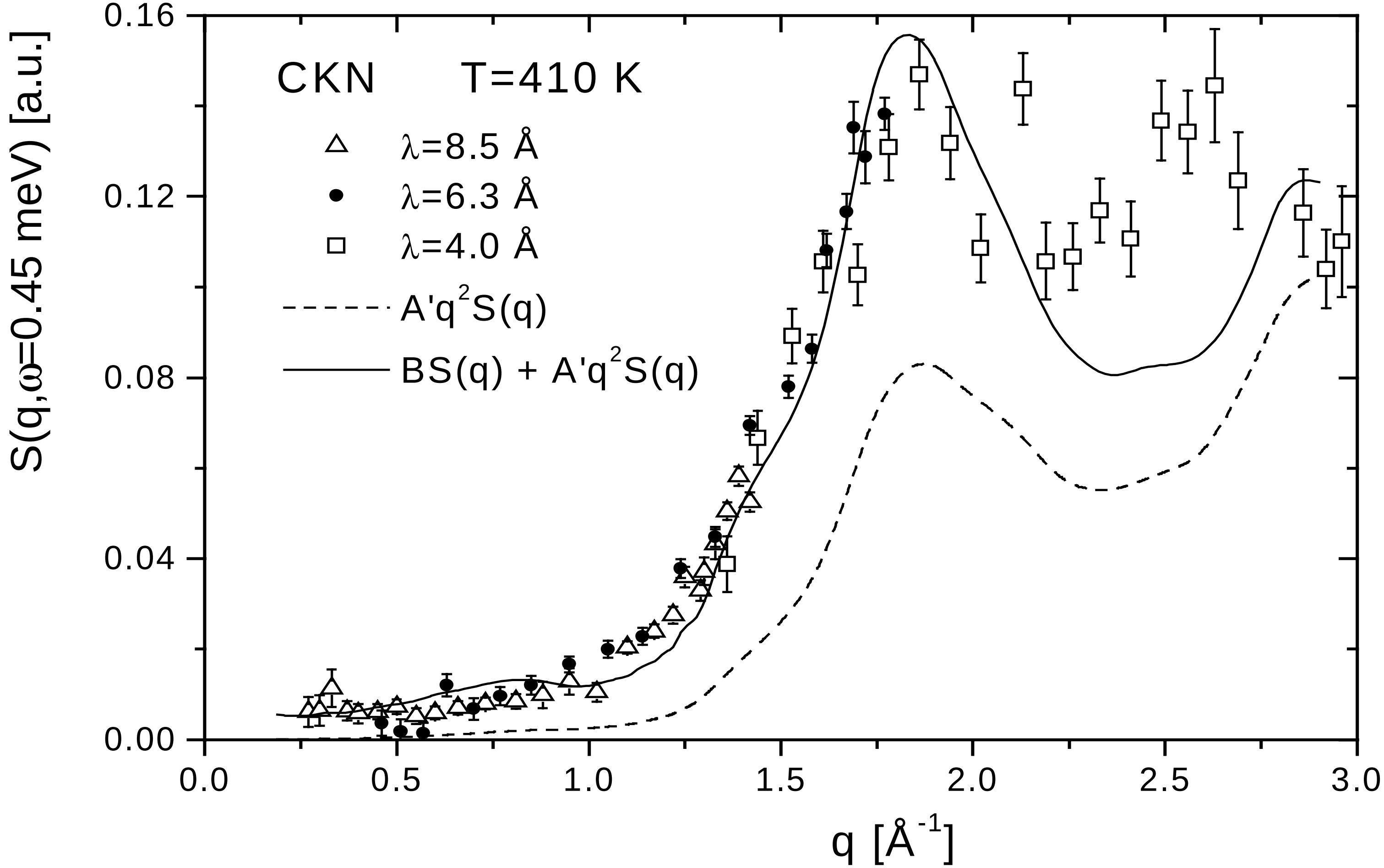
instead of

knowledge of probable absence of danger

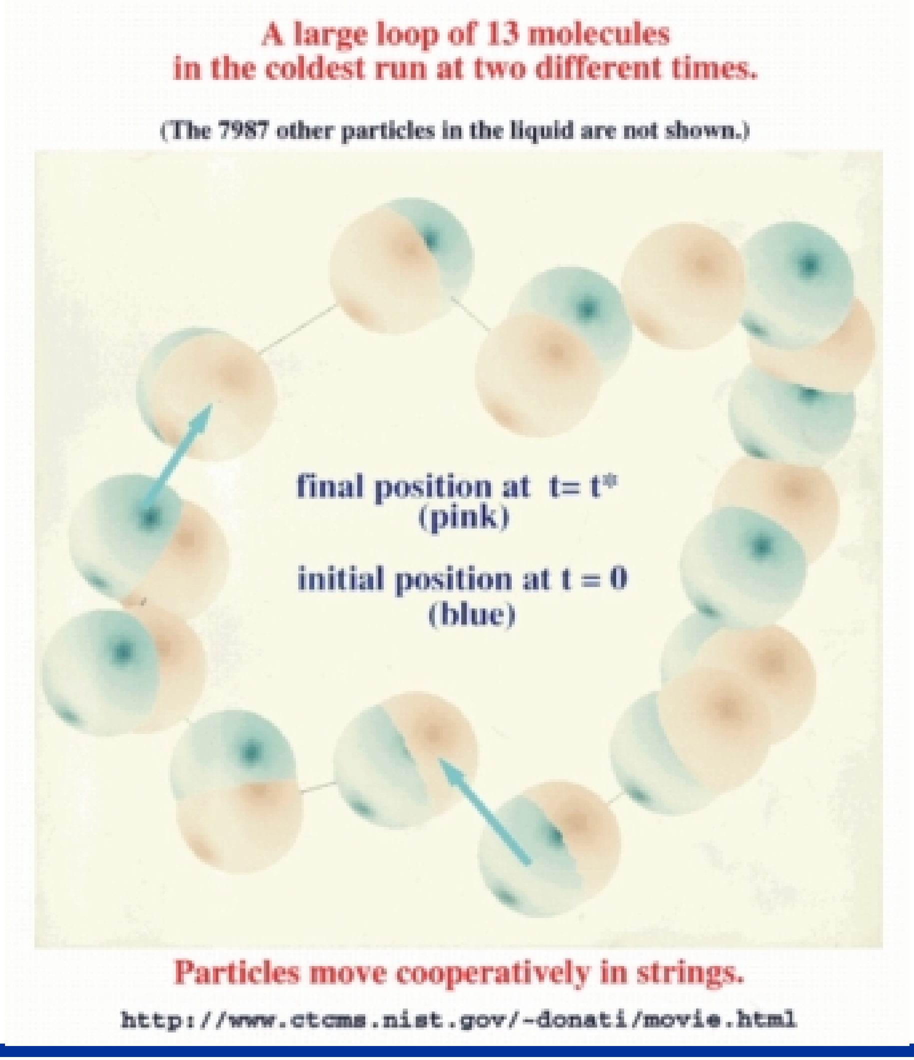
(e.g. environment, genetic modifications, ...)

We badly lack the knowledge needed to act responsibly

ESS will help to pick up the small signals related to molecular functions



Molecular dynamics results on a toy model system: “string flow” is coordinated motion on nanoscale distances



Conclusions

ESS will offer a quantum jump in research capabilities to explore structure and function in condensed matter

ESS is a cost effective approach to put Europe back in leadership position in the face of US and Japanese competition (facilities in construction)

The combination of:

Neutron scattering with 1000 fold enhanced sensitivity offered by ESS,

Advanced data correction/reduction techniques

and

Improved molecular dynamics calculations

will open up ways to tell "where the atoms are and what the atoms do" in non-crystalline matter (*e.g. biological and other functional materials*):

a new adventure in the exploration of matter