

PEPR SCIAM

Réinterprétation d'expériences
intégrales passées

UNCERTAINTY QUANTIFICATION IN THERMAL SCATTERING LAWS

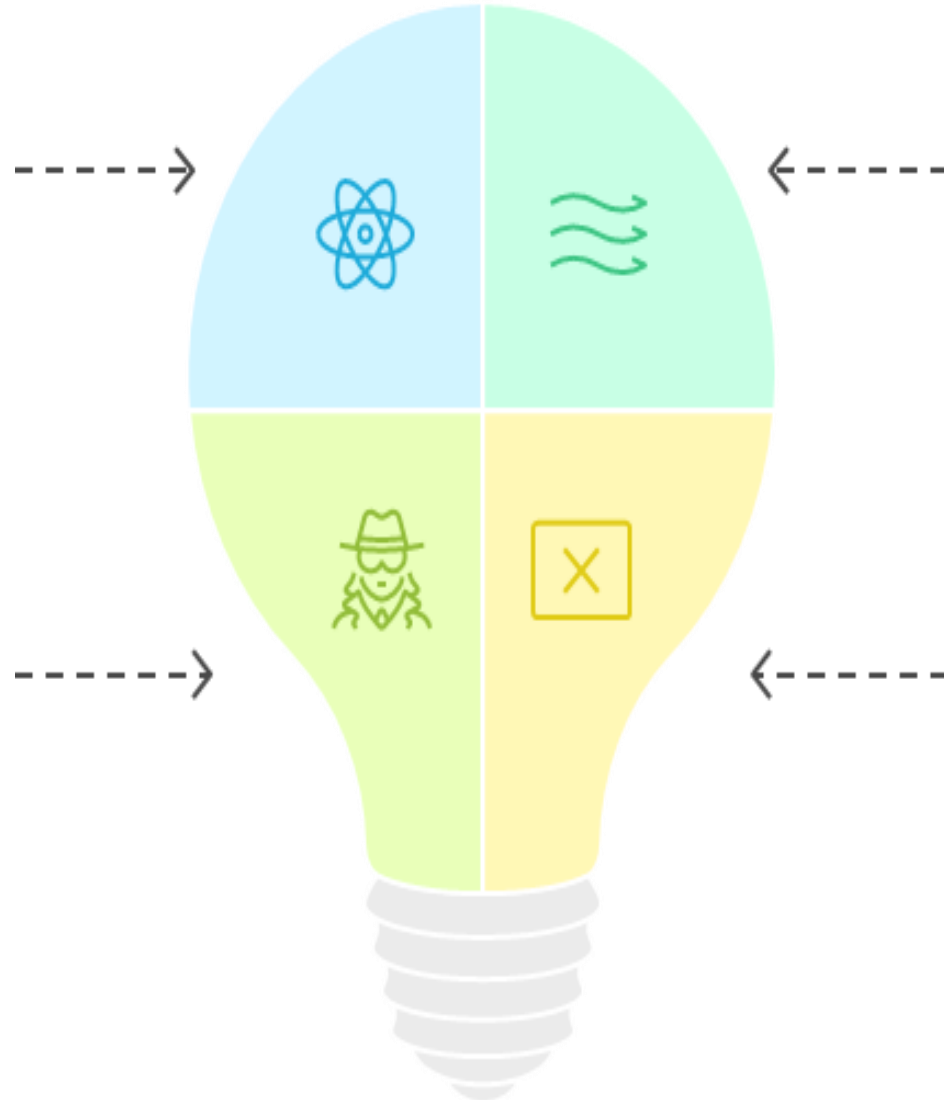
***A JOINT PHD PROJECT:
ASNR/CEA***

Supervisor: Vaibhav JAISWAL
(ASNR/PSN-RES/LN)
Director: Gilles NOGUERE
(CEA/SPRC/LEPh)

WHY DOES THIS MATTER?

TSL governs neutron thermalization
 The physics of how neutrons slow down in moderator materials (H₂O, D₂O, graphite, ice)

JEFF-4.0 has 86 TSLs; ENDF/B-VIII.1 has 114 TSL
 Yet they do not have a covariance matrix or formal uncertainty for TSLs











ΔKeff up to 600 - 800 pcm
 Observed when switching from one TSL library to another (JEFF-3.3 vs JEFF-4) in H₂O sensitive benchmarks

We cannot quantify the uncertainty
 The absence of TSL covariance limits our ability to quantify uncertainty in thermal systems.

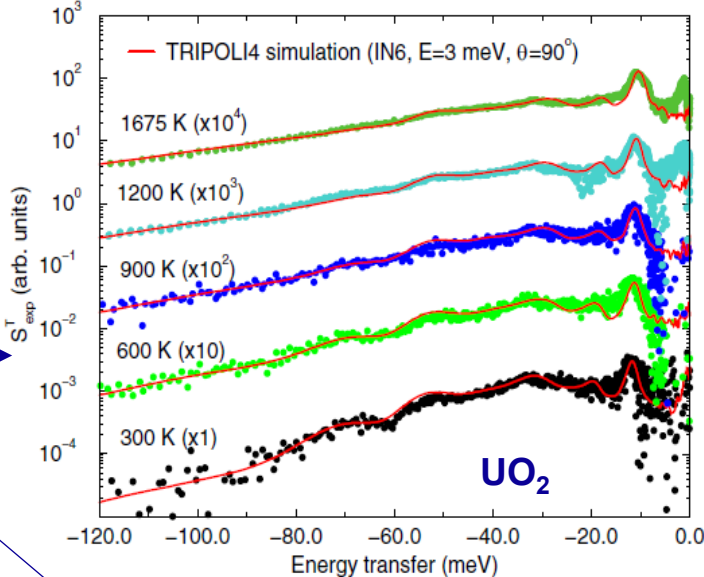
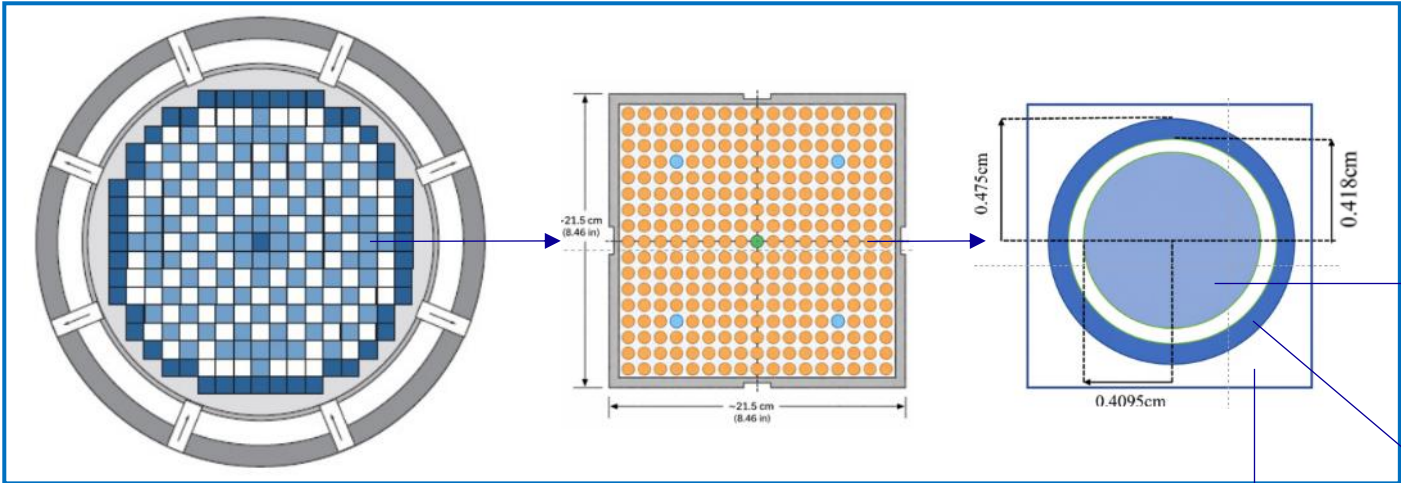
This project changes that — building a systematic uncertainty framework for thermal scattering data

WHAT DO WE HAVE TODAY ?

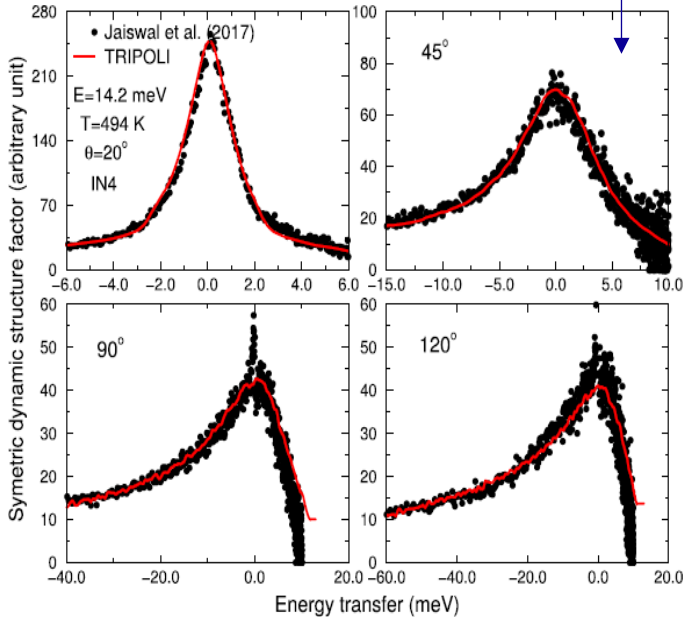
Academic contributions (PhDs) in the last 10 years ..

Analytical Developments of Thermal Scattering Models: Doppler Broadening with CLM and Up-scattering in the Resonance Range	Aitor Bengoechea Fernández (CEA, France)		2025
Nuclear Data Uncertainties Processing and Propagation	Pierre Solé (ASNR, France)		2025
Measurement of the Double Differential Neutron Cross Section of UO ₂ and Determination of the Thermal Scattering Law as a Function of Temperature	Shuqi Xu (CEA), France		2021
Thermal Scattering Law Uncertainties and Propagation into Small Thermal Fission Reactors	Lance Maul (UNSW, Australia)		2018
Amélioration des données neutroniques de diffusion thermique et épithermique pour l'interprétation des mesures intégrales	Juan Pablo Scotta (CEA)		2018
From Experiments to DFT Simulations: Comprehensive Overview of Thermal Scattering for Neutron Moderator Materials	Kemal Ramić (RPI, US)		2018
Theoretical and Experimental Approach Towards Generation of Thermal Scattering Law for Light Water	Vaibhav Jaiswal (IRSN, France)		2018
Thermal Neutron Scattering Evaluation Framework	Chris W. Chapman (ORNL, US)		2017

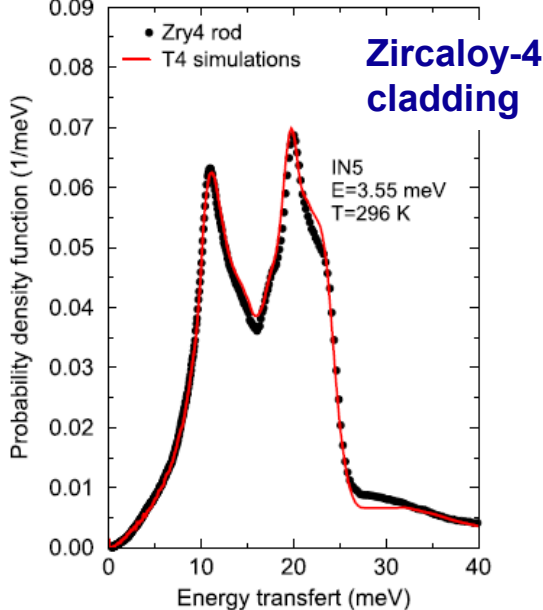
EXPERIMENTAL PROGRAM AT ILL



Experimental studies of each material separately as a function of temperature (300-1700 K) and pressure (P=300 bars)



CINEL model of H₂O (not in JEFF)

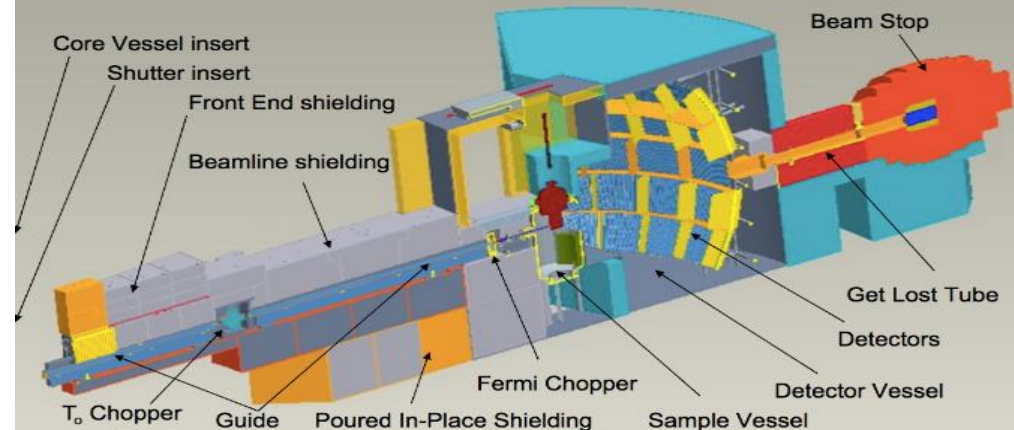


EXPERIMENTAL PROGRAM AT SNS

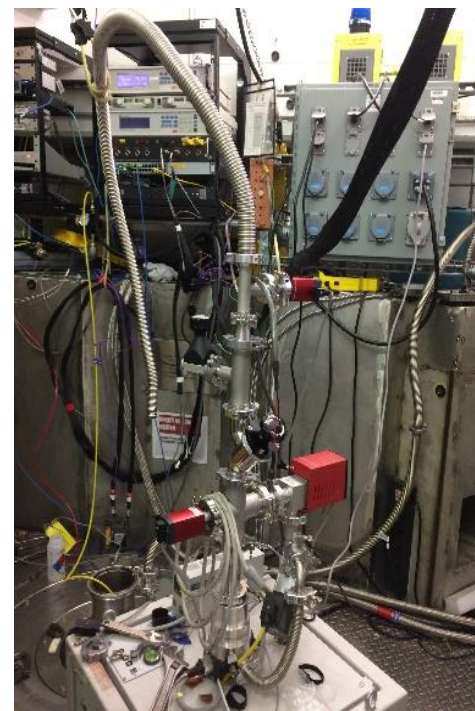
Double differential data measurements for light water
 Double differential and total cross section for Ice-Ih

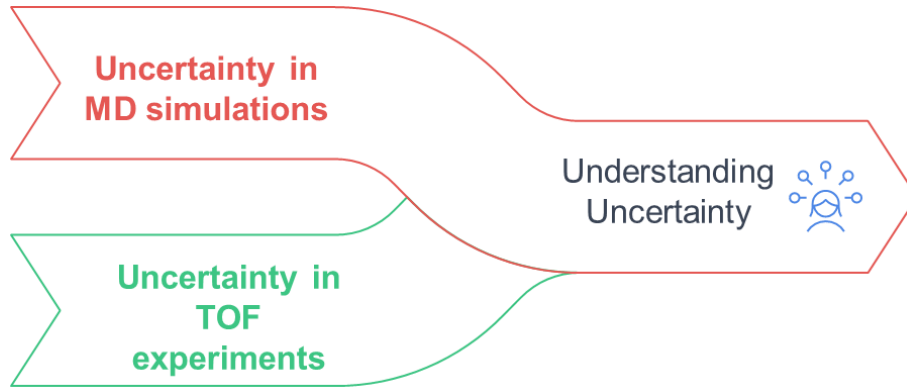
Sample	Temperature (K)	Pressure (bar)	Incident neutron energy (meV)
Water + Cell	295.0	1	60, 160, 280, 800
	323.6	1	60, 160, 280, 800
	350.0	1	12, 60, 160, 280, 800
	350.0	150	8, 60, 160, 280, 800
	400.0	150	8, 60, 160, 280, 800
	450.0	150	8, 60, 160, 280, 800
	500.0	150	8, 60, 160, 280, 800
Cell	550.0	150	8, 60, 160, 280, 800
	600.0	150	8, 60, 160, 280, 800
	295.0, 350.0, 400.0, 450.0, 550.0, 600.0		8, 60, 160, 280, 800
	Vanadium		295.0

Sample	Temperature (K)	Incident neutron energy (meV)
Ice + Cell	6	11, 55, 160, 250, 600
	100	11, 55, 160, 250, 600
	200	11, 55, 160, 250, 600
	233	11, 55, 160, 250, 600
	243	11, 55, 160, 250, 600
	253	11, 55, 160, 250, 600
	263	11, 55, 160, 250, 600
Cell	271	11, 55, 160, 250, 600
	6, 100, 200, 233, 243, 253, 263, 271	11, 55, 160, 250, 600
Vanadium	271	11, 55, 160, 250, 600



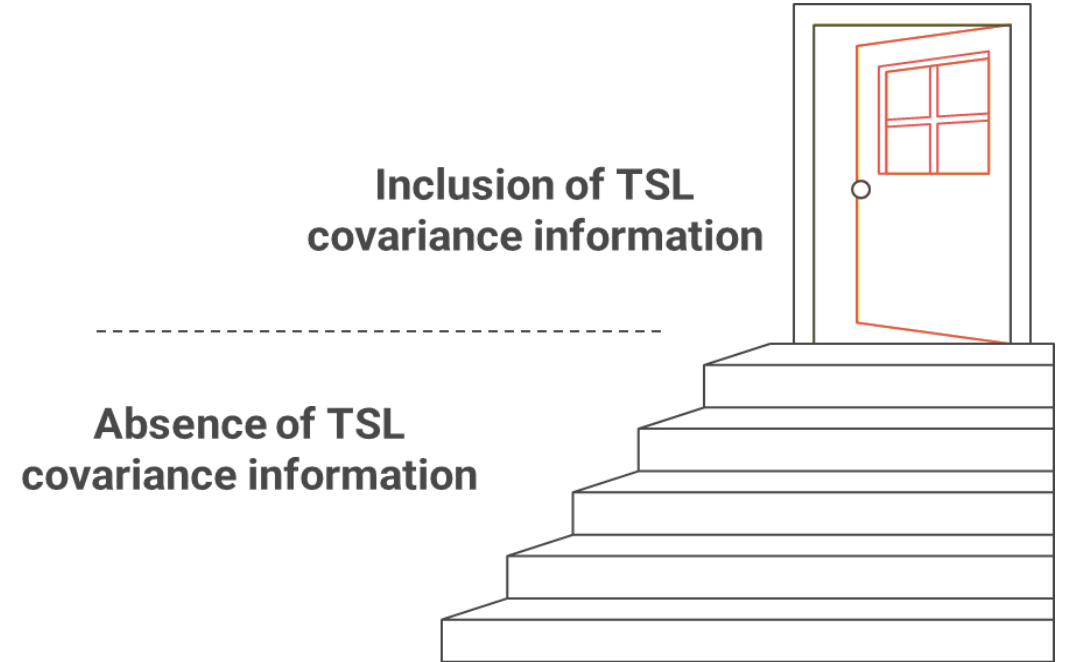
SEQUOIA TOF spectrometer






Scientific Objectives

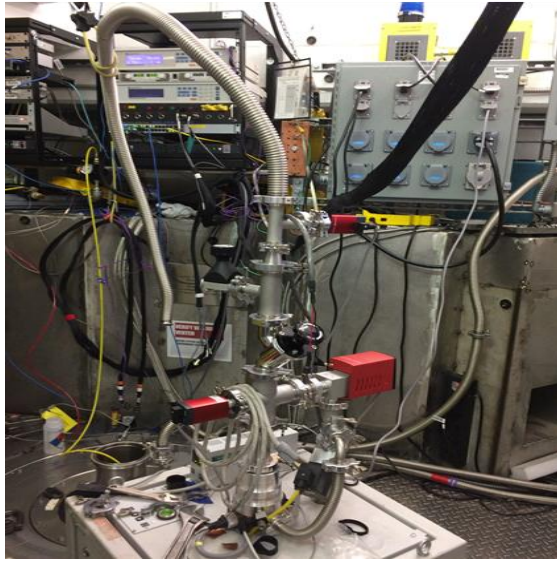
- ❖ **Build the covariance matrices for TSL** : starting from liquid water and ice, then generalizing
- ❖ **Develop a TSL sensitivity framework** : analytical derivatives of LEAPR parameters, phonon sensitivity maps
- ❖ **Propagate uncertainties into safety benchmarks** : ICSBEP and IRPhEP, quantify impact on safety margins
- ❖ **Deliver candidate evaluations** : New TSL evaluation and covariance matrix for ENDF-IX and JEFF-5



Collaboration/partners involved

- FR **ASNR / PSN-RES** project lead, TSL evaluation
- FR **CEA / SPRC** co-supervision, JEFF contributions
- US **ORNL (SNS)** TOF data for ice water
- FR **ILL (Grenoble)** TOF data for liquid water
-  JEFF/ ENDF community

THIS PROJECT



Uncertainty Analysis

Full framework to quantify and propagate thermal scattering law uncertainty

Impact on Criticality

Assess impact on criticality safety and reactor physics benchmarks (ICSBEP/IRPhEP)

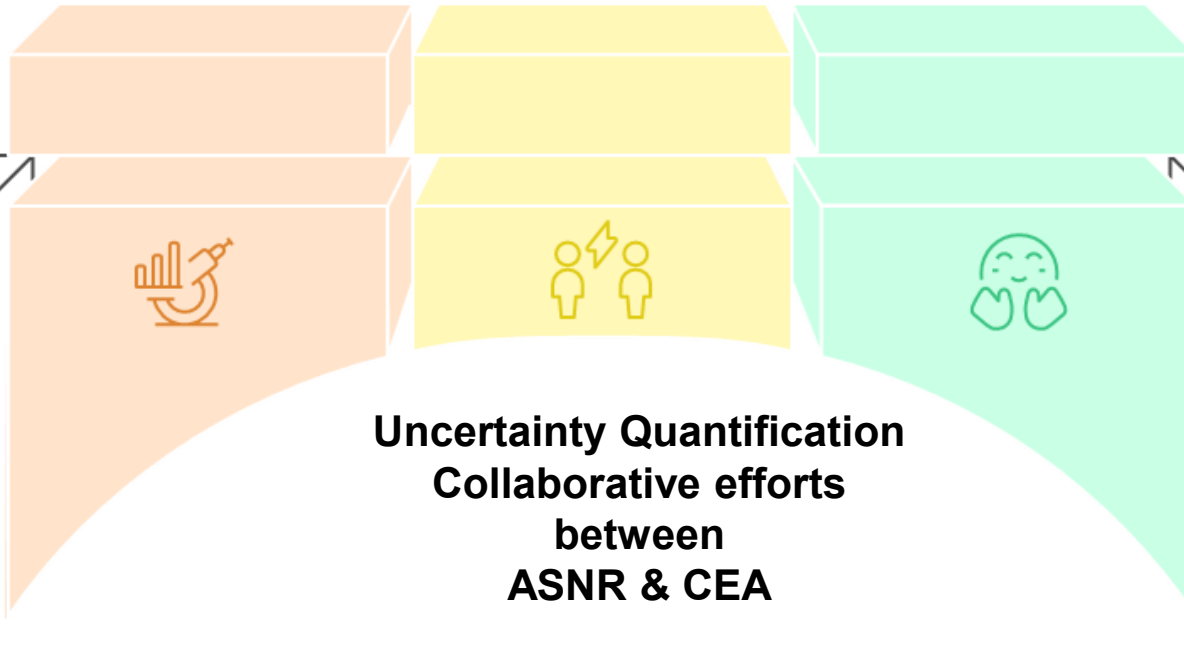
Improve Confidence

Increase confidence in criticality safety and reactor physics margins



Safety Analysis studies (ASNR)

Safety Analysis studies (ASNR)



Uncertainty Quantification
Collaborative efforts
between
ASNR & CEA

WHERE, WITH WHAT, AND WHO

Facilities & Data

- **No new experiment required** : all TOF datasets are already available (with ASNR and CEA)
- **ILL, Grenoble (France)** : high-resolution TOF data for liquid water
- **ASNR access to SNS (USA)** : high-resolution TOF data for liquid light water and ice
- **CEA access to other ILL data** : for UO_2 and PuO_2

Codes & Tools

- LEAPR / NJOY — TSL generation and processing
- NCrystal (ESS) — parameter perturbation
- TARA (ASNR) — TSL sampling tool
- MORET-6 / MCNP — criticality calculations





Human Resources & PEPR Contribution

- **1 PhD student (3 years)** : ASNR/CEA
- **Supervisors:** V. Jaiswal (ASNR), G. Noguère (CEA)
- **PostDoc (APRENDE, EU)** : active since November 2025, shared methodology

PEPR SCIAM Contribution

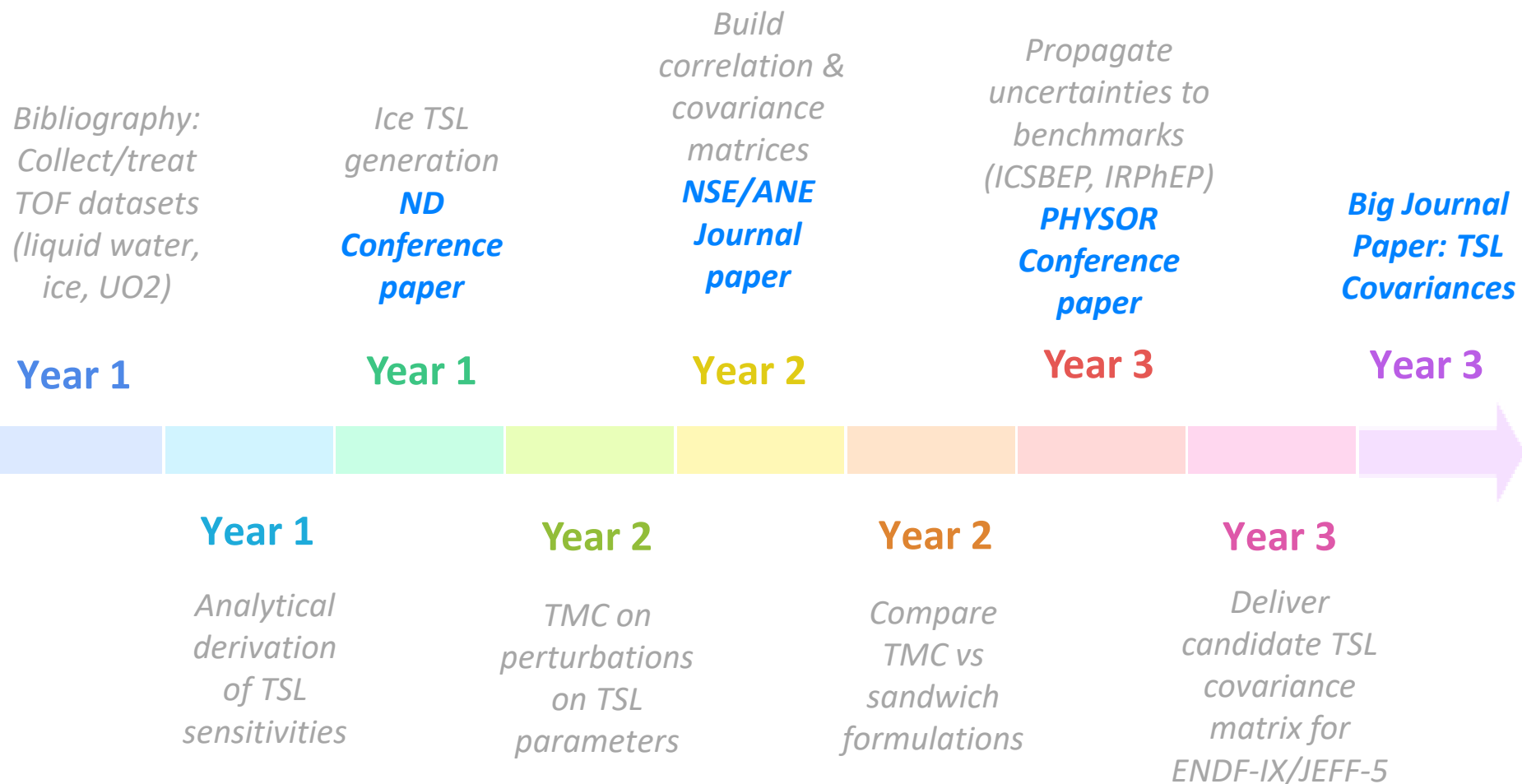
- Funds the PhD contract : APED (50 %), ASNR (50%)
- Connects to the French nuclear data network

RISKS — AND WHY THEY ARE MANAGEABLE

Risk	Level	Mitigation
No new experiment needed : all TOF data already available	 LOW	Data in hand; processing begins immediately
Building formal TSL sensitivity and covariance matrices is analytically complex	 MOD	Builds on TARA framework
Dependence on LEAPR / NCrystal parameterization choices	 LOW	Both codes are mature and actively maintained
3-year coordination between ASNR and CEA	 NA	Collaboration already running (PostDoc APRENDE, prior PhDs)

Overall: low-to-moderate risk profile. All key tools and data are already in place.

PHD TIMELINE



EXPECTED OUTCOMES

Sensitivity maps of TSL

Identify which phonon bands (positions, widths, intensities) most impact $S(\alpha, \beta)$

New Ice TSL evaluation

Candidate for ENDF-IX and JEFF-5 based on reprocessed TOF data.

Covariance matrices for TSL

First systematic covariance construction for liquid and ice water and generalizing on other moderators.

Benchmark propagation

Quantify impact of TSL uncertainties on ICSBEP benchmarks and reactor calculations.

- ❑ **Systematic TSL uncertainty framework**
No covariance exists today in any library for all materials
- ❑ **Direct impact on safety margins** Better-quantified TSL uncertainties improve confidence in criticality safety calculations
- ❑ **Transferable methodology** Developed for water and ice, directly applicable to UO_2 , PuO_2 , graphite, and beyond ..
- ❑ **Legacy in ENDF-IX and JEFF-5**
Deliverables feed directly into the next generation of nuclear data libraries

Thank you !

