Accurate simulations for the CRAB project:
from thermal neutron production to low energy nuclear recoils

L. Thulliez on behalf of the CRAB collaboration

CEA-Saclay/DRF/Irfu/DPhN

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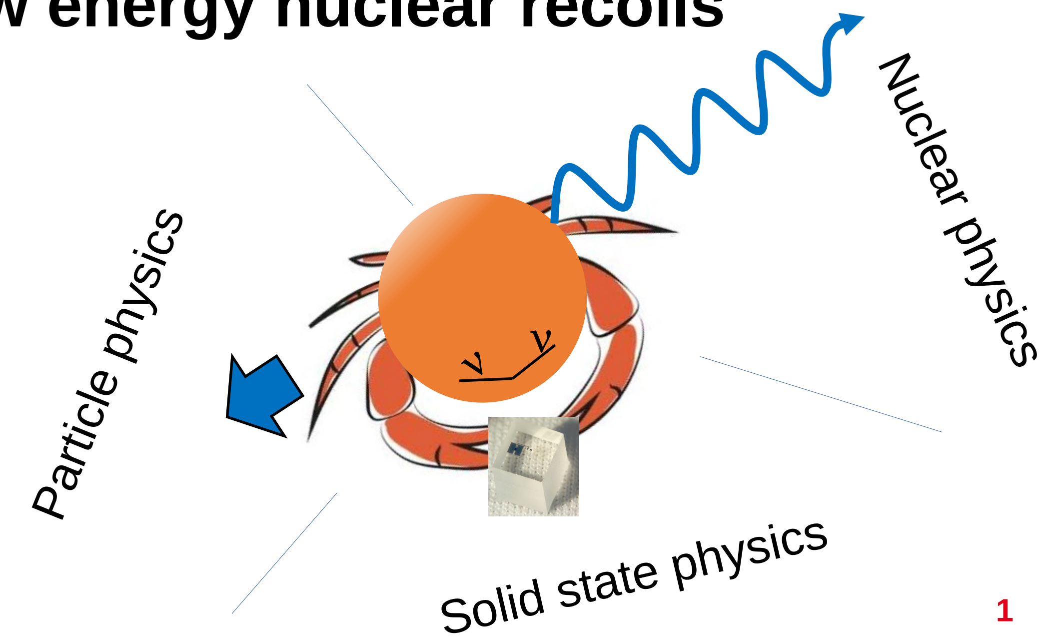
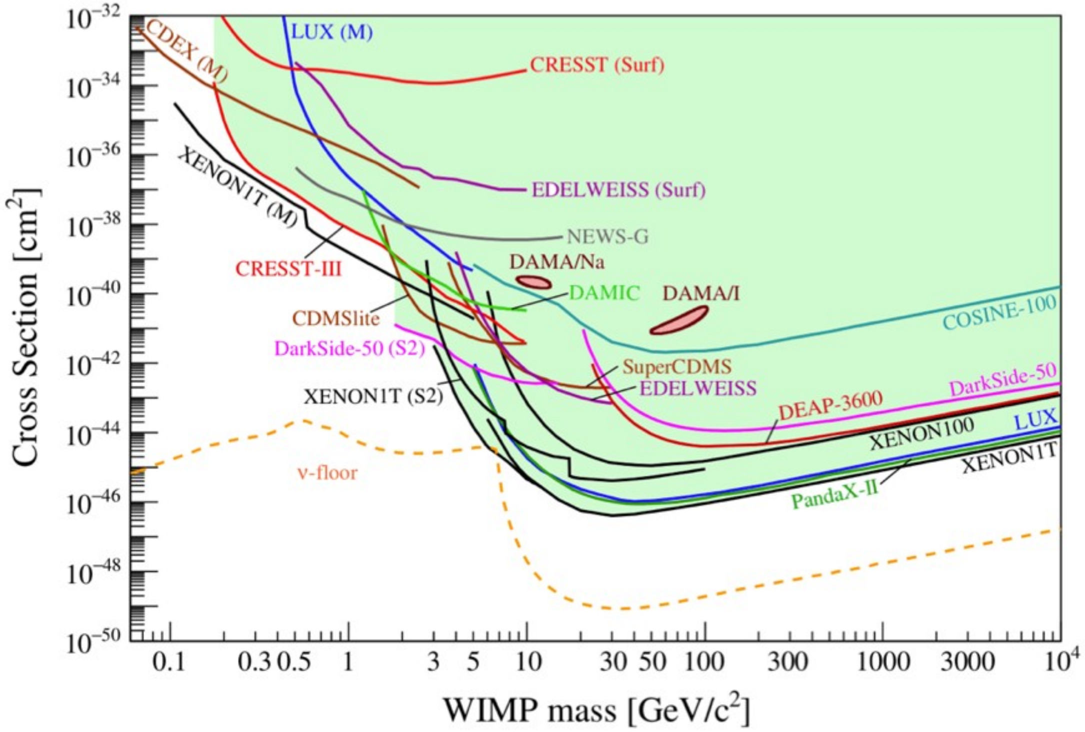


DARK MATTER and CEvNS

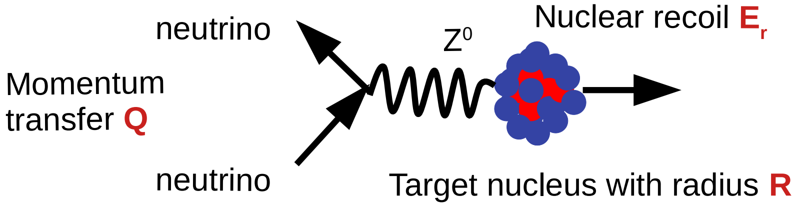
DARK MATTER

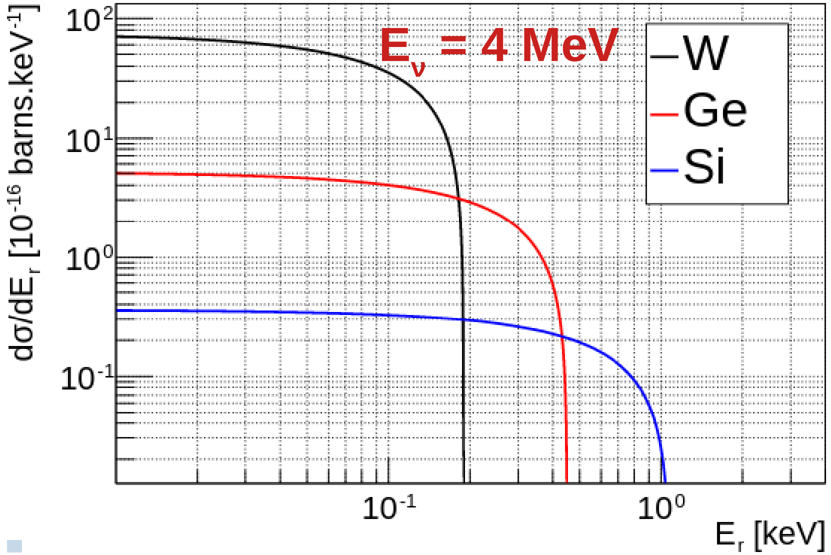


Direct Detection of Dark Matter APPEC Committee Report (2021)

- Moving to lower mass range
- Sensitivity in large mass range approaching the neutrino-floor limit

CEvNS





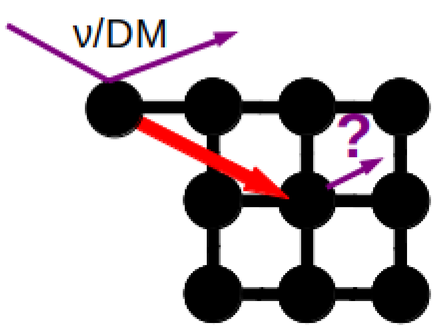
- *test SM (θ_W, etc)*
- *test BSM physics*
  (neutrino magnetic moment, non-standard interaction, etc)
- *Measure nuclear form factor (neutron skin)*
- *Nuclear reactor monitoring*

Need to detect sub-keV nuclear recoil energy

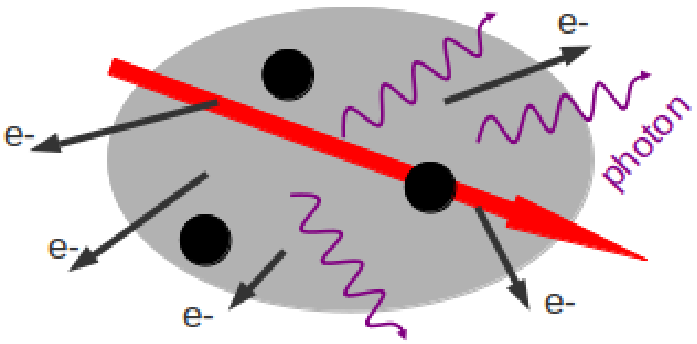
WHAT HAPPEN AFTER A PRIMARY RECOIL (> keV) IN THE DETECTOR ?

Complex solid state physics to understand for precise measurements

Initial interaction

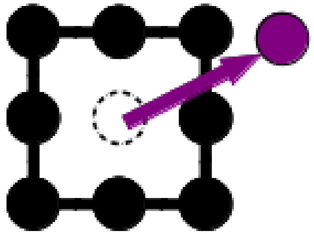


Ionization / Light emission

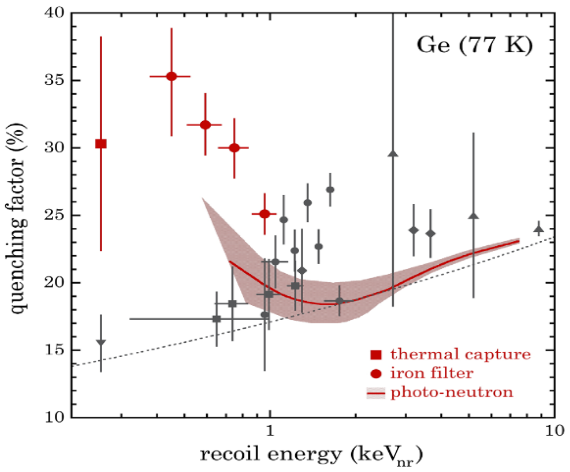


Atomic displacement

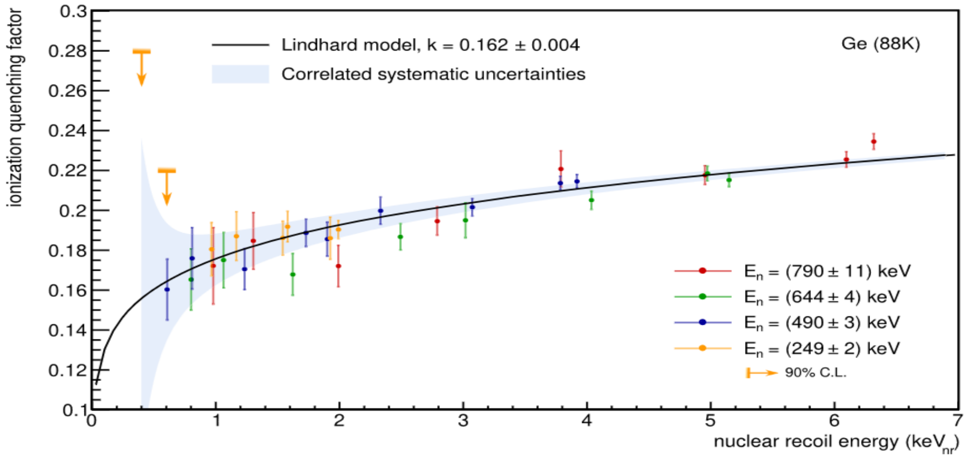
Secondary recoil
cascade



Quenching factor k (= $E_{nr}^{ioni}/E_{e-}^{ioni}$) below 1 keV ?



J. I. Collar Phys. Rev. D 103, 122003 (2021)



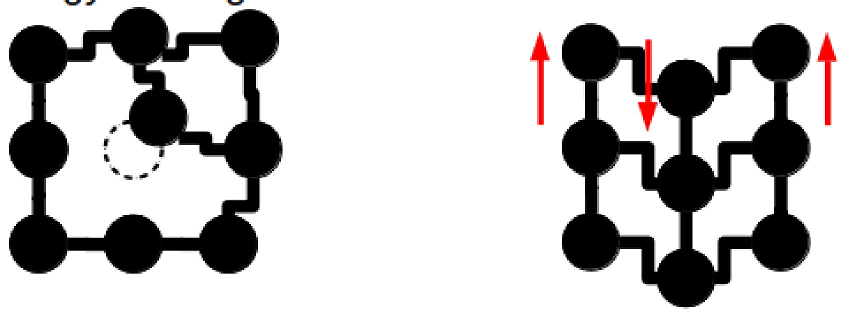
A. Bonhomme et al. Eur. Phys. J. C (2022) 82:815

WHAT HAPPEN AFTER A PRIMARY RECOIL (<keV) IN THE DETECTOR ?

Complex solid state physics to understand for precise measurements

Atomic displacement

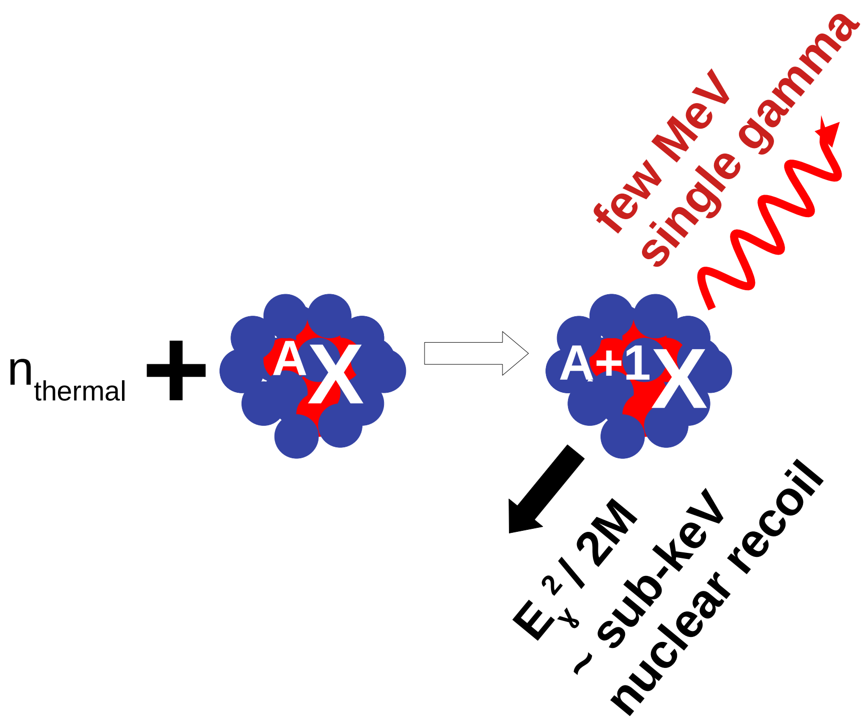
Lattice defect creation	**Phonon excitation**
energy trapped in the detector ⇒ energy biasing	temperature increase



→ Impact of energy stored in lattice defect when reaching 100 eV scale ?
⇒ linearity study

CRAB METHOD [1]

Absolute calibration method with thermal (~25meV) neutron radiative capture



The high-energy gamma leaves the cm scale detector without energy deposition

Advantages

- Pure nuclear recoil ⇒ mimic the neutrino/DM signal
- Allows to probe the whole bolometer
- Accuracy ⇒ well defined peak

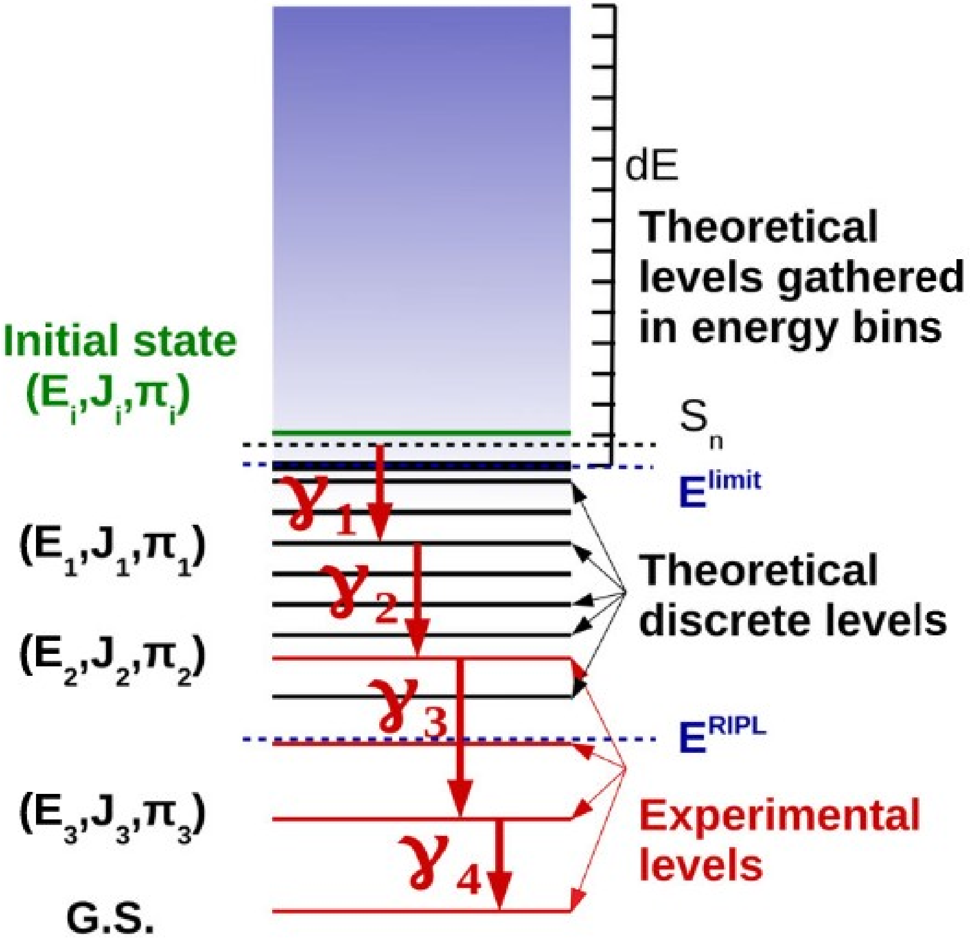
However non-trivial nucleus de-excitation to simulate

- transition probability from S_n to GS ?
  ⇒ signal intensity
- multi-gamma/electron cascade ?
  ⇒ background evaluation in the ROI
  ⇒ dead-time (response time of ~ms for cryo-detectors)

[1] L. Thulliez, D. Lhuillier et al., Calibration of nuclear recoils at the 100 eV scale using neutron capture, JINST, 16, 7 (2021)

FIFRELIN SIMULATION [1]

Fission fragment de-excitation code developed at CEA-Cadarache [1]



- All experimental (evaluated) data from EGAF, ENSDF, RIPL3 databases are taken into account
  ⇒ for light nuclei, *e.g.* Al or Si the nuclear level scheme is known

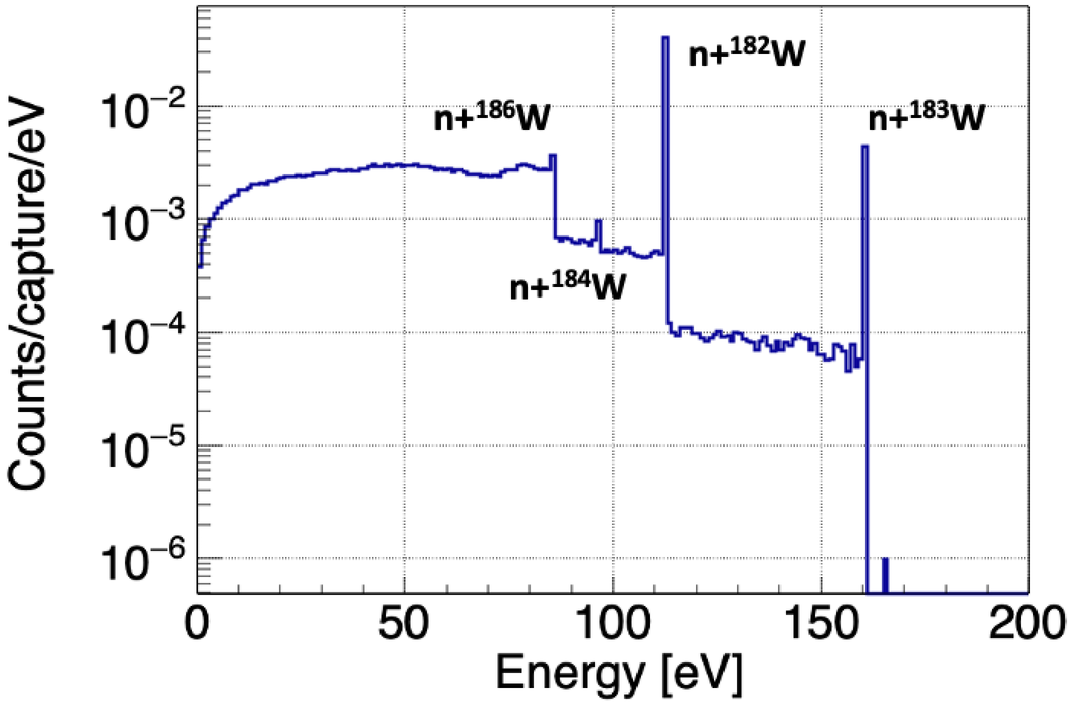
- For heavy nuclei too many levels
  ⇒ every levels cannot be expermentally determined
  ⇒ need theoretical models
    → level density (CGCM, HFB)
    → radiative strength function (EGLO, QRPA)
    → electron conversion coefficient (BrICC)

N. B.: FIFRELIN executable will be released in 2024 *via* the NEA website: https://www.oecd-nea.org/

[1] O. Litaize et al., Fission modelling with FIFRELIN, Eur. Phys. J. A 51, 1 (2015)

STUDIED CRYO-DETECTOR MATERIALS

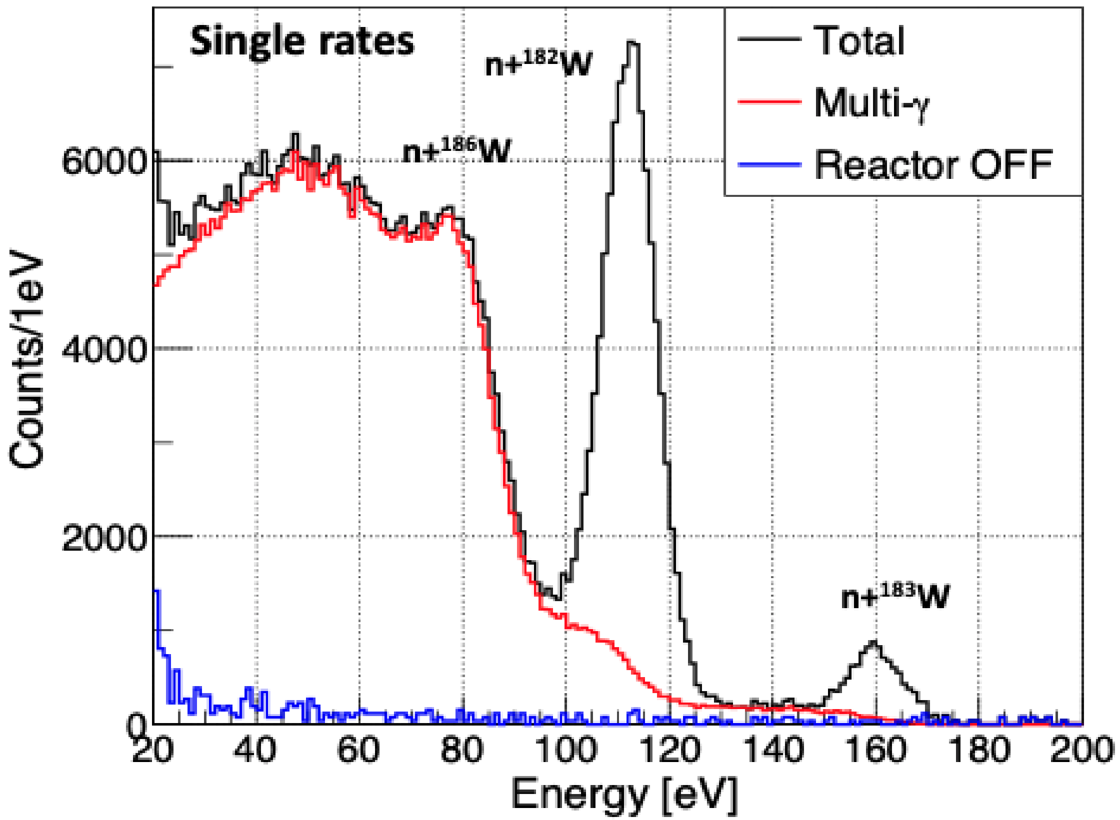
Detector	Target nucleus	E_γ [keV]	FOM = $Y_{abunance} \times \sigma_{(n,\gamma)} \times I_{decay}$	Nuclear recoil [eV]
$CaWO_4$ *CRESST* *NUCLEUS*	^{186}W ^{182}W ^{183}W	~5300 + 150 6191 7411	~4400 7506 823	~80 112.5 160.3



Simulated recoil spectrum with an energy resolution of ***σ=0 eV***

PREDICTED NUCLEAR RECOIL SPECTRA – CaWO4

- Geant4 simulation based on TOUCANS [1] + FIFRELIN
- Mono-directionnal thermal neutron beam



Nuclear recoil spectrum in $CaWO_4$ – 5 eV energy resolution

- One prominent peak at 112 eV
  ⇒ could easily pop-up
- Second small peak at 160 eV
  ⇒ more difficult to get
- Third peak at ~80 eV
  ⇒ burried in multi-ɣ background
  ⇒ how to recover it ?

[1] L. Thulliez, B. Mom and E. Dumonteil, Nuclear Inst. and Methods in Physics Research A , 1051 (2023)

HOW TO ACCURATELY OPTIMIZE A THERMAL NEUTRON SOURCE ?

Neutron phyics in Geant4 Neutron-HP package
is now on-par with reference neutron transport codes such as MCNP, Tripoli-4, etc

Before 2021 : T. Koi (original developper) then E. Mendoza et D. Cano-Ott
E. Mendoza, D. Cano-Ott, T. Koi and C. Guerrero, IEEE Trans. Nucl. Science 61 (2014) 2357

2022 : L. Thulliez, C. Jouanne, and E. Dumonteil. Improvement of Geant4 Neutron-HP package: **From methodology to evaluated nuclear data library**. Nuclear Inst. and Methods Phys. Res., A 1027 (2022) 166187, doi: 10.1016/j.nima.2021.166187

2023 : M. Zmeskal, L. Thulliez, and E. Dumonteil. Improvement of Geant4 Neutron-HP package: **Doppler broadening of the neutron elastic scattering kernel**. Annals of Nuclear Energy, 192, 11 2023, doi: 10.1016/j.anucene.2023.109949

2024 : M. Zmeskal, L. Thulliez, P. Tamagno, E. Dumonteil, Improvement of Geant4 Neutron-HP package: **Unresolved Resonance Region description with Probability Tables**, already on arXiv:2404.16389 submit to Ann.of Nucl. Energy (2024),

On-going : Geant4 speed improvements

Marek ZMESKAL PhD thesis at CTU-Praha

IMPROVEMENTS OF GEANT4 NEUTRON-HP PACKAGE – STATUS BEFORE 2021

Neutron-HP package used to transport low energy neutrons En<20 MeV
⇒ What are the different «models» used to describe the neutron/target interaction?

4 eV — ~100 keV — En [MeV]

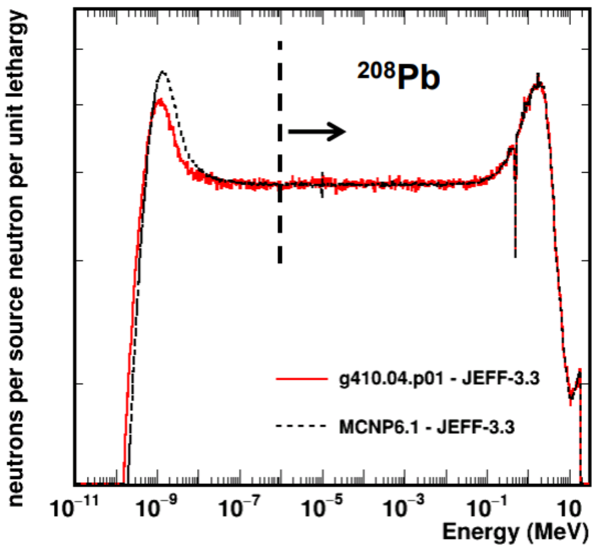
Target nuclei bound in molecules/crystal
⇒ Use of thermal scattering law (TSL)

Target nuclei as a free gas with a Maxwellian distribution
⇒ Use of free gas approximation

Point-like target nucleus
⇒ Use 0K cross-section

TSL not updated since ENDF-BVII.1
⇒ How to use updated and new materials from ENDF-BVIII.0 and JEFF-3.3?

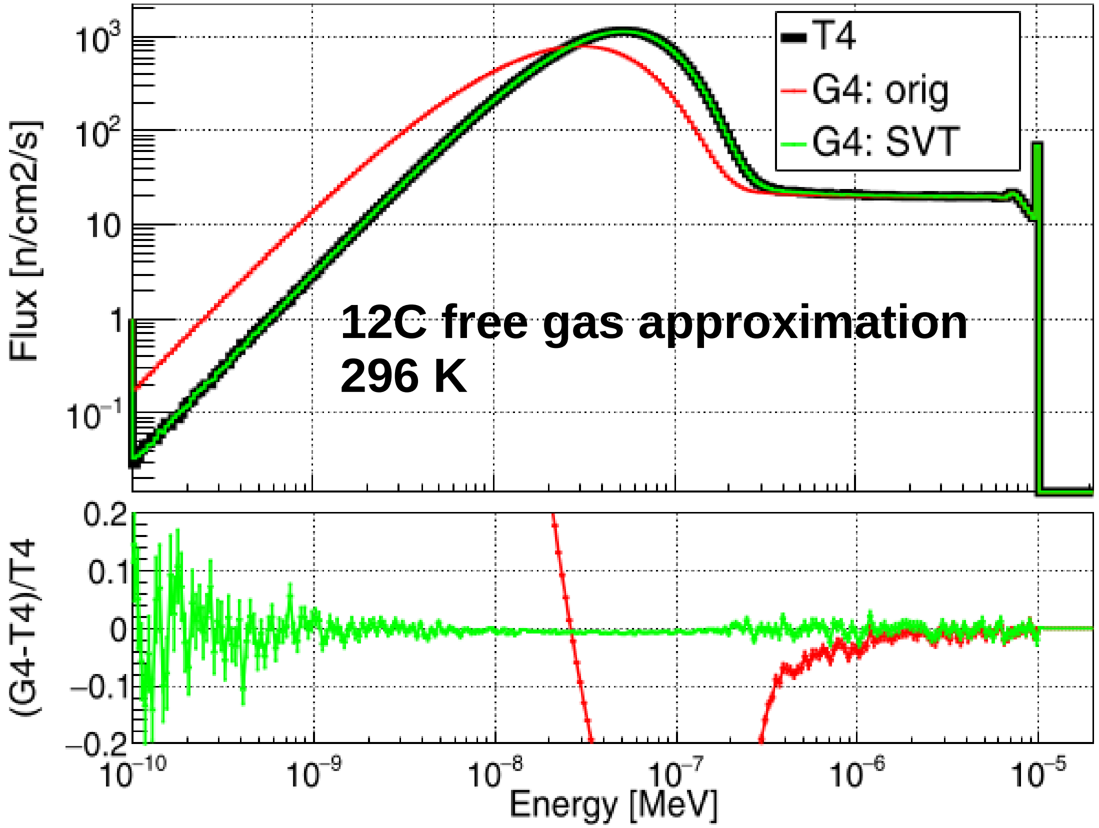
→ New TSL processing code ?
→ Discrepancies between reference neutron codes (MCNP, Tripoli-4) of ~20%



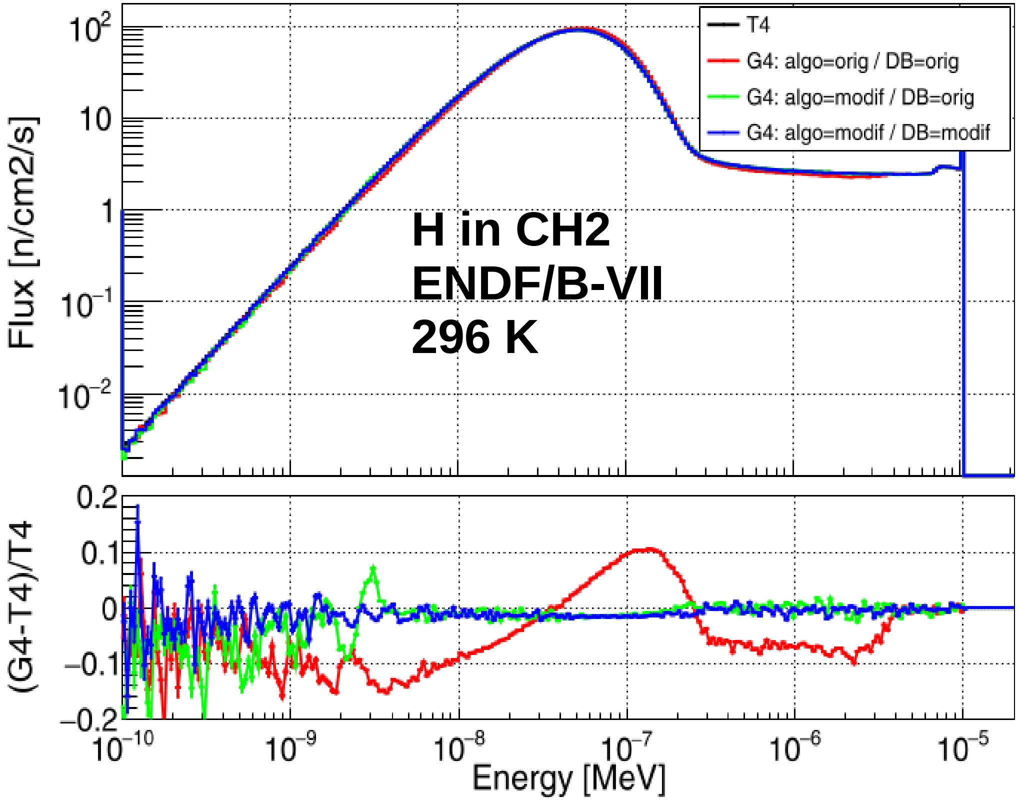
Talk from E. Mendoza Geant4 Hadronic meeting Feb. 2020

→ Free gas approximation implemented in Geant4 has trouble to reproduce MCNP below 1 eV
→ Problem in the algorithm?

IMPROVEMENTS OF GEANT4 NEUTRON-HP PACKAGE – ALGORITHMS



Correction of the Sampling of the Velocity of the Target (SVT) algorithm



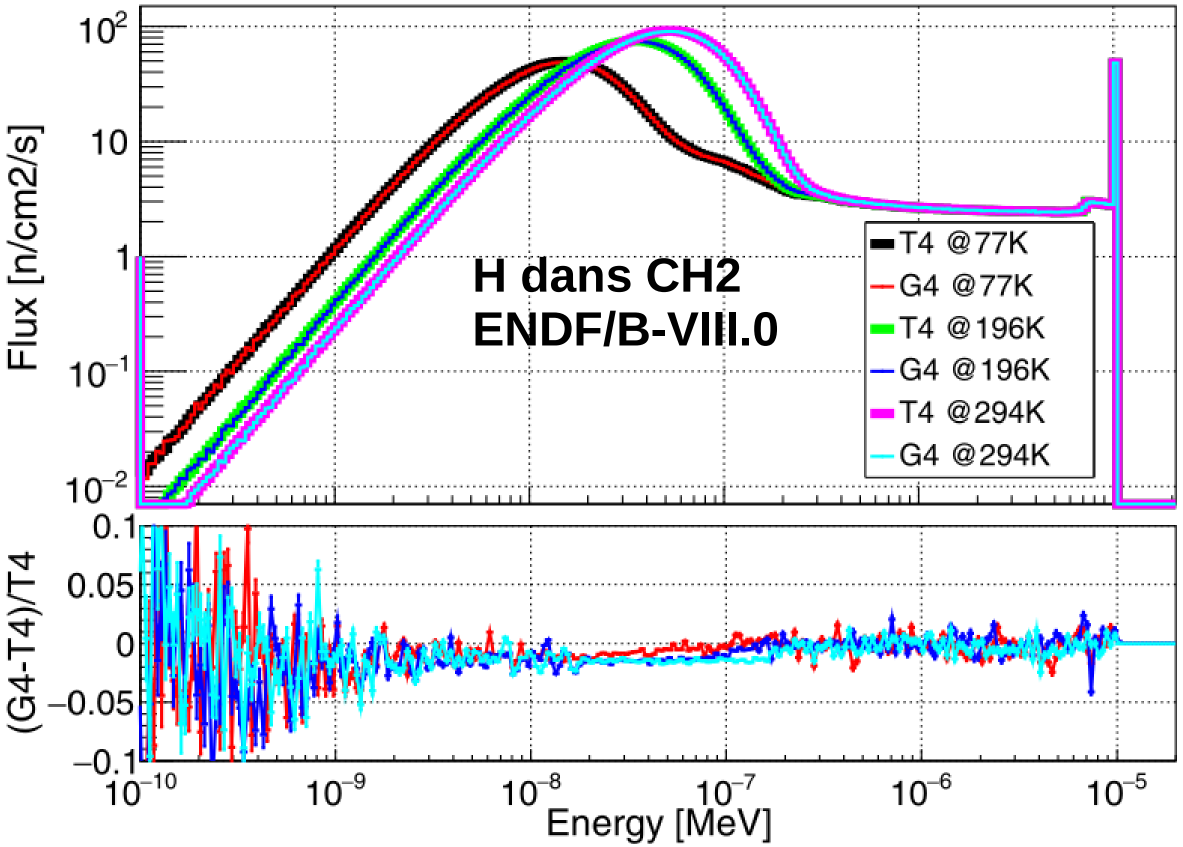
Fix the sampling of the final state of the elastic scattering

Geant4 agrees with reference neutron transport codes such as MCNP or Tripoli4 to better than 1 %

[1] L. Thulliez et al., Nuclear Inst. and Methods Phys. Res., A 1027 (2022) 166187

IMPROVEMENTS OF GEANT4 NEUTRON-HP PACKAGE – NEW TSL DATABASES

Up-to-date databases available in GEANT4 and validated with TRIPOLI4 to better than 1 % – since 2022



ENDF/BVII-1:
TSL_ENDFB71_HighPrecision
TSL_ENDFB71_LowPrecision *(only database before 2022)*

ENDF/BVIII-0:
TSL_ENDFB80_HighPrecision
TSL_ENDFB80_LowPrecision

JEFF-3.3:
TSL_JEFF33_HighPrecision
TSL_JEFF33_LowPrecision

Mix JEFF-3.3 and ENDF/BVIII-0, take all TSL data from JEFF-3.3 and the ENDF/BVIII-0 materials not in JEFF-3.3:
TSL_mix_JEFF33_ENDFB80_HighPrecision
TSL_mix_JEFF33_ENDFB80_LowPrecision

[1] L. Thulliez et al., Nuclear Inst. and Methods Phys. Res., A 1027 (2022) 166187

TOUCANS : a versatile Geant4 based Monte Carlo neutron *(not only)* transport code [1]

All the possibilities offered by Geant4 are leveraged

- Simulation of a setup *via* an input file

⇒ based on key / value

⇒ Easy coupling to other codes

→ multi-objective optimisation code FUNZ

⇒ Import CAD files

⇒ New variance reduction technics: AMS

- Validated with the reference neutron transport codes Tripoli4 and MCNP
- Experimentally qualified (2019 [2]/2022 [3])

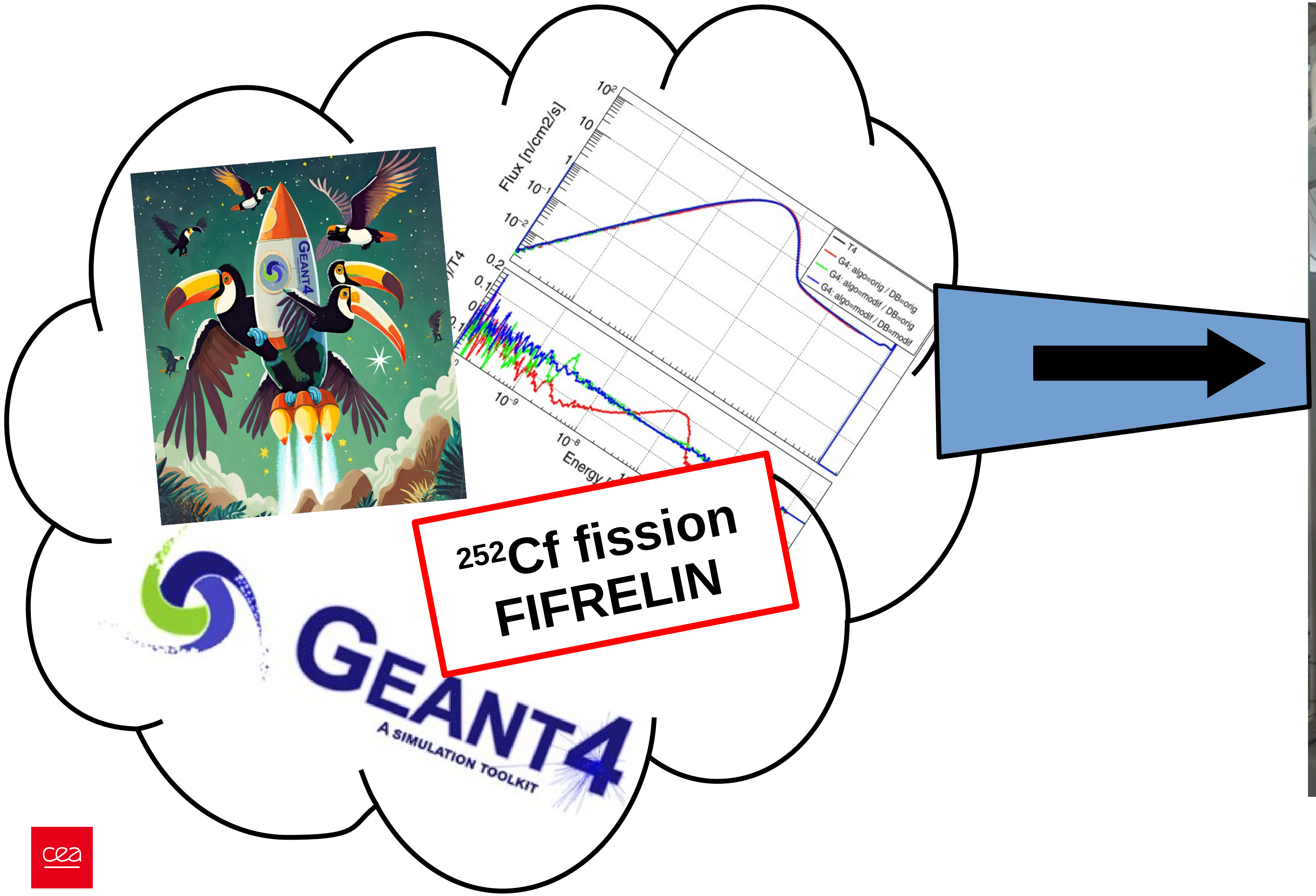
$ STRING	Moderator/Type	BOX			$
$ STRING	Moderator/Material	GRAPHITE			$
$ STRING	Moderator/MotherVolume	experimentalRoom			$
$ DOUBLELIST	Moderator/Dimensions	64	250	219	$
$ DOUBLELIST	Moderator/Position	147.25	-107.2	69.2	$

Soon will be open-source

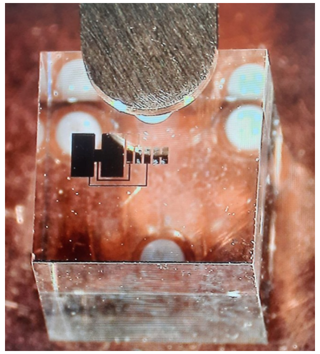
[1] L. Thulliez, B. Mom and E. Dumonteil, Nucl. Inst. and Methods in Phys. Res., A 1051 (2023) 168190
[2] L. Thulliez et al., EPJ Web of Conferences 239, 17011 (2020)
[3] J. Schwindling et al., Journal Of Neutron Research vol. 24, no. 3-4, pp. 289-298, 2022

CRAB PORTABLE THERMAL NEUTRON SOURCE

Thermal neutrons produced with a 3.7 MBq ^{252}Cf in a polyethylene and graphite moderator



FIRST MEASUREMENT CRAB / NUCLEUS COLLABORATIONS



NUCLEUS $CaWO_4$
cryo-detector
E_{th} = 50 eV
σ(E) = 6 eV

Detector in a copper box spring decoupled from cryostat vibration

More copper to thermalize the detector below 100 mK
TES transition ~10 mK

Thermal neutrons produced with a 3.7 MBq ^{252}Cf in a polyethylene and graphite moderator
⇒ 0.25 n_{th}/s on the cryo-detector

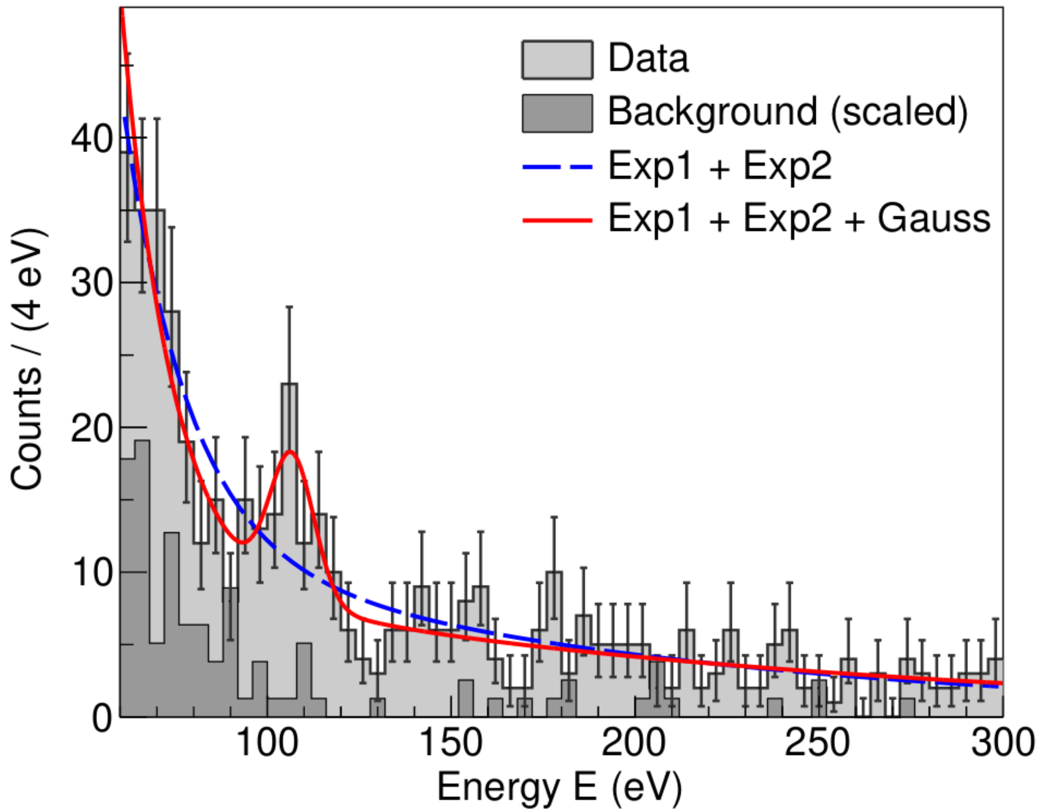
FIRST MEASUREMENT – RESULTS

→ Background data lifetime = 18.9 h
→ Source data lifetime = 40.2 h

Blind search peak

Test the presence of a peak

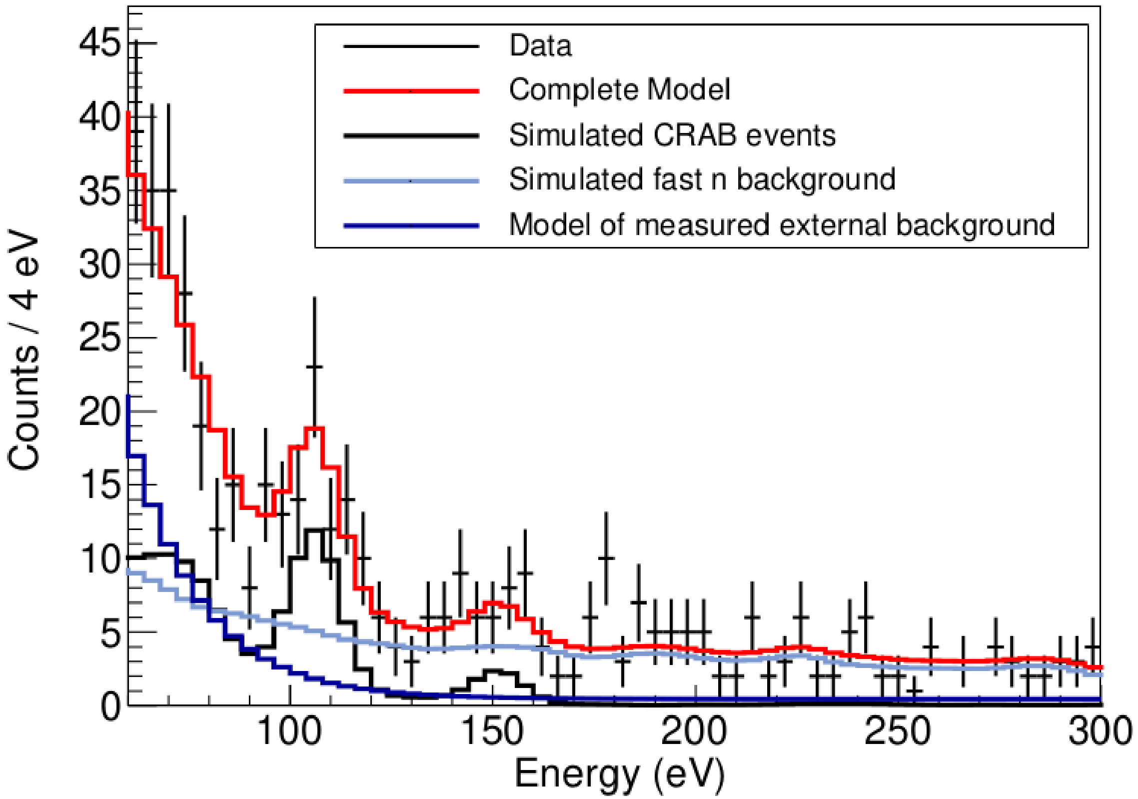
Background = 2 exponentials
Signal = gaussian



Presence of a peak
⇒ 3.1σ significance (2-sided)

Test the presence of nuclear recoils from neutron capture

Background = exponential fit to bkgd data
Signal = GEANT4 + FIFRELIN



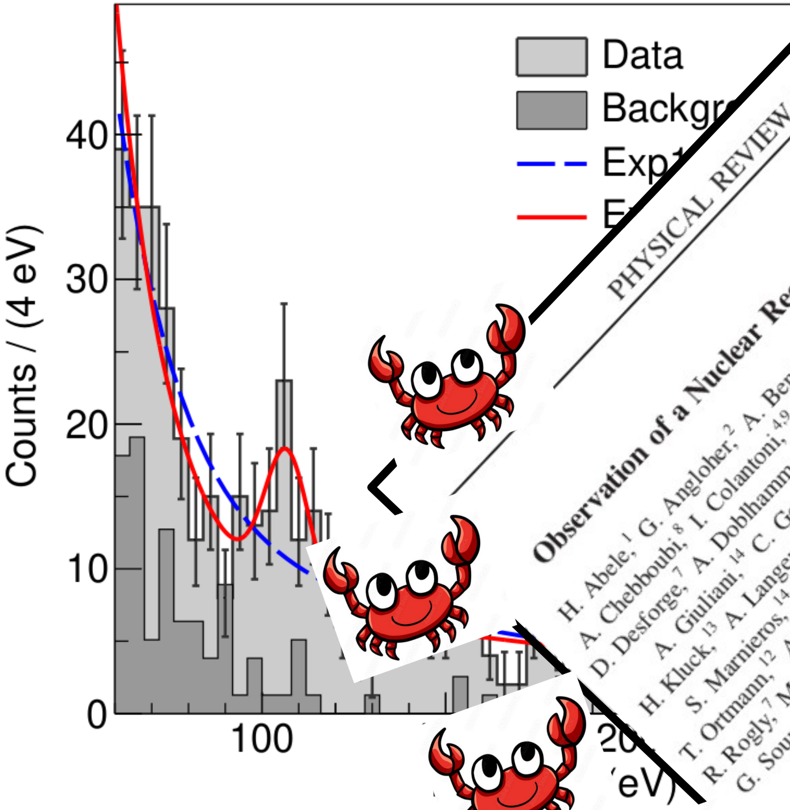
Presence of nuclear recoils from neutron capture
⇒ 6σ significance (2-sided)
⇒ χ^2/NDF = 58.09/59

FIRST MEASUREMENT – RESULTS

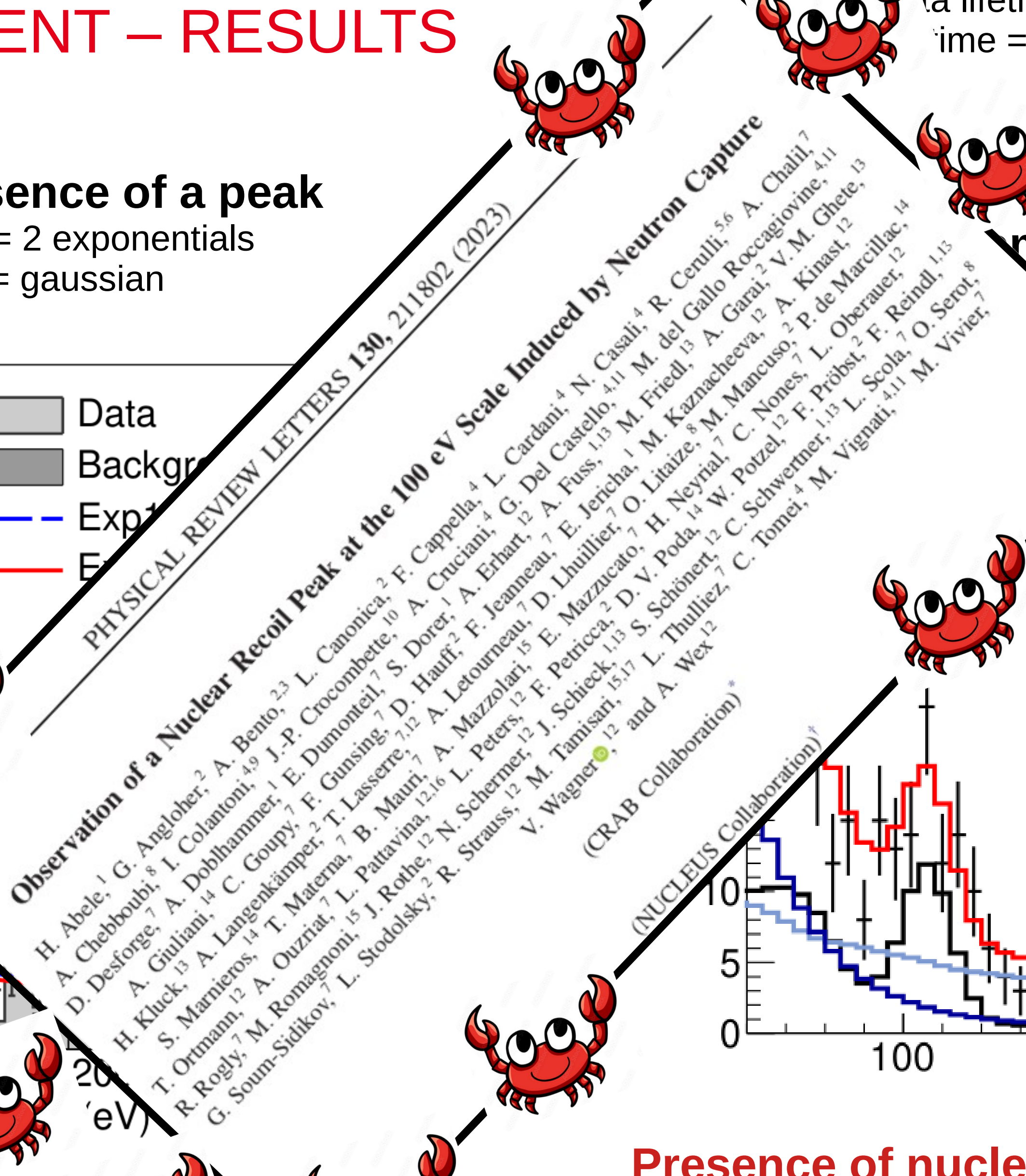
ta lifetime = 18.9 h
ime = 40.2 h

Blind search peak

Test the presence of a peak
Background = 2 exponentials
Signal = gaussian



Presence of a peak
⇒ **3.1σ significance (2**


PHYSICAL REVIEW LETTERS 130, 211802 (2023)

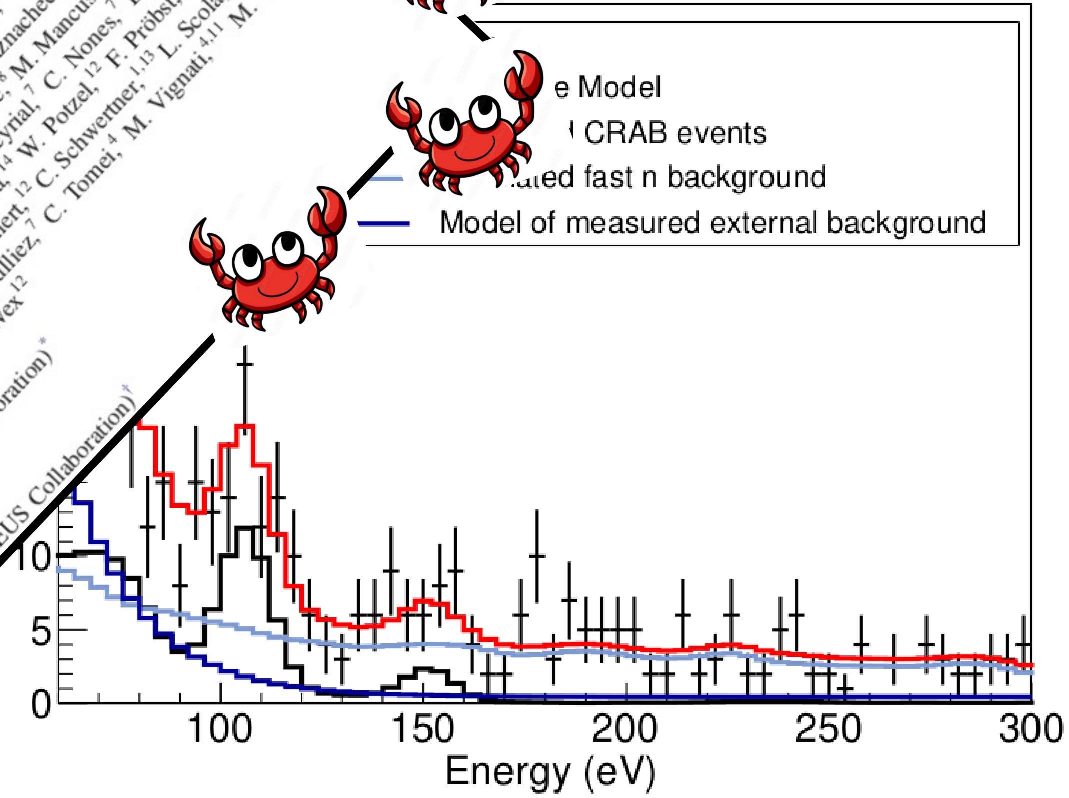
Observation of a Nuclear Recoil Peak at the 100 eV Scale Induced by Neutron Capture

H. Abele,[1] G. Angloher,[2] A. Bento,[2,3] L. Canonica,[2] F. Cappella,[4] L. Cardani,[4] N. Casali,[4] R. Cerulli,[5,6] A. Chalil,[7] A. Chebboubi,[8] I. Colantoni,[4,9] J.-P. Crocombette,[10] A. Cruciani,[4] G. Del Castello,[4,11] M. del Gallo Roccagiovine,[4,11] D. Desforge,[7] A. Doblhammer,[1] E. Dumonteil,[7] S. Dorer,[1] A. Erhart,[12] A. Fuss,[1,13] M. Friedl,[13] A. Garai,[2] V. M. Ghete,[13] A. Giuliani,[14] C. Goupy,[7] F. Gunsing,[7] D. Hauff,[2] F. Jeanneau,[7] E. Jericha,[1] M. Kaznacheeva,[12] A. Kinast,[12] H. Kluck,[13] A. Langenkämper,[2] T. Lasserre,[7,12] A. Letourneau,[7] D. Lhuillier,[7] O. Litaize,[8] M. Mancuso,[2] P. de Marcillac,[14] S. Marnieros,[14] T. Materna,[7] B. Mauri,[7] A. Mazzolari,[15] E. Mazzucato,[7] H. Neyrial,[7] C. Nones,[7] L. Oberauer,[12] T. Ortmann,[12] A. Ouzriat,[7] L. Pattavina,[12,16] L. Peters,[12] F. Petricca,[2] D. V. Poda,[14] W. Potzel,[12] F. Pröbst,[2] F. Reindl,[1,13] R. Rogly,[7] M. Romagnoni,[15] J. Rothe,[12] N. Schermer,[12] J. Schieck,[1,13] S. Schönert,[12] C. Schwertner,[1,13] L. Scola,[7] O. Serot,[8] G. Soum-Sidikov,[7] L. Stodolsky,[2] R. Strauss,[12] M. Tamisari,[15,17] L. Thulliez,[7] C. Tomei,[4] M. Vignati,[4,11] M. Vivier,[7] V. Wagner,[12] and A. Wex[12]

(CRAB Collaboration)*

(NUCLEUS Collaboration)†

ence of nuclear recoils
m n n capture
tial fit to bkgd data
+ FIFRELIN

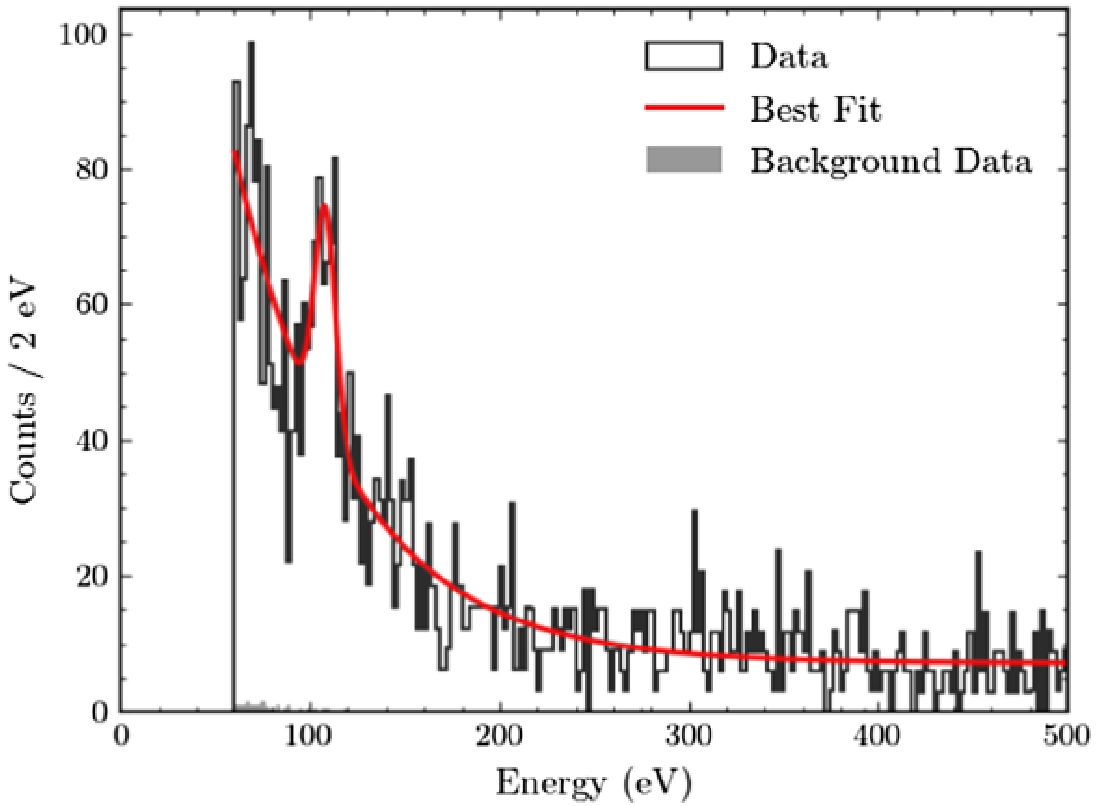


Presence of nuclear recoils from neutron capture
⇒ **6σ significance (2-sided)**
⇒ **χ^2/NDF = 58.09/59**

FIRST MEASUREMENT CONFIRMED BY OTHERS !

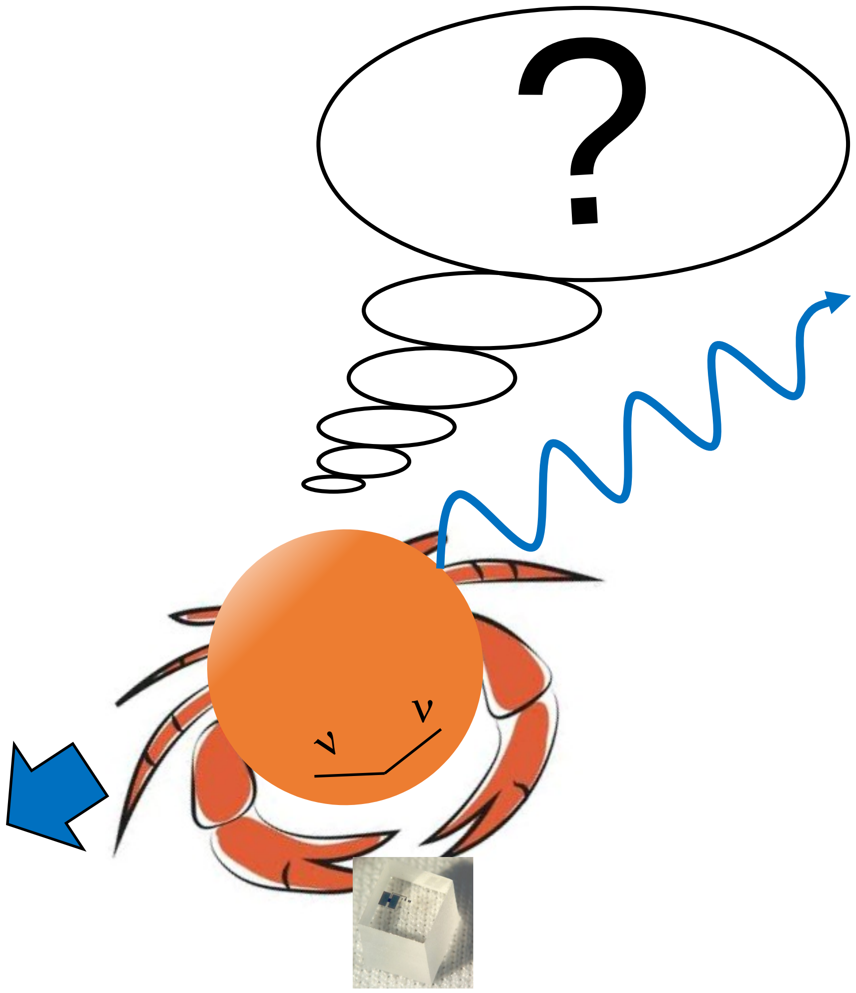
CRESST = dark matter with $CaWO_4$ cryo-detector
→ confirmation of our first CRAB signal with 3 detectors

G. Angloher et al. (CRESST collaboration) Phys. Rev. D 108, 022005 (2023)



CRAB has already a big impact in the dark matter and neutrino communities !

WHAT IS NEXT ?



STUDIED OTHER CRYO-DETECTOR MATERIALS

Detector	Target nucleus	E_γ [keV]	FOM $= Y_{abunance} \times \sigma_{(n,\gamma)} \times I_{decay}$	Nuclear recoil [eV]
Al_2O_3 *MINER* *NUCLEUS*	^{27}Al ^{27}Al	7693 + 30.6 7724	79 616	1135.7 1144.8
Si *SuperCDMS* *DAMIC SENSEI* *Skipper-CCD* *CONNIE*	^{28}Si ^{28}Si	7200 + 1273 8474	116 36	990.4 1330.1
Ge *EDELWEISS* *RICOCHET*	^{74}Ge ^{74}Ge ^{73}Ge ^{70}Ge ^{70}Ge ^{70}Ge	6253 + 253 6506 8733 + 868+ 596 6708 + 708 6117 + 1299 7416	220 54 117 287 261 122	280.6 303.2 561.8 344.3 296 416.2
$CaWO_4$ *CRESST* *NUCLEUS*	^{186}W ^{183}W ^{182}W	~5300 + ~200 7411 6191	~4400 823 7506	~80 160.3 112.5

FIFRADINA datasets available : https://doi.org/10.5281/zenodo.7936552
Fifrelin4Geant4 classes is open-source : https://doi.org/10.5281/zenodo.7933381
https://gitlab.com/lthullie/fifrelin4geant4

CRAB Phase 2 – HIGH PRECISION MEASUREMENTS (in 2024)

TRIGA Mark-II nuclear reactor (250 kW)
TU-Wien – Atominstitut

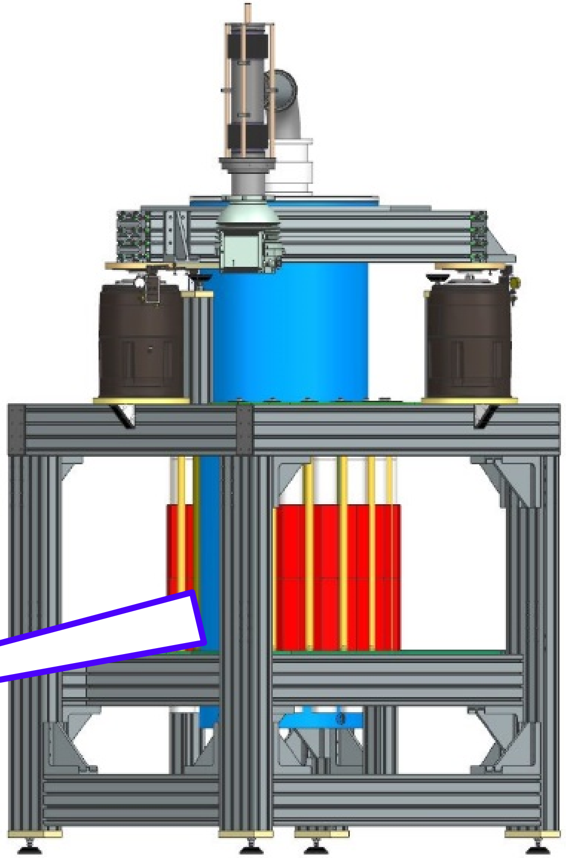
Thermal neutron beam line

$10\,000\ n_{th}/cm^2/s$

$100\ n_{th}/s$

Monochromator
Graphite crystal

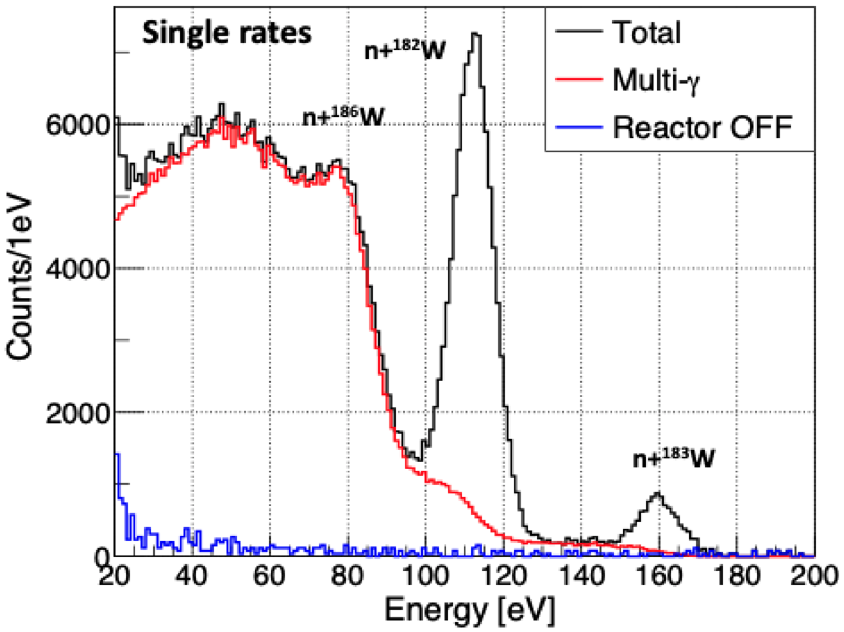
Wet cryostat
Oxford kelvinox 400



Array of 28 hexagonal BaF2 gamma detectors (2” x 6”)

STUDY OF THE DETECTOR LINEARITY

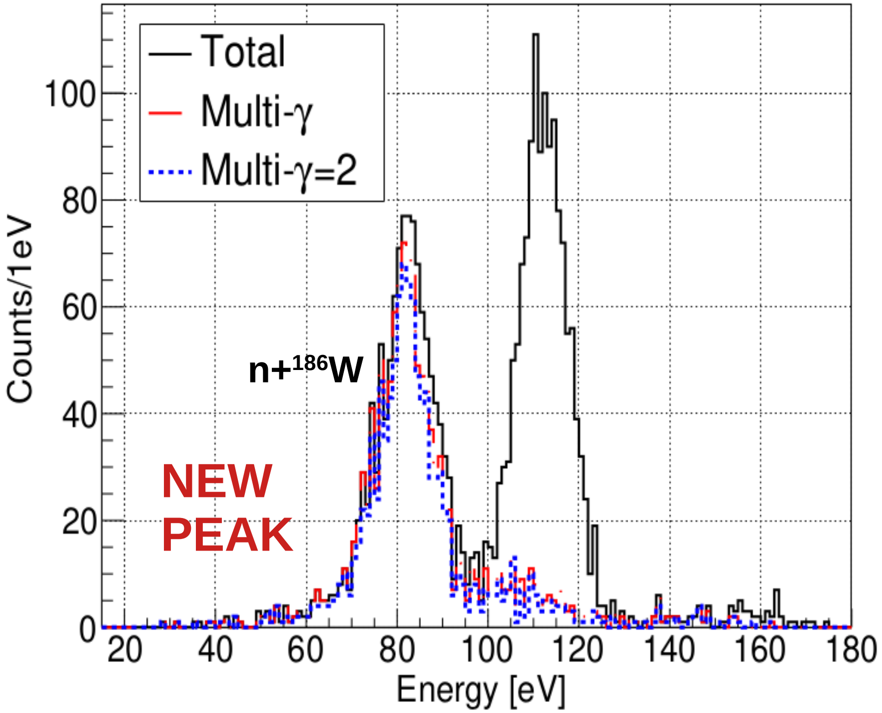
Single spectrum with high statistics



~6 full days of data taking
⇒ sub- % statistical precision

ɣ-coincidence !

Gamma tagging is a powerful tool



Recoil spetrum after gamma tagging with $E_ɣ$=5.5 ±0.2 MeV

ɣ-tagging is a powerful tool to get a **3rd peak at 80 eV** for CaWO4
⇒ **study of the detector linearity !**

CRAB SENSITIVE TO CRYSTAL DEFECT CREATIONS

Gabrielle Soum-Sidikov PhD thesis
J.-P. Crocombette (CEA/DES)

How to quantify the energy stored in the crystal lattice ?

Machine learning inter-atomic potential

Training database from DFT calculations (VASP)

MiLaDy

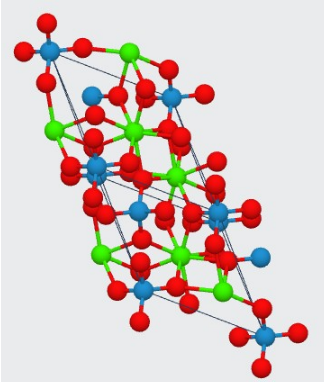
A.M. Goryaeva, J.-B. Maillet, M.-C. Marinica
Comp.Mater.Sci.166:200 (2019)

+

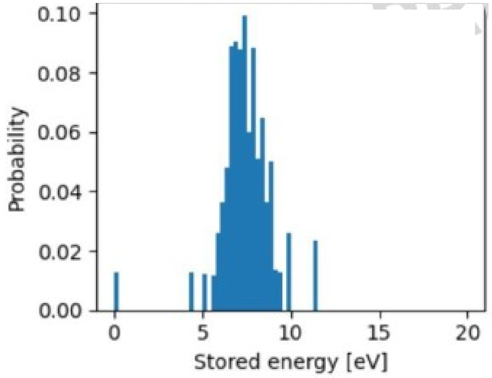
Molecular dynamics simulations

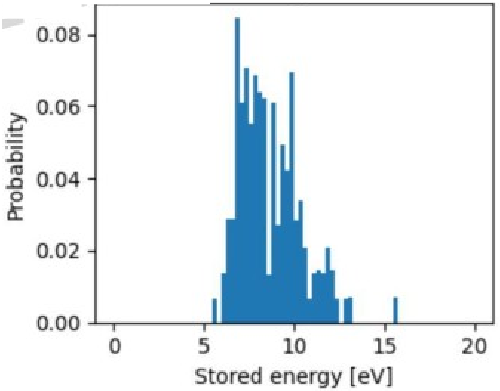
80 A size box with 50000 atoms
Simulation time ~8 ps
Zero point energy taken into account

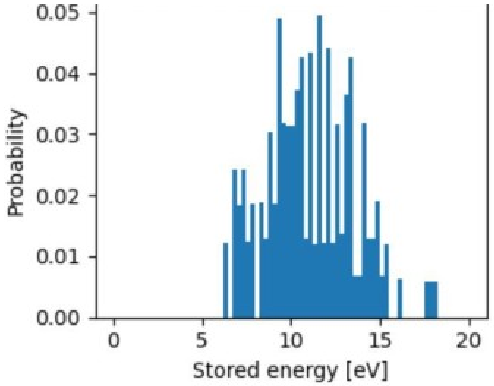
LAMMPS



E_{recoil} [ev]	81	112	160
E_{stored} [eV]	7.4	8.9	11.0
If linear E_{stored} [eV]	7.4	10.23	14.6





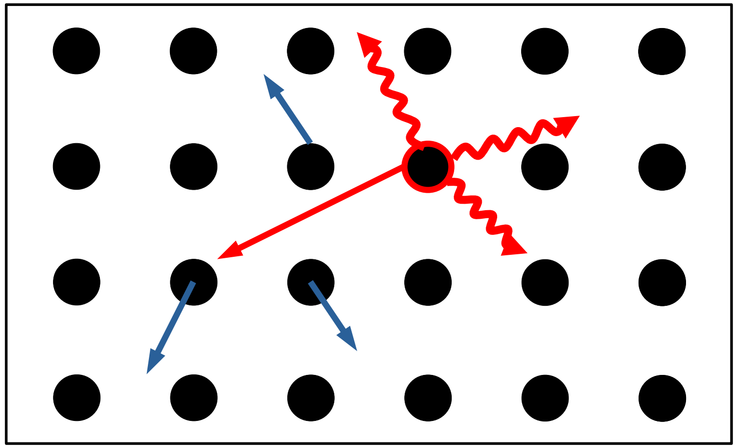


⇒ Unique sensitivity to single crystal defect with the very low E recoils in CaWO4

TIMING EFFECT – EXTREME HYPOTHESES

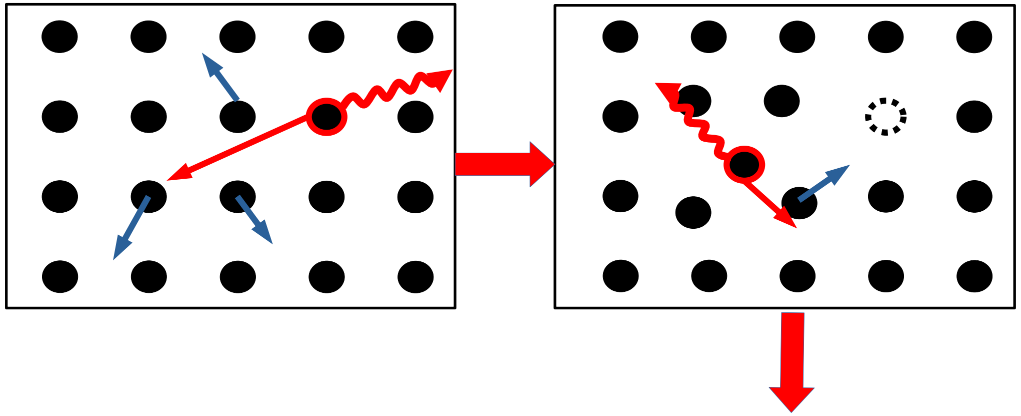
Fast hypothesis

$\tau_{recoil} \gg \tau_{cascade}$ $E_{recoil} = \left(\sum_i \vec{p}_i\right)^2 / 2M$



Slow hypothesis

$\tau_{recoil} \ll \tau_{cascade}$ $E_{recoil} = \sum_i E_{recoil,i} = \sum_i p_i^2 / 2M$



etc ...

TIMING EFFECT – EXTREME HYPOTHESES

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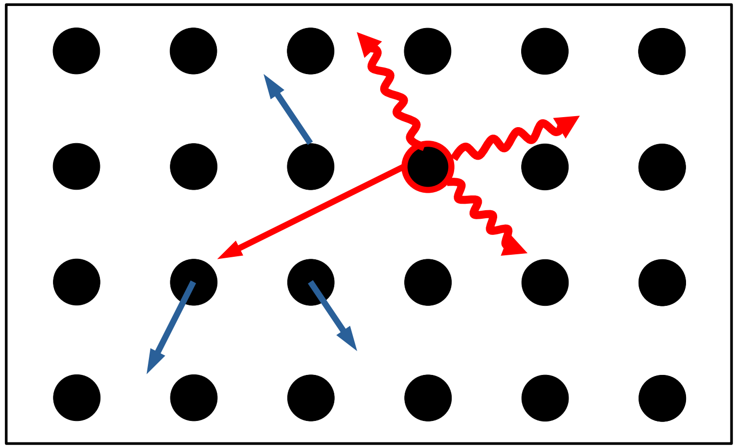
$\tau_{recoil} \gg \tau_{cascade}$ $\qquad E_{recoil} = \left(\sum_i \vec{p}_i\right)^2 / 2M$

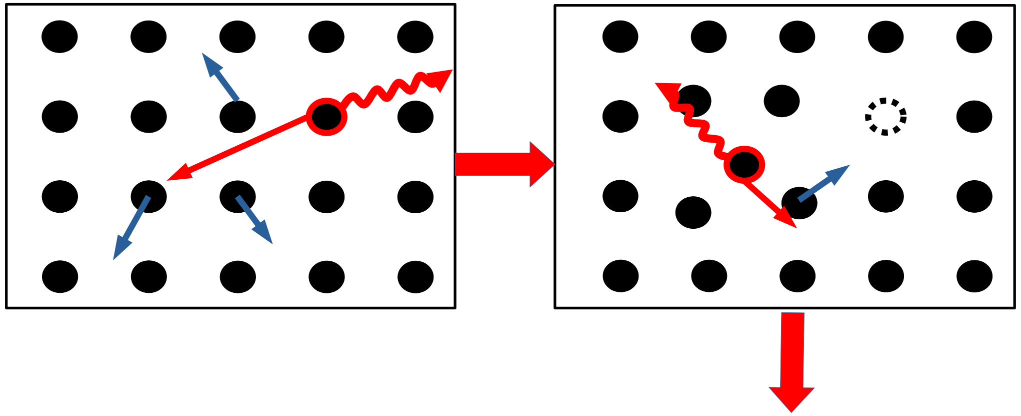


Reality in between

Coupling FIFRELIN and IRADINA [1]

Slow hypothesis

$\tau_{recoil} \ll \tau_{cascade}$ $\qquad E_{recoil} = \sum_i E_{recoil,i} = \sum_i p_i^2 / 2M$



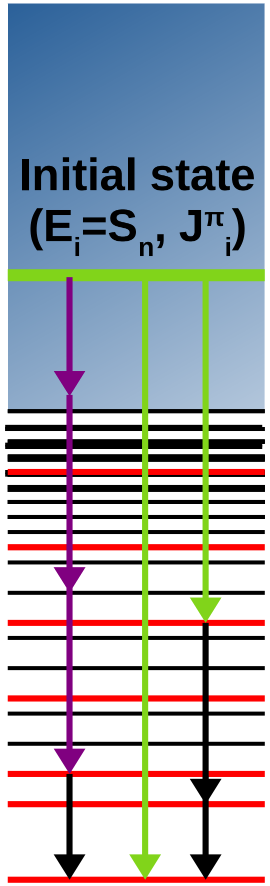
etc ...

[1] G. Soum-Sidikov et al., Study of collision and γ-cascade times following neutron-capture processes in cryogenic detectors, Phys. Rev. D 108, 072009 (2023)

FIFRELIN + IRADINA = FIFRADINA [1]

Gabrielle SOUM PhD thesis at CEA

FIFRELIN : Fission fragment de-excitation code



Level scheme

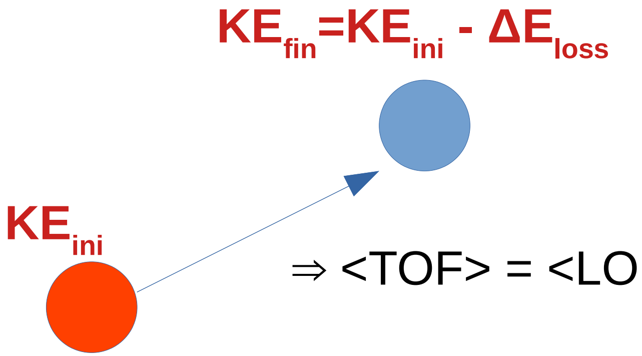
- Continuum
- Sampled levels
- RIPL-3 levels

Transition probability

- EGAF (primary) transition
  Timing : Weisskopf estimate
- RSF transition
  Timing : radiative partial width
- RIPL-3 transition
  Timing :
  RIPL-3 if known
  else Weisskopf estimate

IRADINA (similar to SRIM):
Binary Collision Approximation code
Ingredients: → amorphous structure
→ atoms described as a free gas

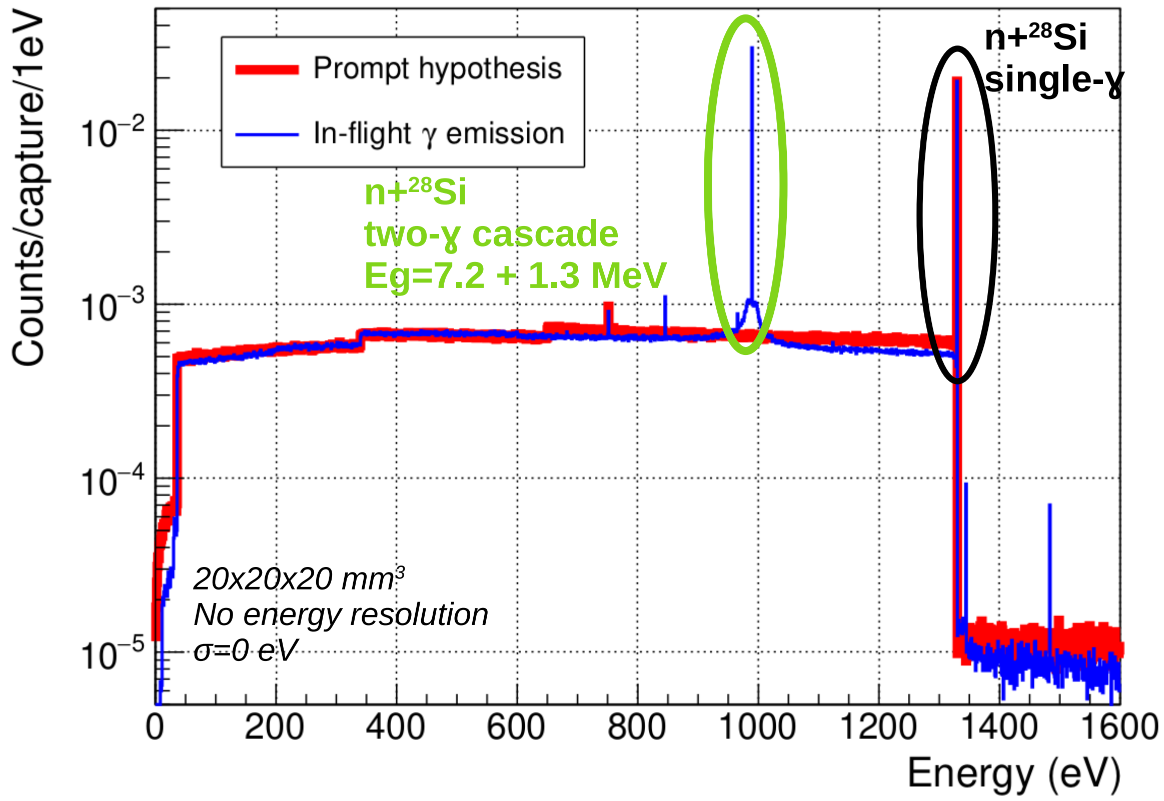
Sample a target (and collision parameters)

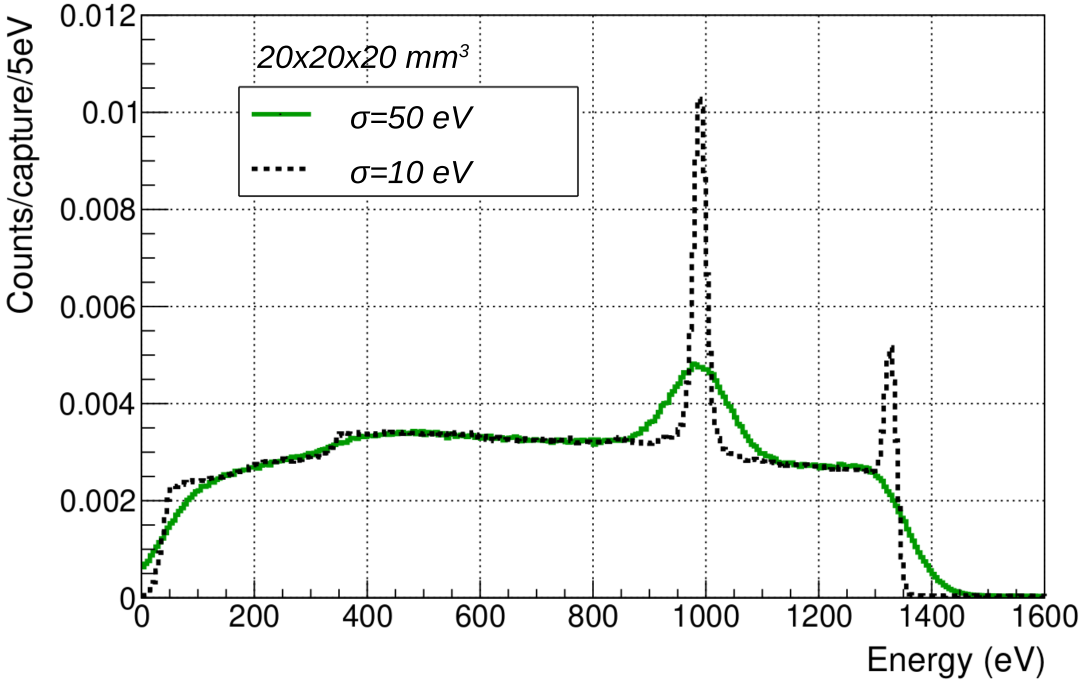


⇒ <TOF> = <LOF> / <V>

[1] G. Soum-Sidikov et al., Study of collision and γ-cascade times following neutron-capture processes in cryogenic detectors, Phys. Rev. D 108, 072009 (2023)

TIMING EFFECTS – SILICON





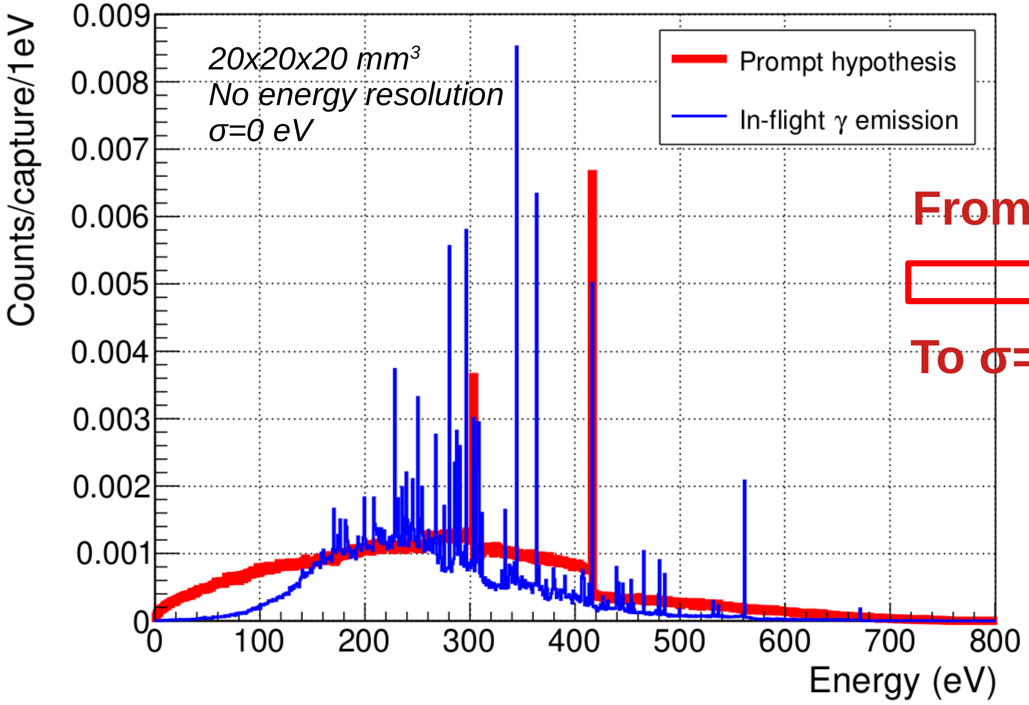
Most of the half-live are in the databases (collective effects taken into account)

Two-ɣ cascade robust against poorer energy resolution

In-flight gamma emission ⇒ probe nucleus de-excitation time
⇒ sensitive to directionnality effects

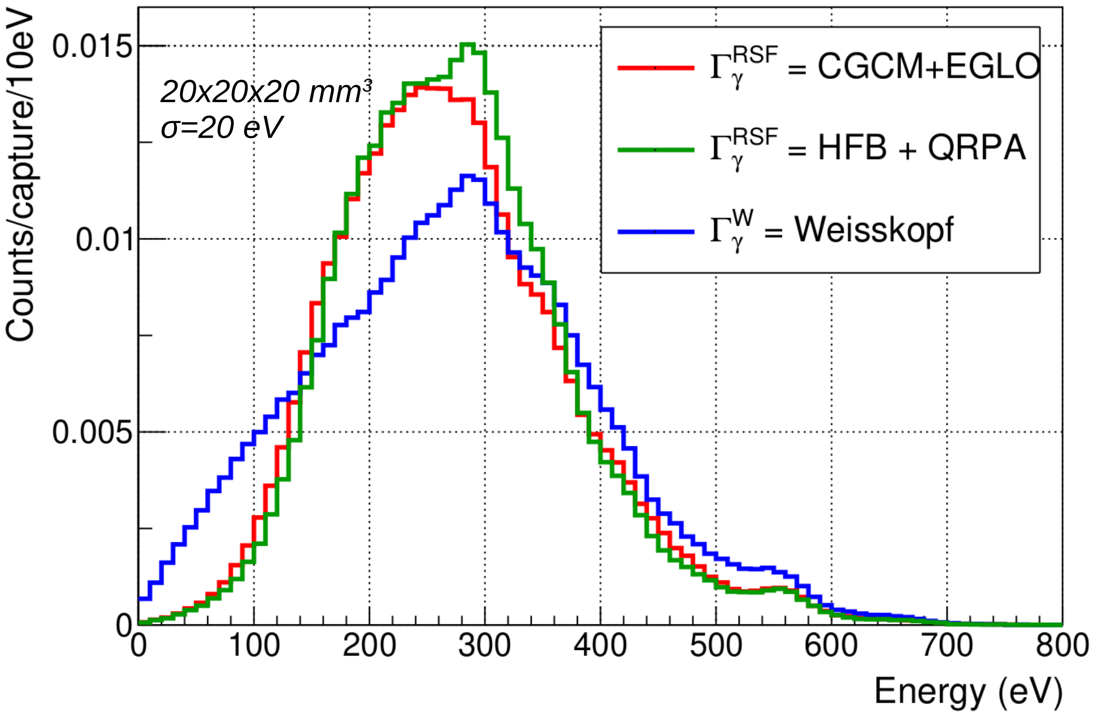
[1] G. Soum-Sidikov et al., Study of collision and γ-cascade times following neutron-capture processes in cryogenic detectors, Phys. Rev. D 108, 072009 (2023)

TIMING EFFECTS – GERMANIUM



From σ=0 eV

To σ=20 eV



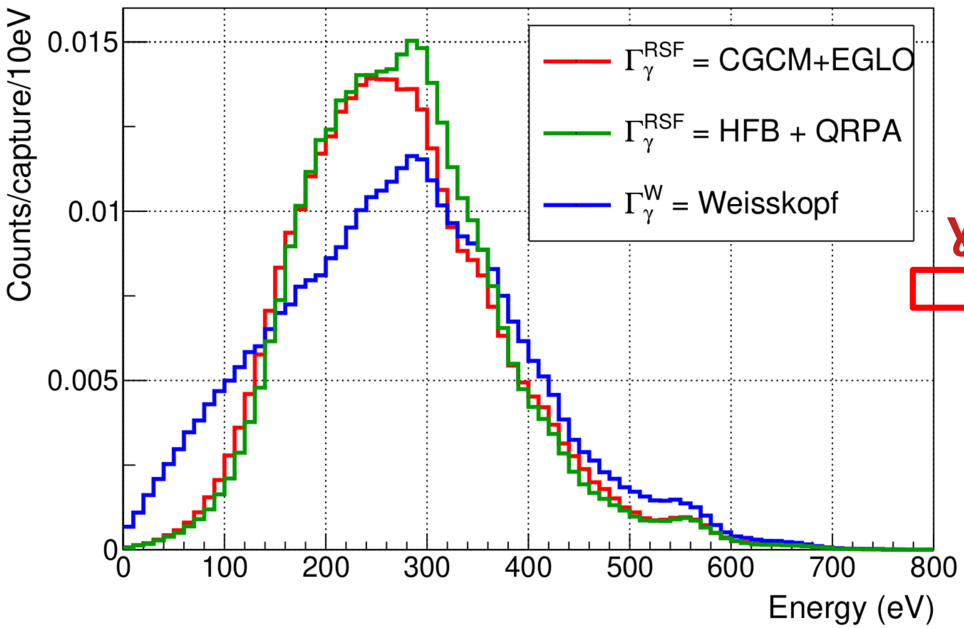
In-flight γ emission ⇒ more calibration peaks

Recoil energy spectrum sensitive to nuclear models !
⇒ could help set constraints on models

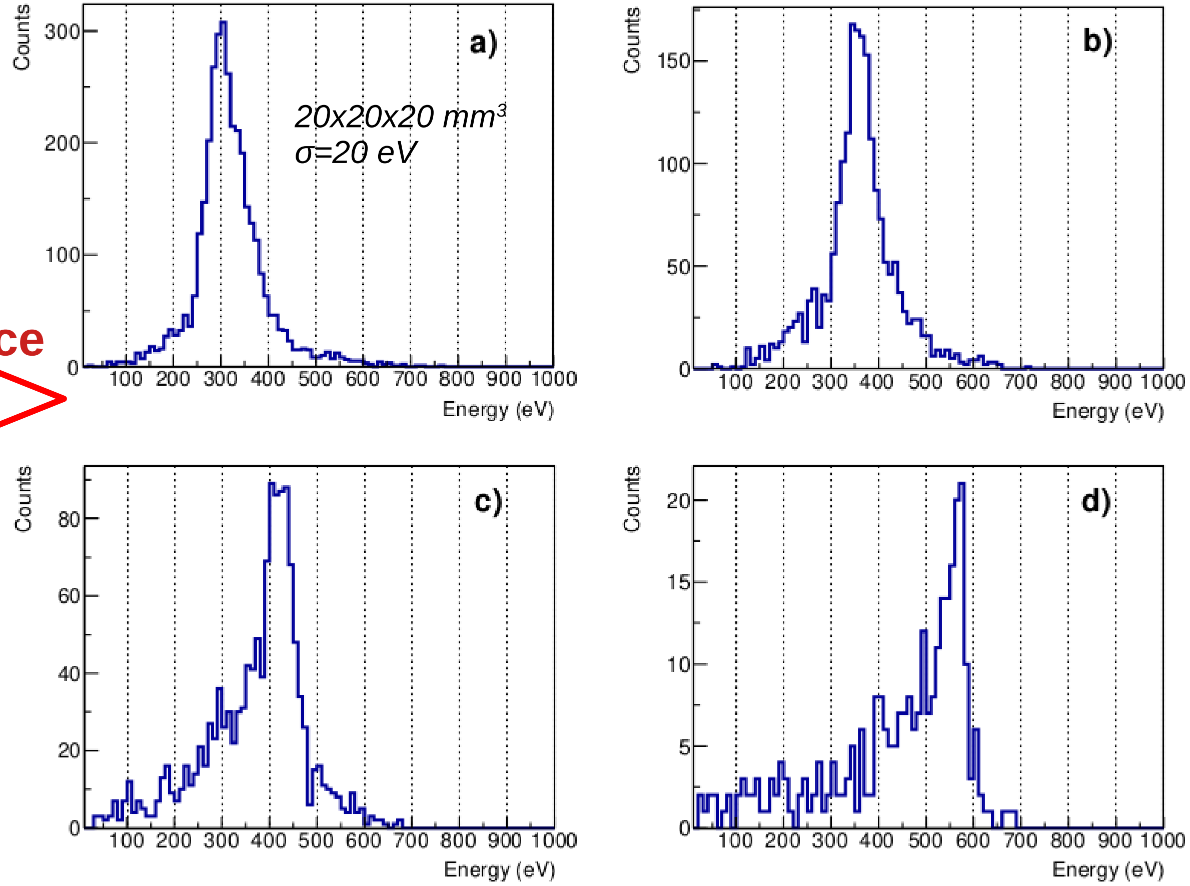
- **With timing effects, more calibration peaks !**
- **Timing modelling sensitive to the underlying nuclear physics**
  ⇒ test of nuclear models
- **Resolution is a critical parameter**

[1] G. Soum-Sidikov et al., Study of collision and γ-cascade times following neutron-capture processes in cryogenic detectors, Phys. Rev. D 108, 072009 (2023)

TIMING EFFECTS – GERMANIUM



γ-coincidence



Resolution is a critical parameter
BUT gamma coincidence allows to overcome this limitation !

[1] G. Soum-Sidikov et al., Study of collision and γ-cascade times following neutron-capture processes in cryogenic detectors, Phys. Rev. D 108, 072009 (2023)

CONCLUSIONS

- **CRAB method** promising for a **sub-kev calibration** of the majority of cryo-detector materials in DM/CEvNS communities currently used (**$CaWO_4$**, **Ge**, **Si**, **Al_2O_3**)

- Successfull first measurement with a NUCLEUS $CaWO_4$ and a portable neutron source
  - ⇒ presence of a peak at ~112 eV with 3.1σ significance (confirmation by the CRESST collaboration)
  - ⇒ presence of nuclear recoils with 6σ significance : agreement between data and GEANT4-FIFRELIN

- CRAB with **gamma tagging** is a powerul tool to **increase S/B** and **access lower energy** recoils, study the linearity of the bolometer response and tag the direction of the recoil (directionality)

CODES / DATA TO TAKE AWAY

- Liquid scintillator experiments (STEREO collaboration) :
  Gadolinium thermal neutron capture **FIFRELIN** dataset : https://doi.org/10.5281/zenodo.6861341

- Cryo-detectros experiments (CRAB collaboration):
  W / **Ge** / **Al** / **Si** thermal neutron capture **FIFRADINA** datasets : https://doi.org/10.5281/zenodo.7936552

- **Fifrelin4Geant4** classes is open-source (STEREO/CRAB): https://doi.org/10.5281/zenodo.7933381
  https://gitlab.com/lthullie/fifrelin4geant4

- All the improvements of the Neutron-HP package are in the latest Geant4 release !
  ⇒ stay tune for the incoming speed improvements

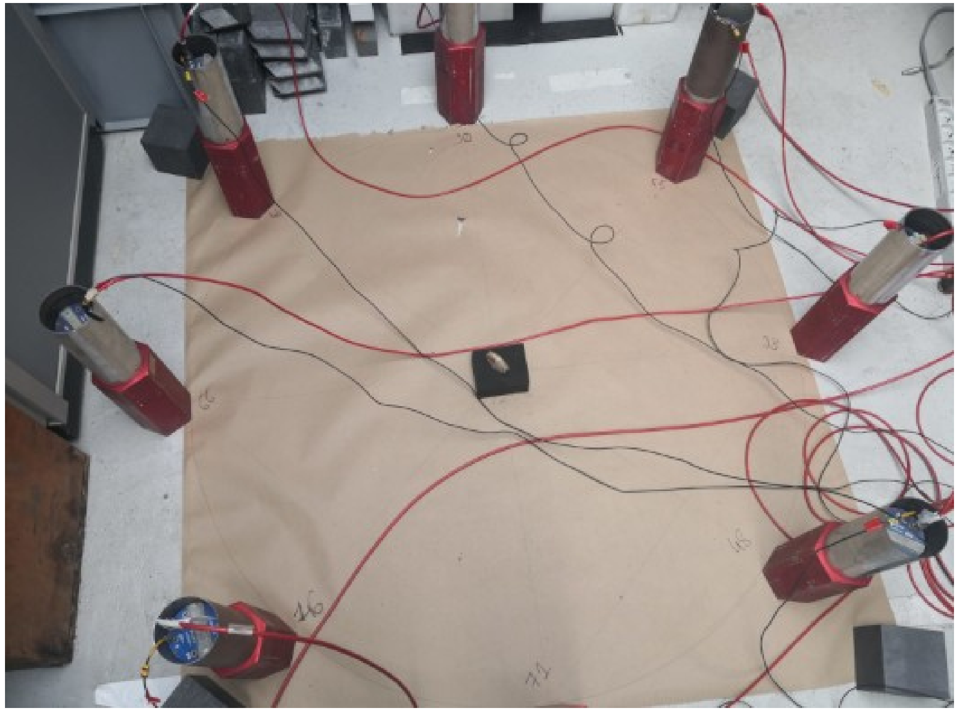
- FIFRELIN executable will be released in 2024 *via* the NEA website: https://www.oecd-nea.org/

Do not hesitate to contact us if you want to study specific isotopes !

PERSPECTIVES

- CRAB High Precision measurements at the TRIGA-Mark II reactor at TU-Wien in 2024 with CaWO4
- Promissing case of Ge detectors. Impact of crystal defects to be calculated soon.
- On the long term, it will be a facility available to the community to characterise their detectors

Wet cryostat @TUM



Gamma tagging development @CEA-Saclay

Neutron beam line construction and characterisation @TU-Wien

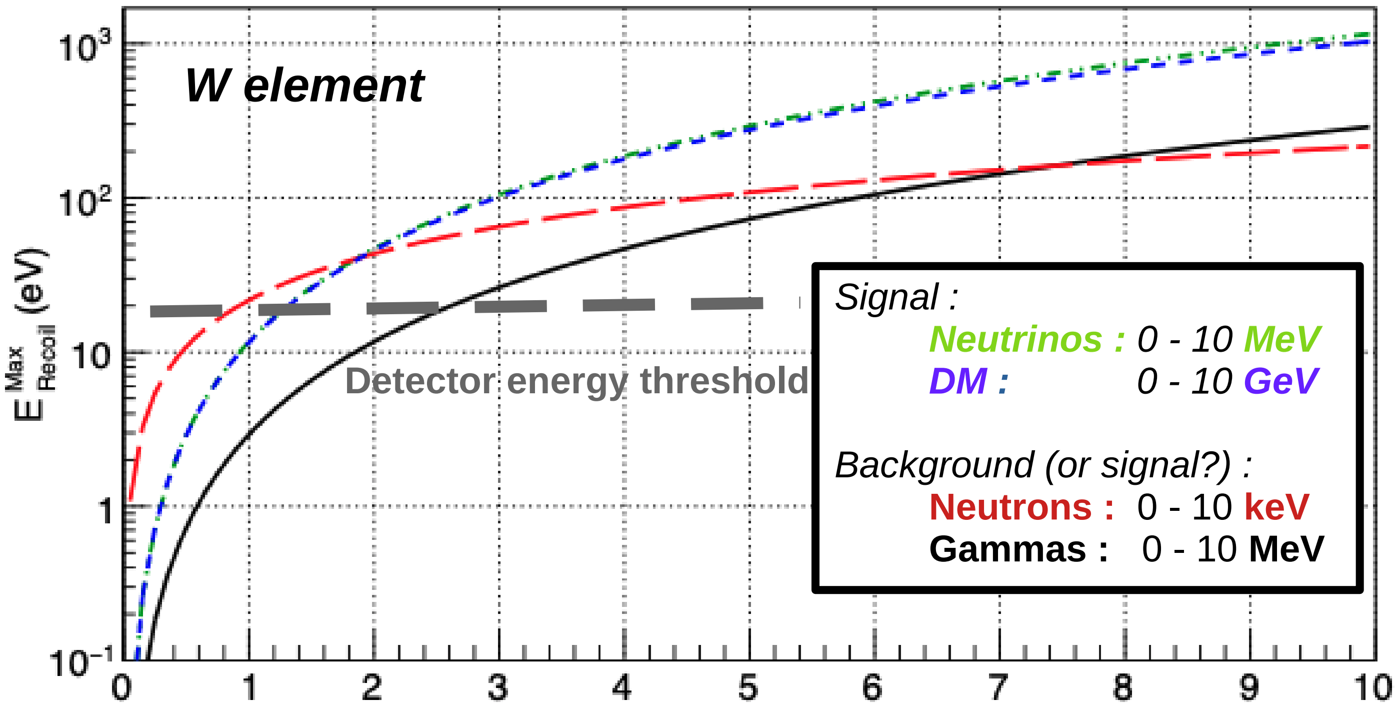
THANK YOU

The CRAB collaboration

NEED SUB-keV CALIBRATION METHODS

State-of-the-art calibration techniques :

- mainly electron recoils for *in-situ* calibration with LED [1], XRF source BUT surface calibration
- alphas BUT surface calibration
- epithermal/fast neutrons produced at accelerator are limited by TOF and angular precisions



What about thermal neutrons ?

- gammas from (n,ɣ) reaction

First indirect measurement by Jones and Kramer [2]

[1] L. Cardini et al., Eur. Phys. J. C 81 (2021) 7, 636
[2] K.W. Jones and H.W. Kraner, Phys. Rev. A, 11 4, 1975