

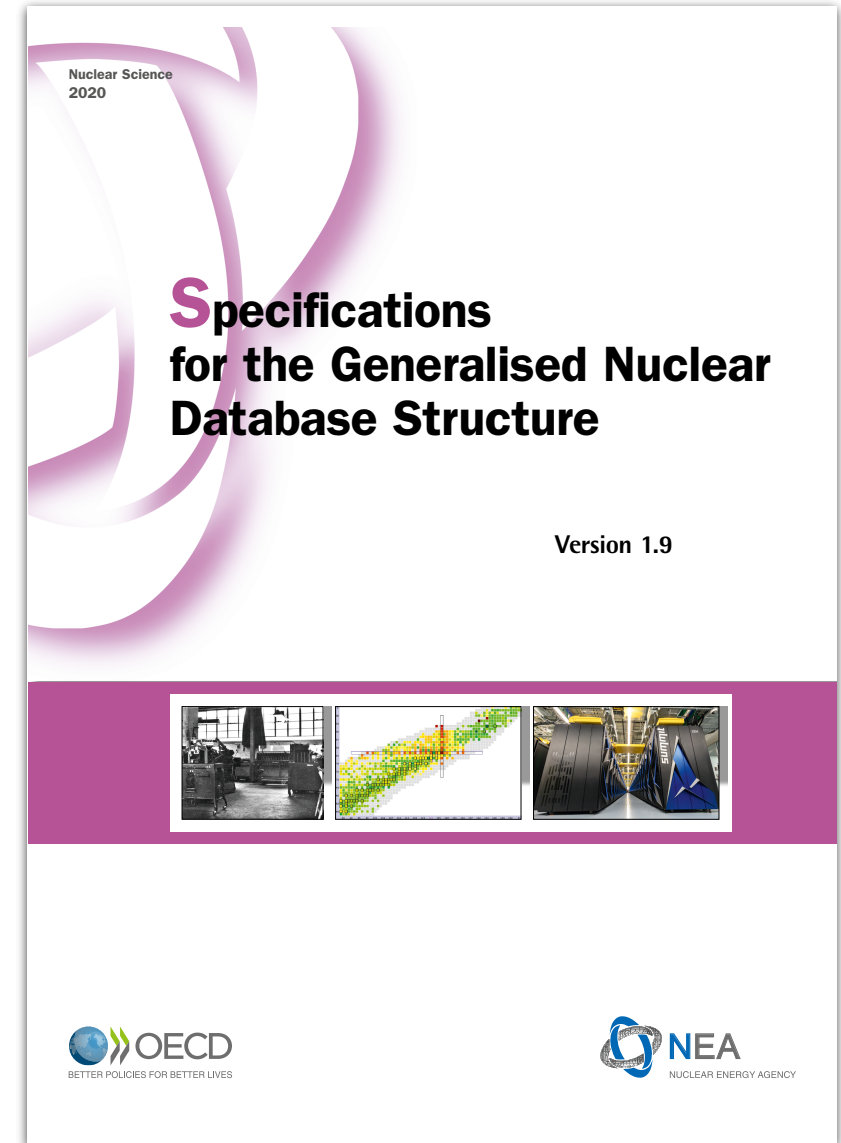
**David Brown (BNL)**

# **GNDS Expert Group Report**

**CSEWG Meeting, Virtual Nuclear Data Week 2020  
30 Nov. 2020**

# GNDS-1.9 specifications published Summer 2020

- Specifications: <https://oecd-nea.org/download/wpec/documents/7519-GNDS.pdf>
- XML Schema for GNDS-1.9: <https://www.oecd-nea.org/download/wpec/gnds/gnds.xsd>
- GNDS Webinar: <https://www.youtube.com/watch?v=h9Byrkxr8LE&feature=youtu.be>



# Thank you webinar participants

<https://www.youtube.com/watch?v=h9Byrkxr8LE&feature=youtu.be>

The NEA hosted an expert roundtable webinar on GNDS on 8 July 2020. The discussion was moderated by William D. Magwood, IV, NEA Director-General and Dr David Brown (BNL), Chair of the NEA Expert Group on the Recommended Definition of a General Nuclear Database Structure (GNDS). The panellists included:

- Dr Osamu Iwamoto (JAEA)
- Dr Jean-Christophe Sublet (IAEA)
- Dr Dorothea Wiarda (ORNL)
- Dr Caleb Mattoon (LLNL)
- Dr Fausto Malvagi (CEA)

**Nuclear data are the "secret sauce" that enable our understanding of nuclear systems**

Nuclear reactions are too complex to model from first principals and must be tabulated for use in simulations

The size and complexity of reaction data has increased markedly in the last 20 years

Year	Energy angle distributions	Energy distributions	Angular distributions	Charged particle reactions	Resonances	Uncertainties
1990	0.5	0.5	0.5	0.5	0.5	0.5
2000	1.5	1.5	1.5	1.5	1.5	1.5
2010	3.5	3.5	3.5	3.5	3.5	3.5
2020	15.0	15.0	15.0	15.0	15.0	15.0

VERA simulation of Xe-135 production in WB2 reactor core, from "Predictive Power" <https://www.ornl.gov/news/predictive-power> (2017)

# GNDS-2.0 Goals

- Satisfy remaining SG-38 goals
  - `<map>` format
  - `<documentation>` format (handled in May)
  - Major TNSL rewrite (handled in May)
- Ensure “forwards compatibility” with ENDF-6
- Respond to user needs
  - TNSL Covariance

## Detailed requirements for a next generation nuclear data structure

OECD/NEA/WPEC SubGroup 38\*

(Dated: June 28, 2016)

This document attempts to compile the requirements for the top-levels of a hierarchical arrangement of nuclear data such as found in the ENDF format. This set of requirements will be used to guide the development of a new data structure to replace the legacy ENDF format.

### CONTENTS

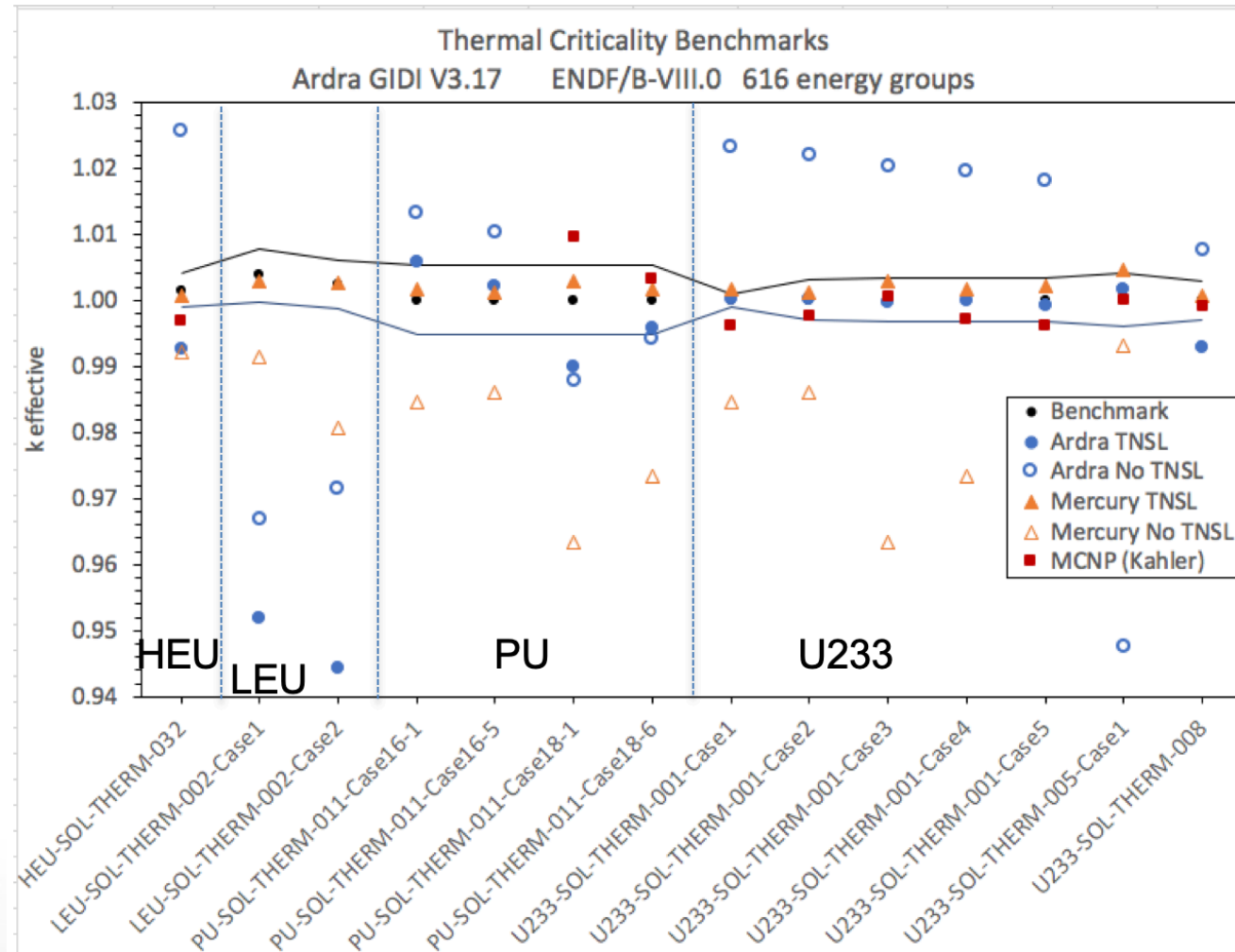
I. Introduction	3	6. How to use the RRR elements in special circumstances	55
A. Use cases	4	IV. Covariance Data	56
B. How to use these requirements	5	A. Covariance definitions	56
C. Organization of this document	6	B. Covariance between different variables	59
D. Connection to ENDF-6 data types	6	C. Covariance of continuous functions	59
II. General Features	8	D. Covariance of multi-dimensional functions	59
A. Design philosophy	8	E. Covariance and correlation matrices	60
B. Complications	8	F. Weighted sums of covariance	61
1. Is it a material property or a reaction property?	9	G. The “Sandwich Formula”	63
2. Different optimal representation in different physical regions	10	H. Monte Carlo sampling	64
3. Ensuring consistency	10	I. Examples of covariance data usage in this hierarchy	64
4. Elemental targets	11	V. Special Cases	67
5. Legacy data	11	A. Atomic scattering	67
C. Top of the hierarchy	11	1. Incoherent photon scattering	68
D. Particle and/or material properties database	12	2. Coherent photon scattering	68
E. Documentation	16	B. Charged particle elastic scattering	69
F. Representations	20	1. Legendre series expansion approach:	69
G. What data are derived from what other data?	21	2. “Fake cross section” approach	70
H. Prototyping functions	22	C. Fission reactions	71
I. Required low-level containers	25	D. Fission product yields	73
1. General data/functional containers	26	1. Introduction	73
2. Text	27	2. Existing ENDF format	74
3. Hyperlinks	27	3. Detailed FPY requirements	74
III. Evaluations	29	4. Discussion of possible implementations	75
A. <code>&lt;evaluation&gt;</code> elements	29	E. Spallation reactions	77
B. “Meta” evaluations	32	F. Radiative capture	78
C. Reactions and reaction lists	34	G. Thermal scattering law	78
1. <code>&lt;reactions&gt;</code> and <code>&lt;summedReactions&gt;</code>	35	1. Introduction	78
2. <code>&lt;productionReactions&gt;</code> lists	38	2. Theoretical background	79
3. <code>&lt;reaction&gt;</code> elements	38	3. Gaussian approximation of the self part of the scattering kernel	81
4. Reaction designation	39	4. Coherent elastic scattering	81
D. Cross sections	40	5. Incoherent elastic scattering	82
1. Integrated cross sections: $\sigma(E)$	40	6. Incoherent inelastic scattering in the short collision time approximation	83
2. Differential cross sections: $d\sigma(E)/d\Omega$ and $d^2\sigma(E)/d\Omega dE'$	41	7. Discussion of TSL covariance	83
E. Products and product lists	41	VI. Derived Data For Applications	85
1. Product list elements	41	A. General transport data	85
2. <code>&lt;product&gt;</code> elements	42	1. Product average kinetic energy and forward momentum	85
F. Distribution and distribution lists	44	2. $\bar{\mu}_{ab}(E)$	85
1. <code>&lt;distributions&gt;</code> and <code>&lt;distribution&gt;</code> elements	44	3. CDF’s from PDF’s	85
2. Multiplicities	45	4. Probability tables in the URR	86
G. Resonances	45	B. Grouped transport data	86
1. Designating channels	49	1. Inverse speed	87
2. Resolved resonances	51	2. Multiplicity	87
3. Unresolved resonances	52	3. Q-value	87
4. Correcting reconstructed cross sections and distributions	53	4. Projectile kinetic energy and momentum	87
5. Expected resonance processing workflow	54	5. Bondarenko factors	87
		C. Production data	88
		D. Radiation heating and damage	89
		Acknowledgments	90

\* Edited by D.A. Brown (dbrown@bnl.gov)

# Status 2020

## Demonstration of capability

LLNL transport codes have been updated to run problems using GNDS data via GIDI API

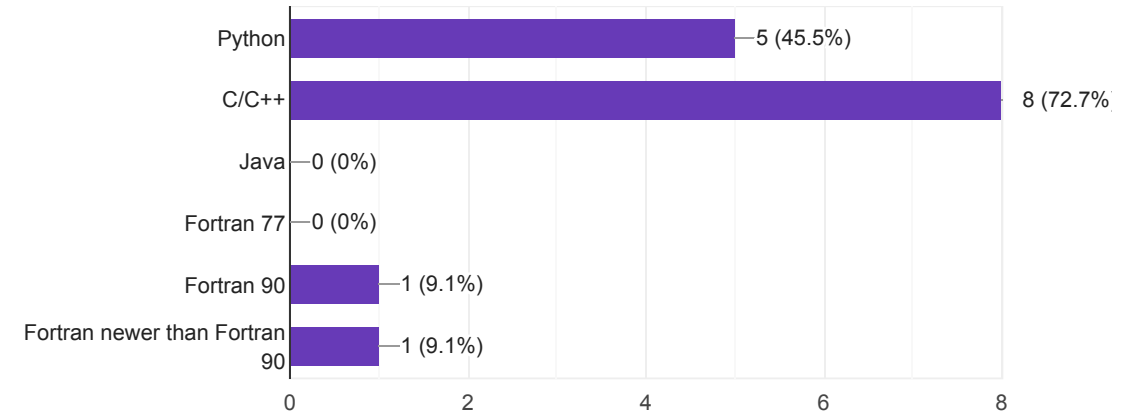


# We did a little poll to find out more about how GNDS is being implemented

- AMPX
- SAMMY
- brownies (FUDGE extensions)
- FRENDY
- GIDI+
- OpenMC
- GALILEE
- TAGNDS (TALYS to GNDS)
- FUDGE
- NJOY

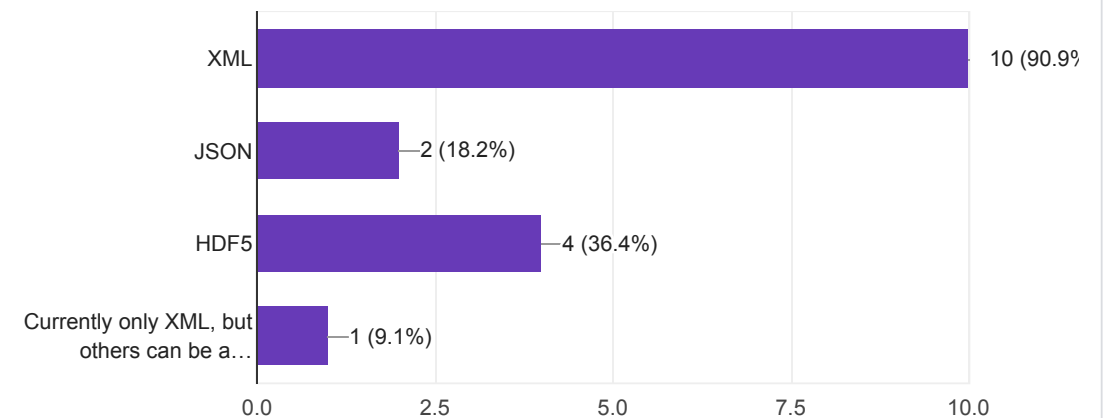
What languages is your application developed in?

11 responses

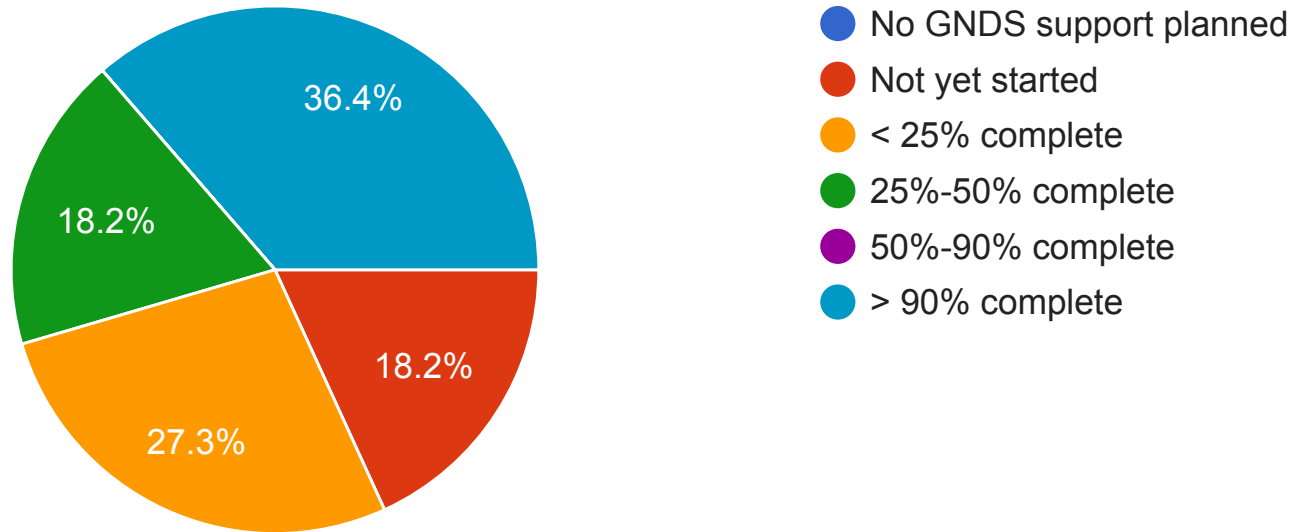


What formats will you use to interact with your GNDS data?

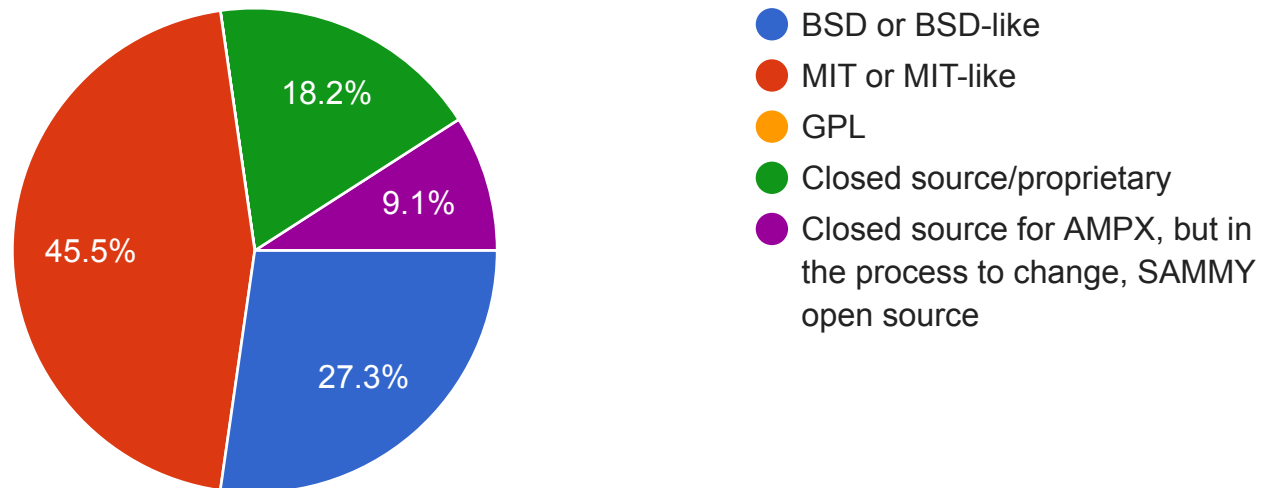
11 responses



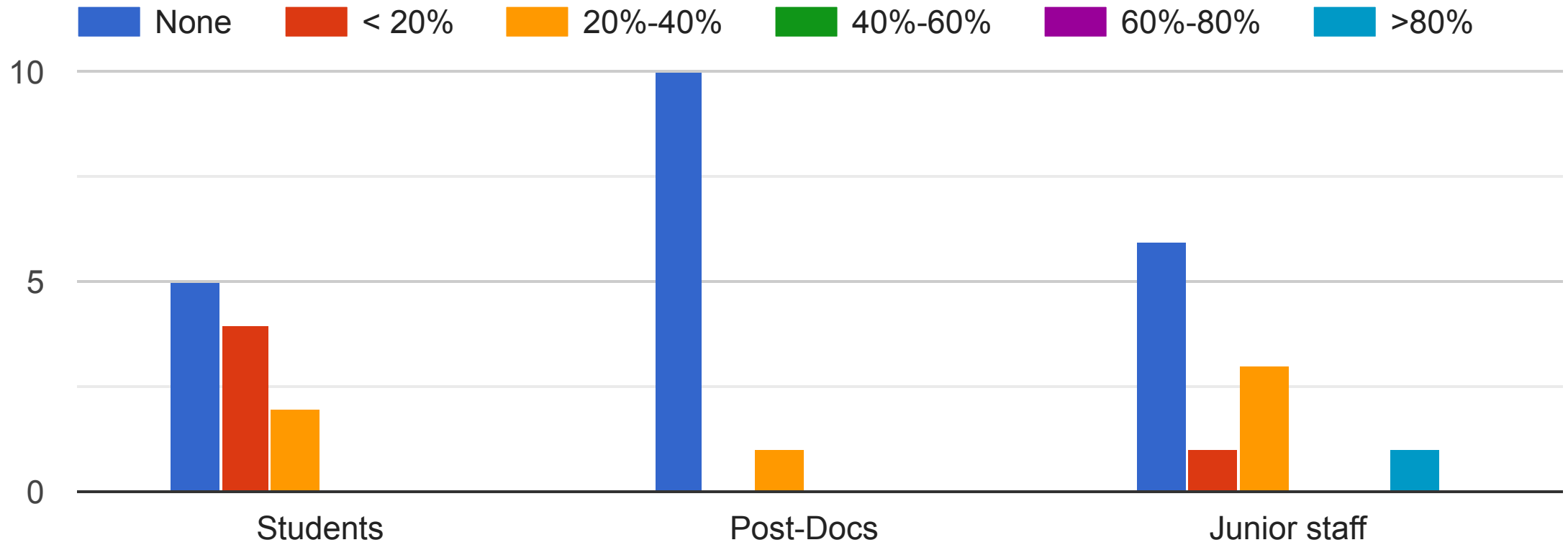
# Some projects are far along in their GNDS support



**Most are open source! Only ~20% of applications are closed source**



Part of GNDS's purpose is inspiring younger scientists. What fraction of your developers are





# What's next

- **Expect major format changes post-GNDS-2.0:**
  - Synchronize nuclear structure formats with ENSDF as part of ENSDF modernization
  - Revamp uncertainty/covariance to make more ML friendly
  - Atomic data additions
  - FPY formats per FIRE collaboration/CSEWG recommendations
- **ENDF to GNDS transition:**
  - ENDF/B-VIII.0 released in GNDS-1.9
  - Expect at least next release to be in both ENDF-6 and GNDS formats
  - Transition is slow; we must walk together and we can only go as fast as the slowest among us