Status of GForge and ADVANCE

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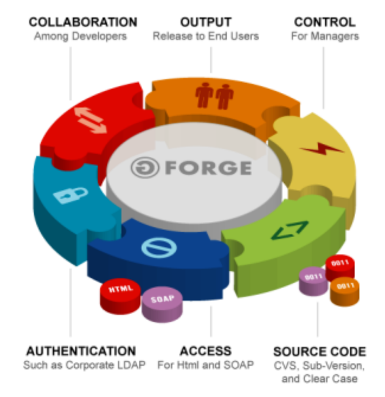
U.S. DEPARTMENT OF ENERGY

Things to discuss

- GForge: hardware & software
- ADVANCE hardware
- ADVANCE software
- ENDF review system
- ENDF evaluation quality standards



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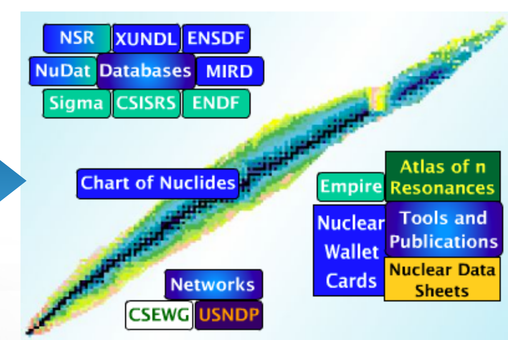

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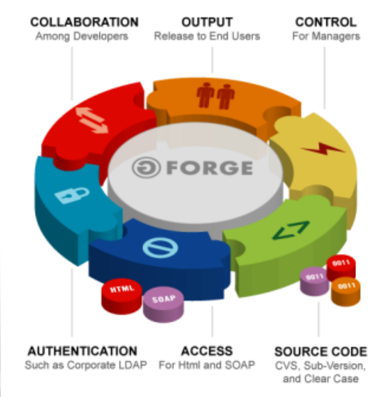

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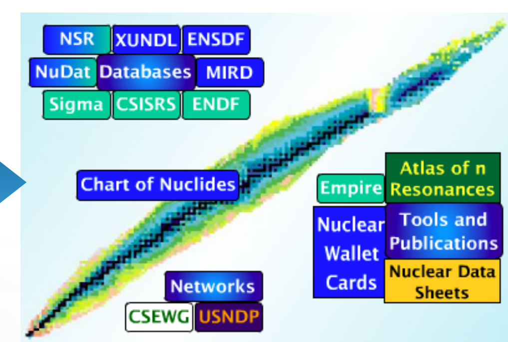

CSEWG has obvious need to GForge like functionality

- **Hosted projects:**
  - ENDF
  - ENDF Formats manual
  - SG-38 (GNDS)
  - Various evaluation projects (Fe, Cr, …)
  - ENDF checking codes
  - Much more…
- **Features we use regularly**
  - Revision control
  - Bug trackers
  - Release management
  - Workflow management
  - Unlimited seats
- **Features we'd like to have**
  - Review mechanism upon commit

NNDC’s GForge system is long in the tooth

- **GForge machine**
  - 2011, nearly 8 years old
  - 800 Gb of data
- **GForge software**
  - Annual license, $4.8k, unlimited number of seats paid for by USNDP (10-15% increase/yr.)
  - SSL Certificate, ~$450/year, paid for by USNDP
  - Maintenance done in-house by R. Arcilla
- **It is time to revisit this system**

Options

- **Continue GForge as is (but buying new server)**
- **Upgrade to GForgeNext (must buy new server)**
  - $10.5k/yr., 100 seats
  - Ramon manages
  - Has review mechanism
- **Open GitHub not viable** — until data has gone through proper DOE/BNL reviews, data cannot be freely distributed (even if it will be freely distributed eventually)
- **Closed GitHub/GitLab**
  - $7-$20/mo./seat
  - GitHub/GitLab manages or we manage
  - Has review mechanism
- **Many other options, needs proper review**
- **A BNL institutional resource?**

Ultimately this is NNDC/BNL decision, but we want your input

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New ADVANCE server: advance2

- Dell PowerEdge R640
- 2 CPUs/24 Cores
- 32Gb RAM x4
- 480 Gb SSD x2
- 900 Gb HD x6 (RAID)

Quite zippy

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also rinky dink compared to NNSA lab computers

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ENDF quality assurance

- **Phase 0 testing (svn hooks)**
  - yes ASCII, no unicode, no Microsoft
  - Unix linefeeds
  - checks if evaluation different from what in repo (taking into consideration ENDF line numbers)
- **Phase I testing**
  - see next page
- **Phase II testing**
  - Validation with integral tests, coordinated by CSEWG validation committee

Code	Test	pre-VII	Now
	File summary complete & correct	🤔	
STAN, STANEF, CHECKR, fudge	**ENDF format compliance**	🖥️	🖥️
FIZCON, fudge	**Mathematical correctness** (e.g. probabilities valid, covariances positive)	🖥️	🖥️
FIZCON, PSYCHE, fudge	**Physical correctness** (e.g. Q, thresholds, energy deposition/KERMA)	🖥️	🖥️
INTER, fudge (inter.py)	**Compute & check integral metrics** (e.g. RI, thermal cross sections, MACS)	🖥️	🖥️
fudge	**Completeness** (all outgoing particles, including gammas)	🤔	🖥️
ADVANCE	**Comparisons to microscopic experimental data** (EXFOR)	🤔	🖥️
	Assessment of application suitability (e.g. usable for fast reactors or spaceflight)	🤔	
	Reasonable (e.g. covariances, angular distributions)	🤔	
fudge (grokres.py)	**Resonance quality** (missing resonances? widths realistic?)		🖥️
PREPRO, fudge, NJOY, SCALE	**Can process for user codes**		🖥️
	Is state of the art? Is best we can do?	🤔	

Large fraction of Phase I testing automated with `ADVANCE` software

- **`ADVANCE` Standalone**
  - Includes NNDC codes, `PREPRO`
  - Needs Python2-3, make, `fudge`, `x4i`, `NJOY`
- **Full `ADVANCE`**
  - Uses `buildbot`
  - Best with standalone build server
  - Needs access to subversion repository

Changes to **ADVANCE** software coming this FY

- Much of **ADVANCE** uses Python2, Python2 end-of-life is 1 Jan. 2020, so we are upgrading to Python3.7
  - **ADVANCE** software itself is done (both stand alone & **buildbot** version)
  - **fudge** in progress
  - **x4i** is next
- DOE-wide http -> https transition means changes to **ADVANCE** build report js & css usage
- Addition of resonance report
- NCSP funds most of development of **ADVANCE**, but USNDP purchases the server(s)

Resonance Quality Assurance

Brookhaven National Laboratory Report
BNL-209313-2018-INRE

A tale of two tools: `mcres.py`, a stochastic resonance generator, and `grokres.py`, a resonance quality assurance tool

David Brown,[1,*] Declan Mulhall,[2,†] and Rishi Wadgoankar[3]

[1] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY*
[2] *University of Scranton, Scranton, PA*
[3] *G.W. Hewlett High School*
(Dated: October 19, 2018)

We detail two software tools, now integrated into the **`fudge`** code system. The first tool, **`mcres.py`**, can be used to generate stochastic ensembles of resonances which are both consistent with the expectations of the Gaussian Orthogonal Ensemble of Random Matrix Theory and with the level densities and widths encoded in ENDF formatted files. The second tool, **`grokres.py`**, can be used to assess global and local features of sequences of resonances found in ENDF files and make comparisons to known results from Random Matrix Theory. We apply these tools to ^{54}Fe and other nuclei.

CONTENTS

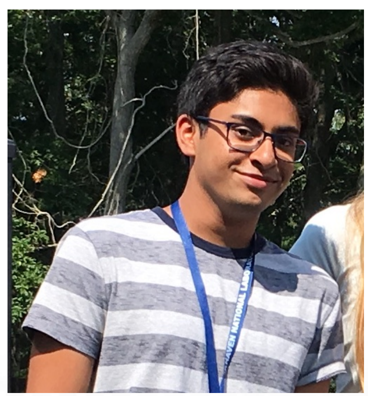
Resonance metrics considered

<u>Measures of energies</u>

- **Long range behavior**
  - Average spacing vs. E
  - Cumulative level distribution
- **Short range behavior**
  - Nearest neighbor spacing distribution
  - Spacing-spacing correlation, ρ
  - Dyson-Mehta Δ_3 statistic
  - Other statistics

<u>Measures of widths</u>

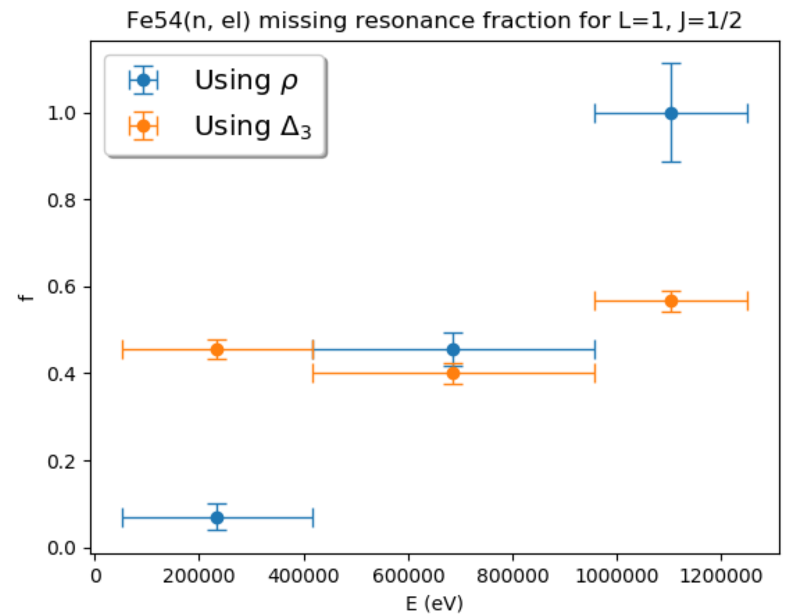
- **Long range behavior**
  - Average width vs. E
  - Width distribution
- **Short range behavior**
  - Are there short range correlations in the widths?

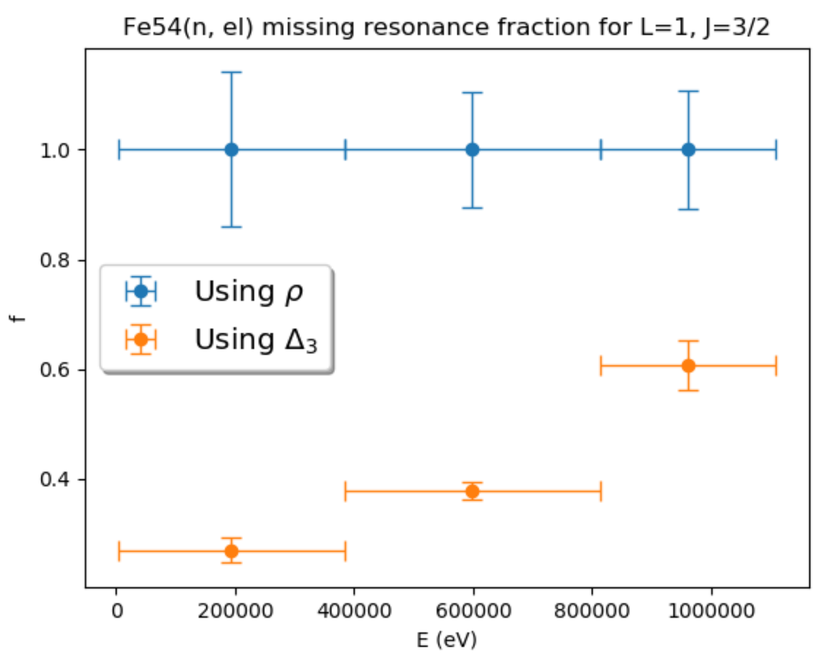


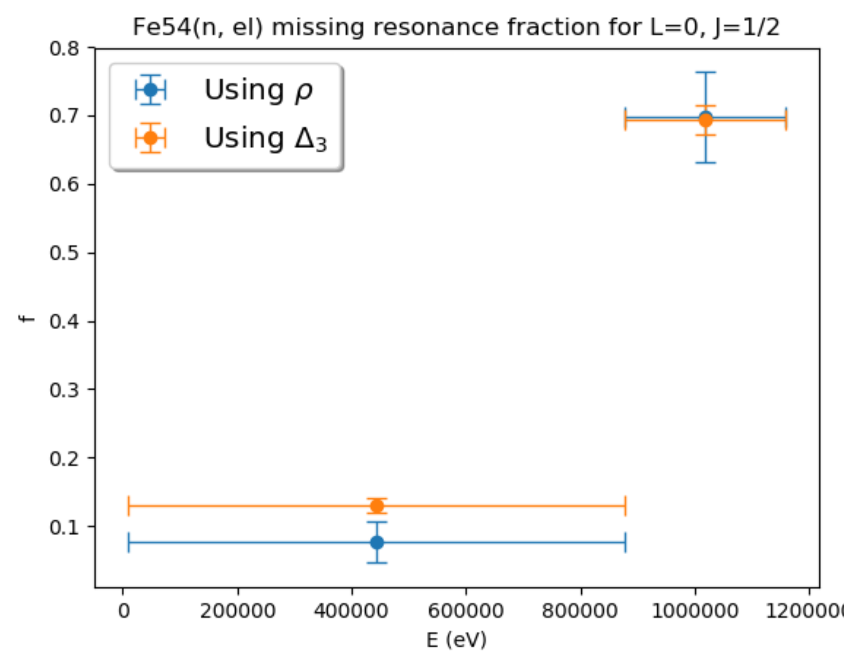
Rishi Wadgoankar (HSRP student)

Declan Mulhall (Univ. Scranton)

Can we use these to assess the fraction of missing resonances?







Issues with ADVANCE

- **Test coverage**:
  - all sublibraries needs more plots vs. data
  - neutrons considerable number of tests
  - other sublibraries need substantially more testing than is done
- **Usability:** does organization of reports meet our needs?
- **Turn around time:** old machines mean turn-around time erratic (sometimes > 1 week for actinides); hopefully is resolved!
- **Phase II testing:** can/should be automated too

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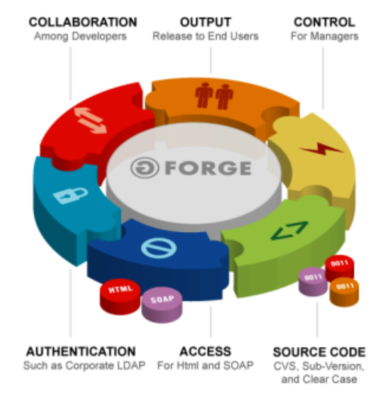

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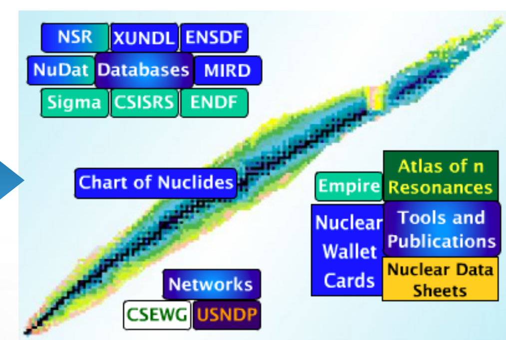
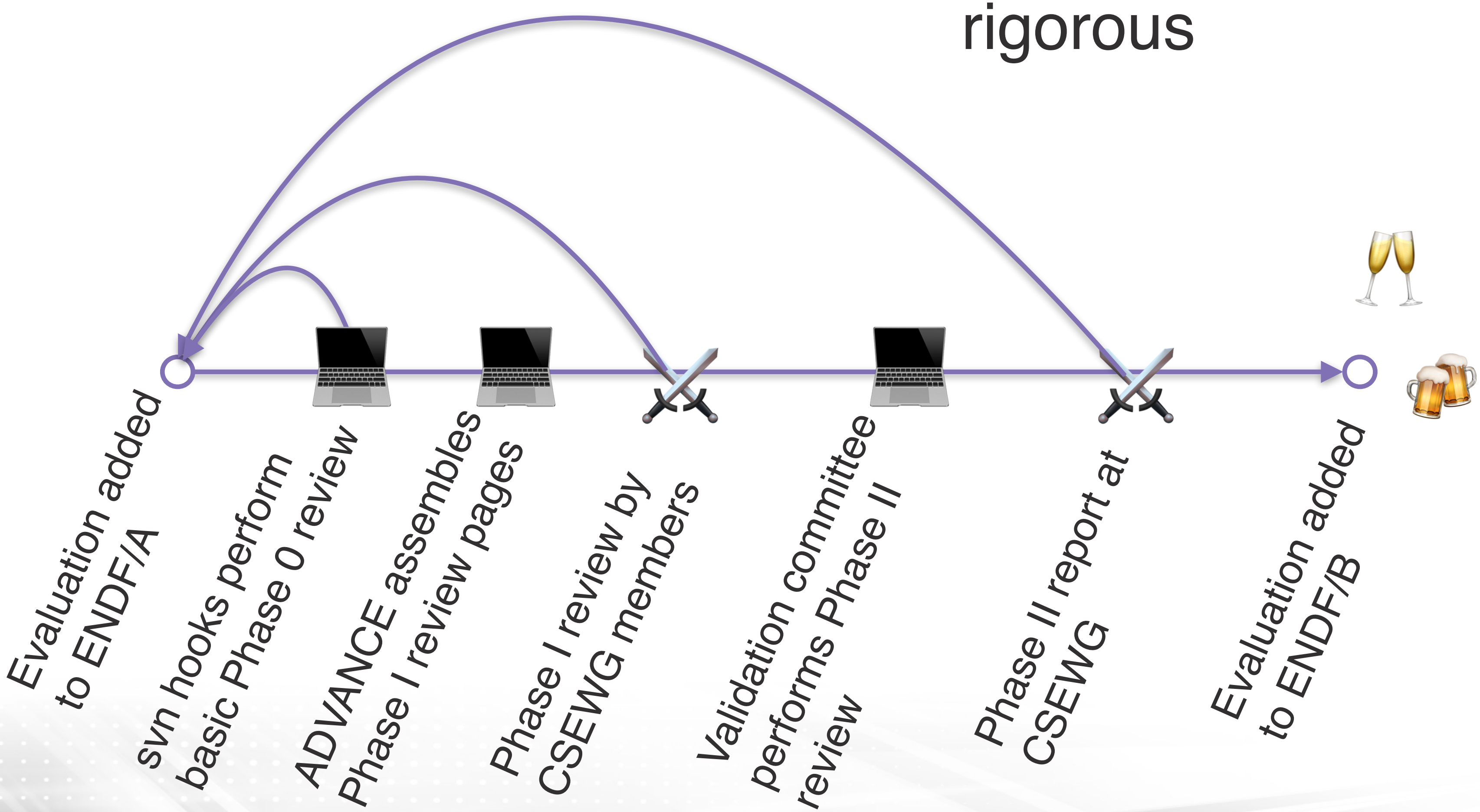
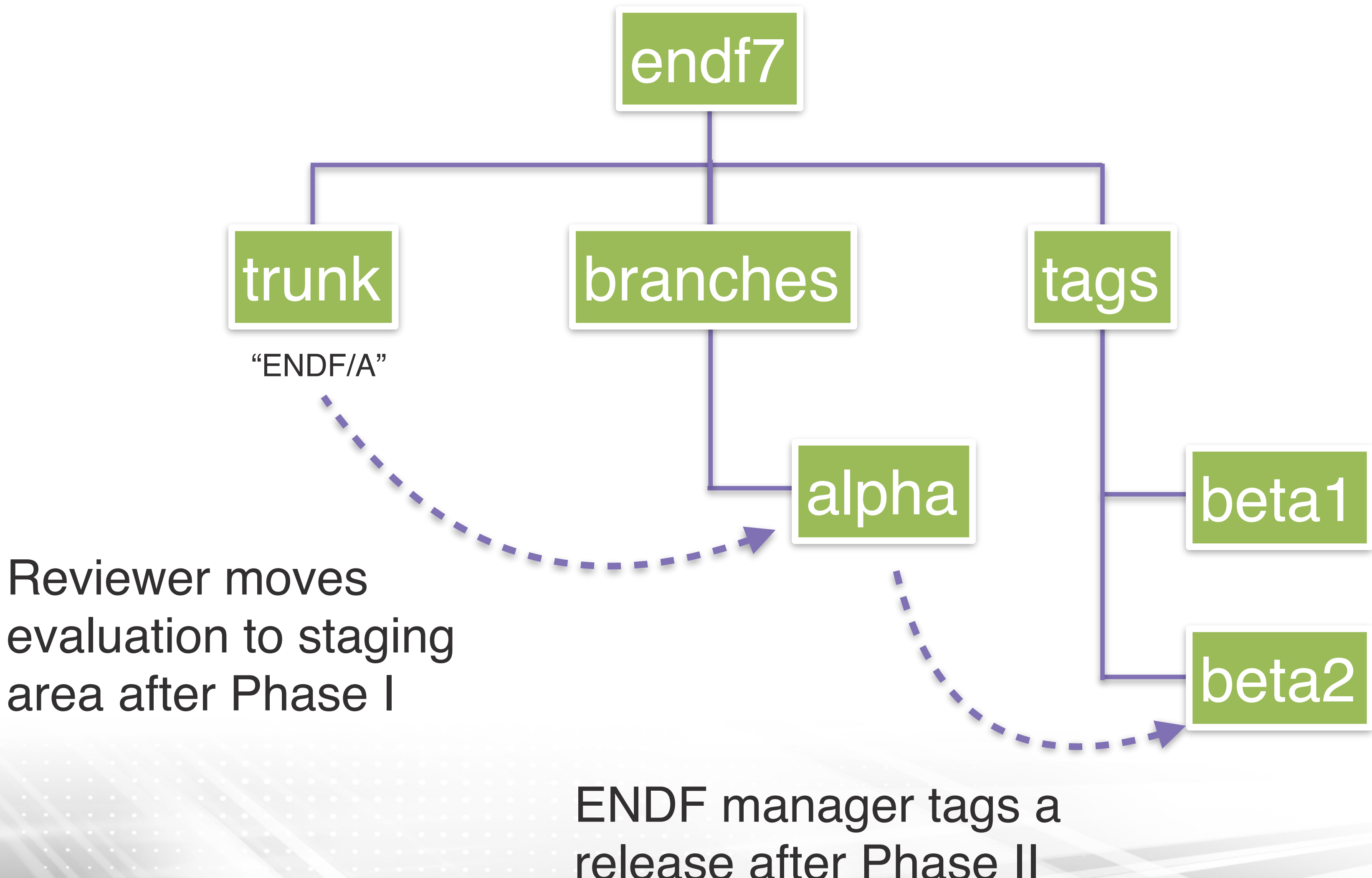


For ENDF/B-VIII.1, want to bring back formal reviews

want fast AND rigorous



Plan is to tie subversion to review process



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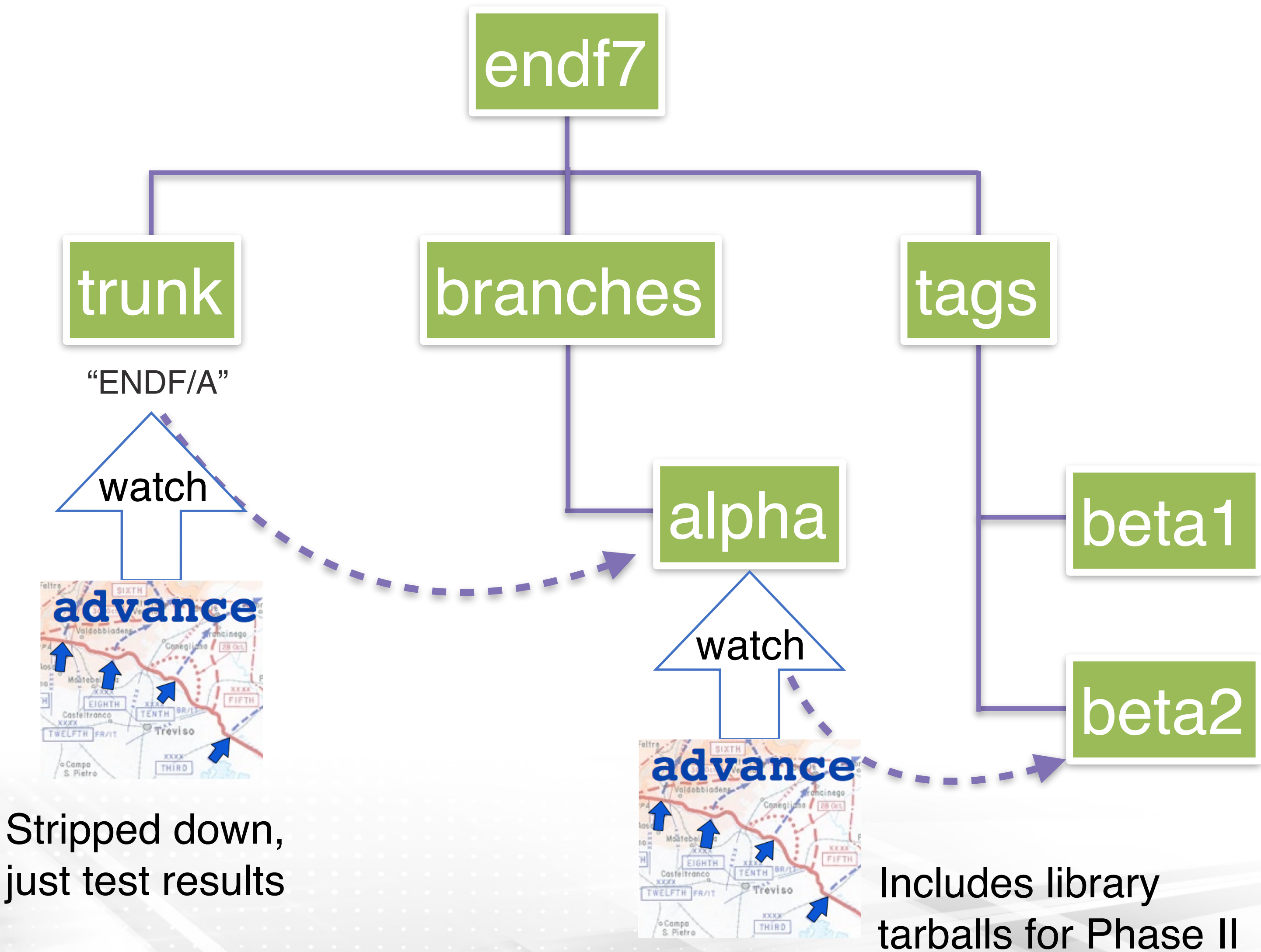

Plan is to tie subversion to review process

endf7

This is all easy and I will get it set up rapidly once other issues dealt with…

Stripped down,
just test results

watch

beta2

Includes library
tarballs for Phase II

Status of ENDF review system

- **Nice idea, but needs more fleshing out**
  - not really clear what needs to be checked!
  - not really clear who's going to be doing the checking
- **Chadwick model:**
  - the lead of previous evaluation becomes reviewer of future changes to that evaluation (provided the changes are coming from elsewhere)
  - ENDF Lib. Mgr. picks reviewer otherwise

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Establishing ENDF Quality standards for entire library (not just neutrons)

- **For neutrons, should of course check the ADVANCE build reports, but what else?**
- **Other sublibraries need quality standards**
  - example 1: Paris & Hale reviewing the LLNL CP evaluations now. What standards should they apply? Demanding R-matrix for everything impractical
  - example 2: SG-42 establishing standards for TSL, but not fleshed out beyond basic format checks and consistency between cross sections
  - example 3: Covariance committee developed standards for neutron library, but no other sublibraries

Establishing ENDF Quality standards for entire library (not just neutrons)

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Item for discussion: draft an ENDF QA standards document?