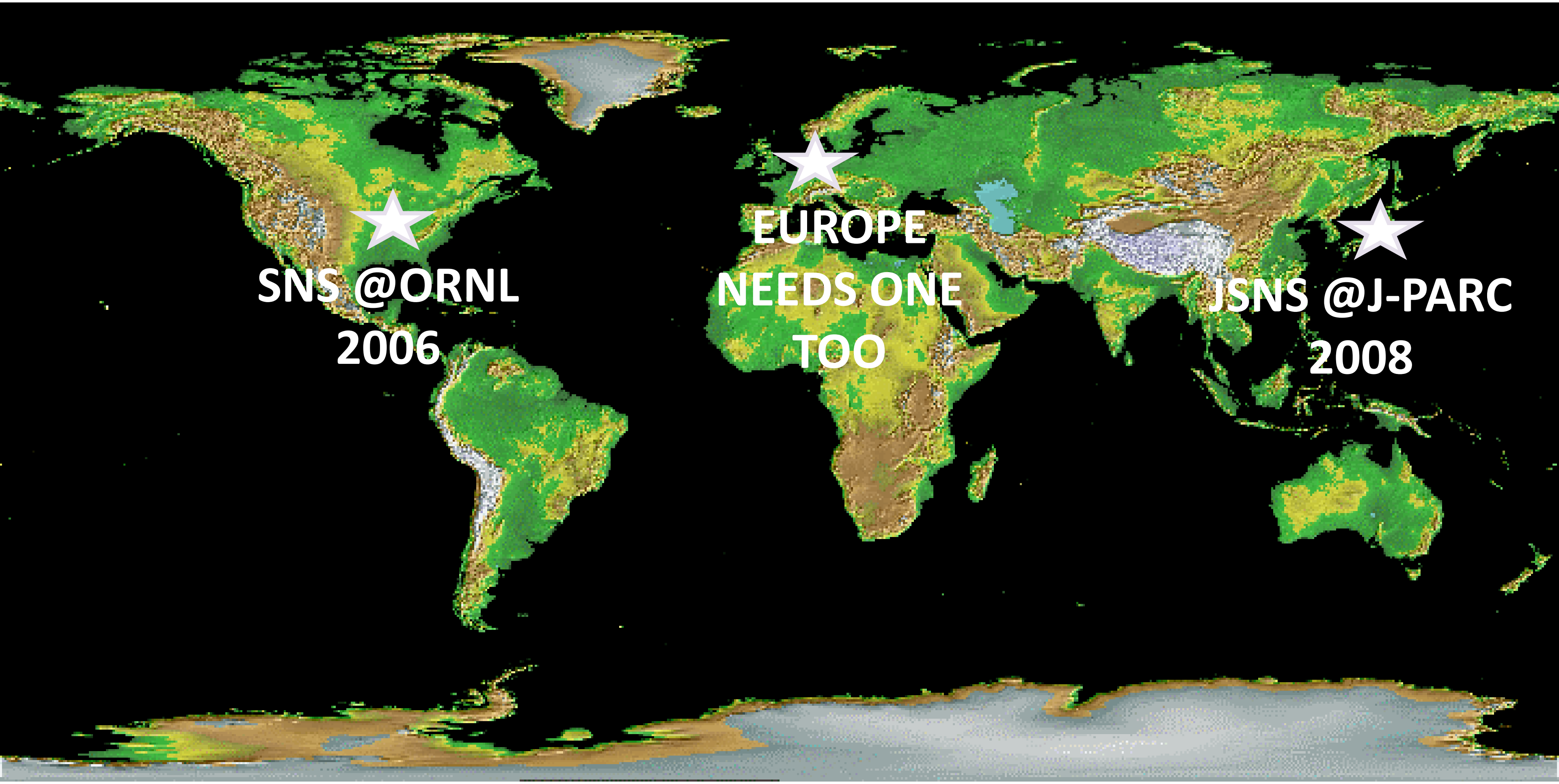
Preliminary formulation of a nuclear data roadmap for designing the ESS

Mary PW Chin[1,2] Francois Plewinski[1]
Cyril Kharoua[1,2] Etam Noah[1,2] Mats Lindroos[1]

[1] E S S S
(European Spallation Source Scandinavia)
Lund University
SE-22100 Lund
Sweden

[2] C E R N
(European Centre for Nuclear Research)
Department EN/STI
CH-1211 Geneva 23
Switzerland

MEGAWATT SPALLATION NEUTRON SOURCES



28 MAY 2009 Meeting of Research Ministers in Brussels

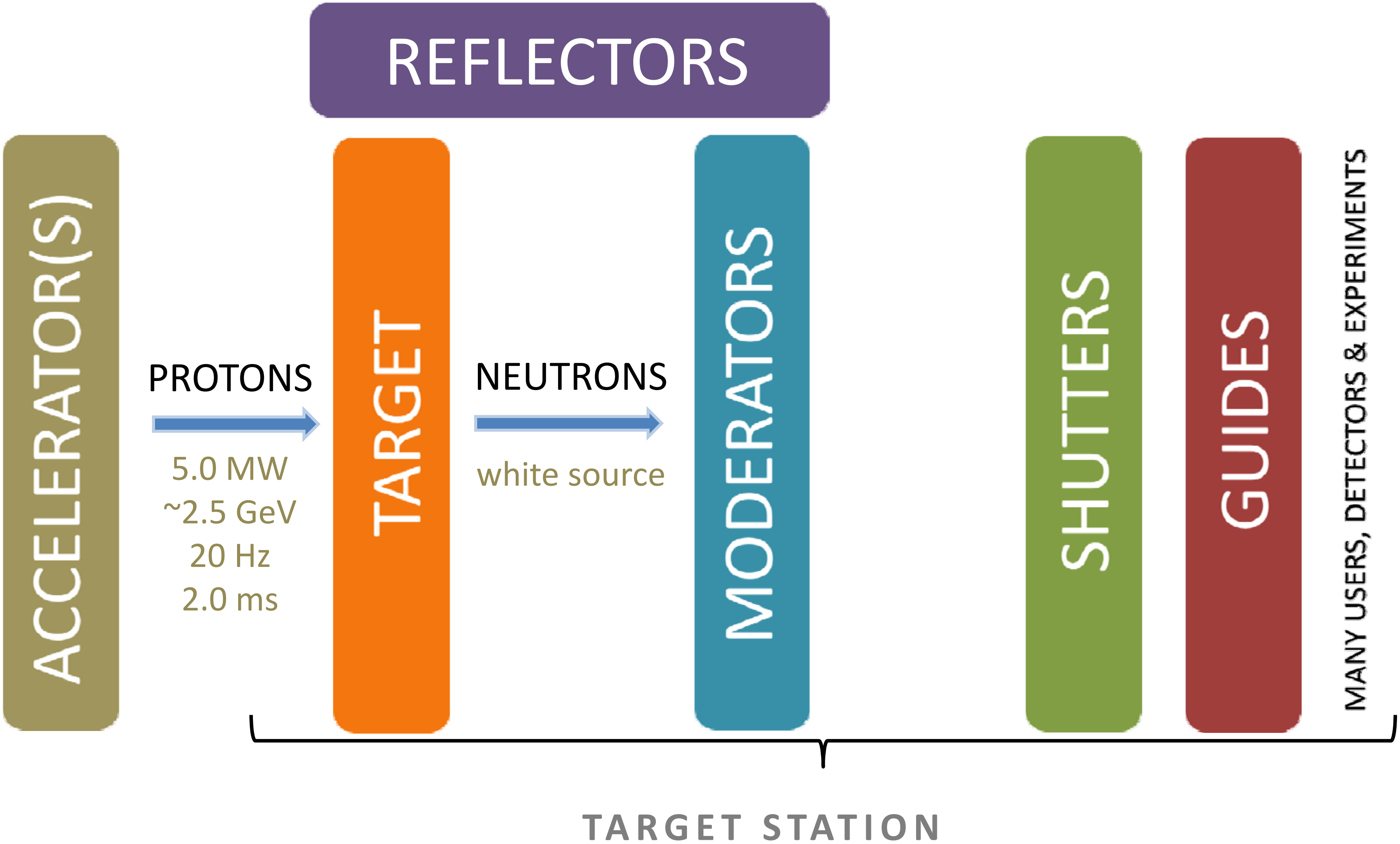
- YES, WE WILL DESIGN AND BUILD ONE
- LUND WINS THE BID TO HOST

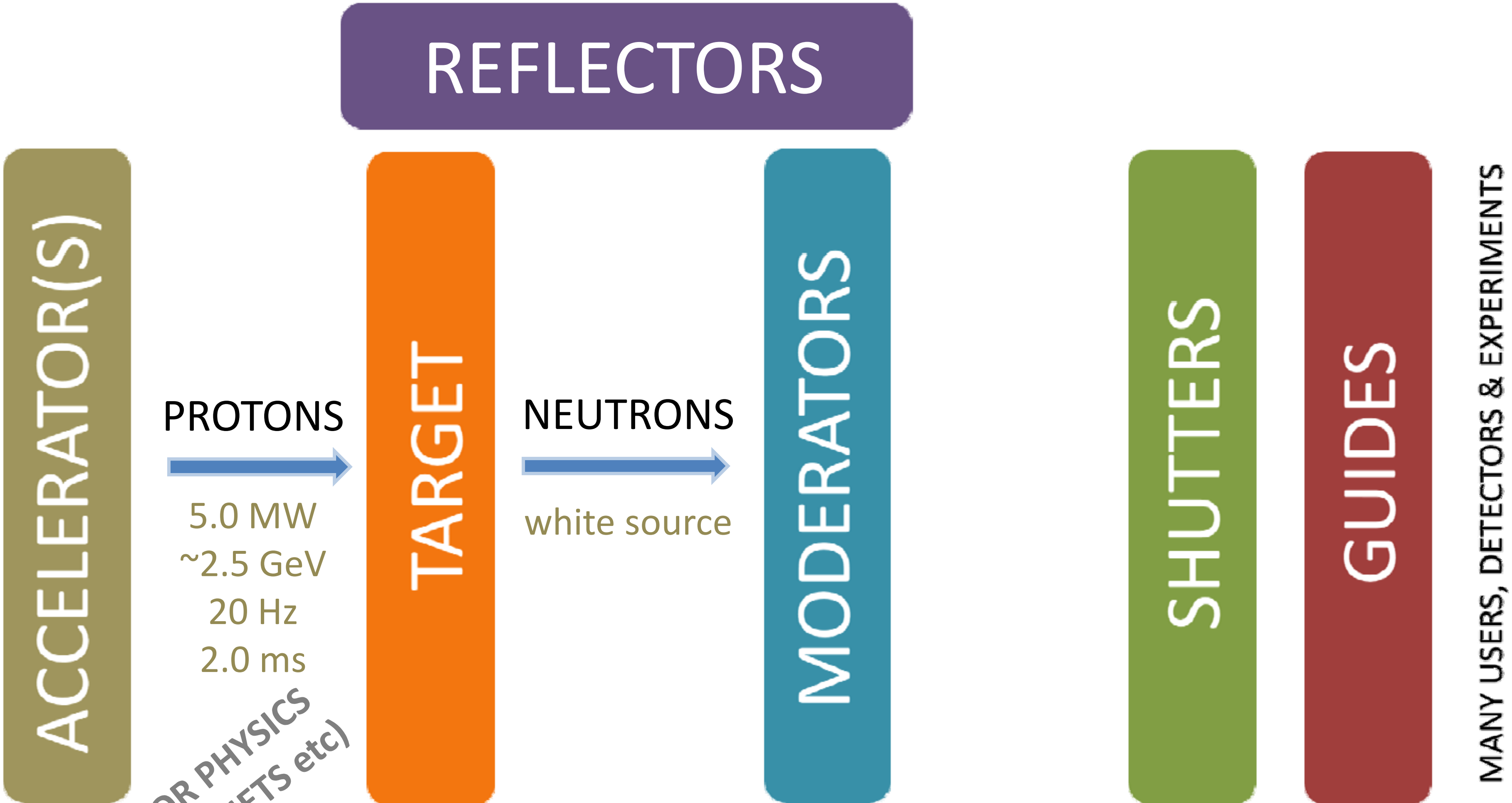
OUR LEGOLAND

GPS N 55° 44,013 E 013° 14,829

CURRENTLY AN OLD FARMLAND

TOWARDS THE 1^{ST} NEUTRON IN 10 YEARS' TIME


REFLECTORS
ACCELERATOR(S)
PROTONS
5.0 MW
~2.5 GeV
20 Hz
2.0 ms
TARGET
NEUTRONS
white source
MODERATORS
SHUTTERS
GUIDES
MANY USERS, DETECTORS & EXPERIMENTS
TARGET STATION



ACCELERATOR PHYSICS
(RF, MW, MAGNETS etc)

PARTICLE TRANSPORT
RADIATION
INTERACTIONS (ATOMIC) &
REACTIONS (NUCLEAR)
WITH MATTER

+

WAVE NATURE OF
NEUTRONS
(not MCNP/FLUKA/
GEANT4, but McSTAS)

DESIGN

VIRTUAL SIMULATIONS

- ANSYS
- FLUKA + MCNPX
- McSTAS
- _ _ _ _ _ _

TEST CELLS / MOCK-UPS

SUPPORTING TECHNIQUES

FINAL CONSTRUCT

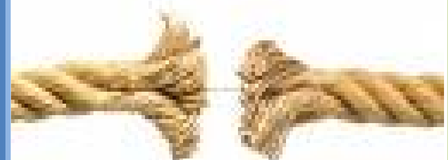
DESIGN

VIRTUAL SIMULATIONS

- ANSYS
- FLUKA + MCNPX
- McSTAS
- _ _ _ _ _ _ _

TEST CELLS / MOCK-UPS

SUPPORTING TECHNIQUES



THE GRAND CHALLENGE

FINAL CONSTRUCT

1. TO IDENTIFY HIDDEN TRAPS now
2. TO AVOID BUILDING CASTLES in the air
3. TO TAKE CARE OF ERROR BARS

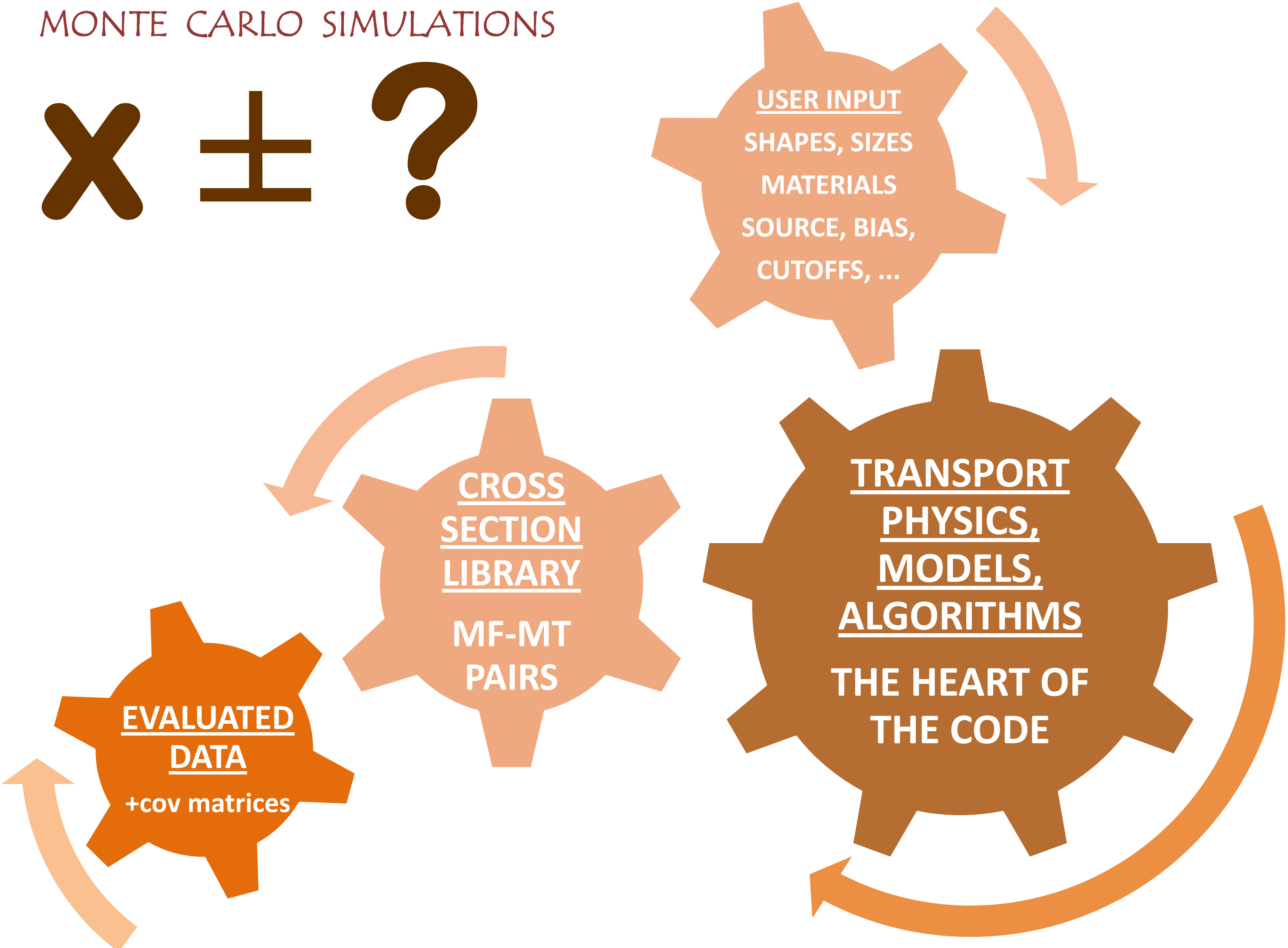
THE GRAND CHALLENGE

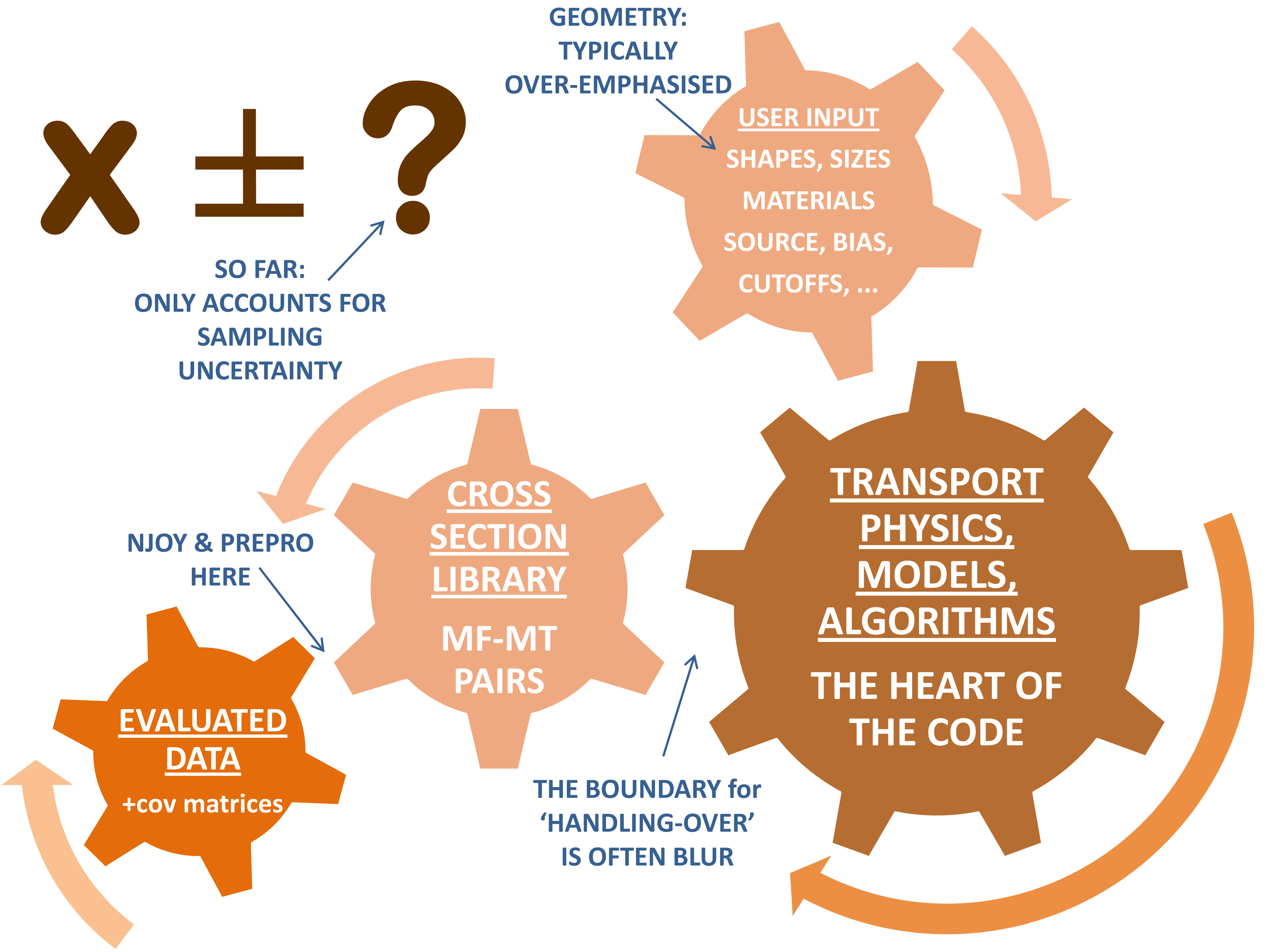
THIS WORK:

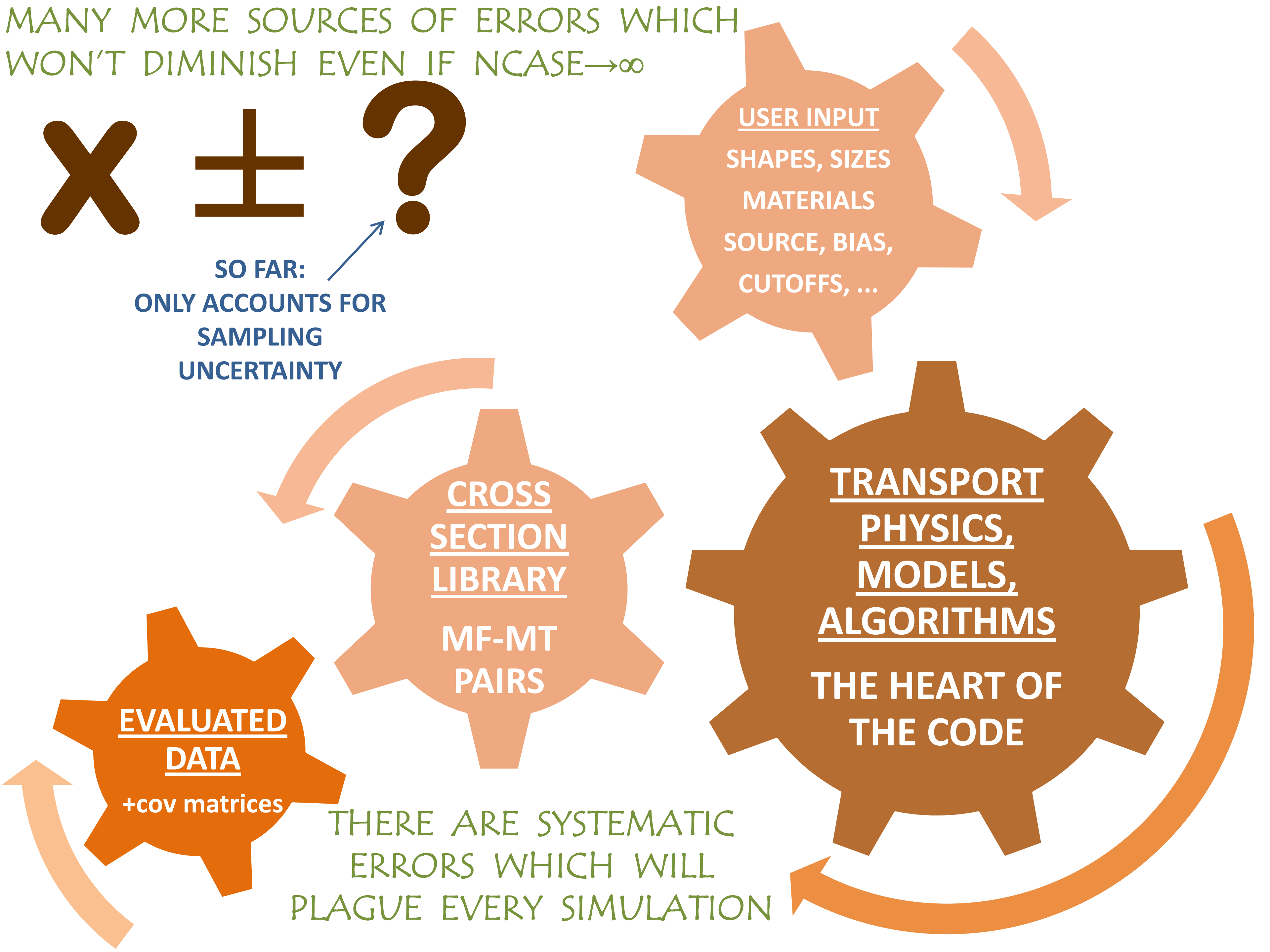
1. TO IDENTIFY ISSUES
2. TO RULE-OUT NON-ISSUES

MONTE CARLO SIMULATIONS

$x \pm ?$




X ± ?
GEOMETRY:
TYPICALLY
OVER-EMPHASISED
USER INPUT
SHAPES, SIZES
MATERIALS
SOURCE, BIAS,
CUTOFFS, …
SO FAR:
ONLY ACCOUNTS FOR
SAMPLING
UNCERTAINTY
CROSS
SECTION
LIBRARY
MF-MT
PAIRS
NJOY & PREPRO
HERE
TRANSPORT
PHYSICS,
MODELS,
ALGORITHMS
THE HEART OF
THE CODE
EVALUATED
DATA
+cov matrices
THE BOUNDARY for
'HANDLING-OVER'
IS OFTEN BLUR


MANY MORE SOURCES OF ERRORS WHICH WON'T DIMINISH EVEN IF NCASE→∞
x ± ?
SO FAR: ONLY ACCOUNTS FOR SAMPLING UNCERTAINTY
USER INPUT
SHAPES, SIZES
MATERIALS
SOURCE, BIAS,
CUTOFFS, ...
CROSS SECTION LIBRARY
MF-MT PAIRS
TRANSPORT PHYSICS, MODELS, ALGORITHMS
THE HEART OF THE CODE
EVALUATED DATA
+cov matrices
THERE ARE SYSTEMATIC ERRORS WHICH WILL PLAGUE EVERY SIMULATION

NOTE: MCNPX's PERT does not propagate covariance data

MCNPX User's Manual
Version 2.5.0, April. 2005
LA-CP-05-0369

TALLY SPECIFICATION

5.6.21 PERT Perturbation

Form: `PERTn:<pl> KEYWORD=value(s) ...`

Basic Keywords	Description
CELL	Comma or space delimited list of cells, c_1 ... c_K, to which to apply perturbation. Required.
MAT	Single material number, m, with which to fill all cells listed in CELL keyword.† Must have a corresponding M card.

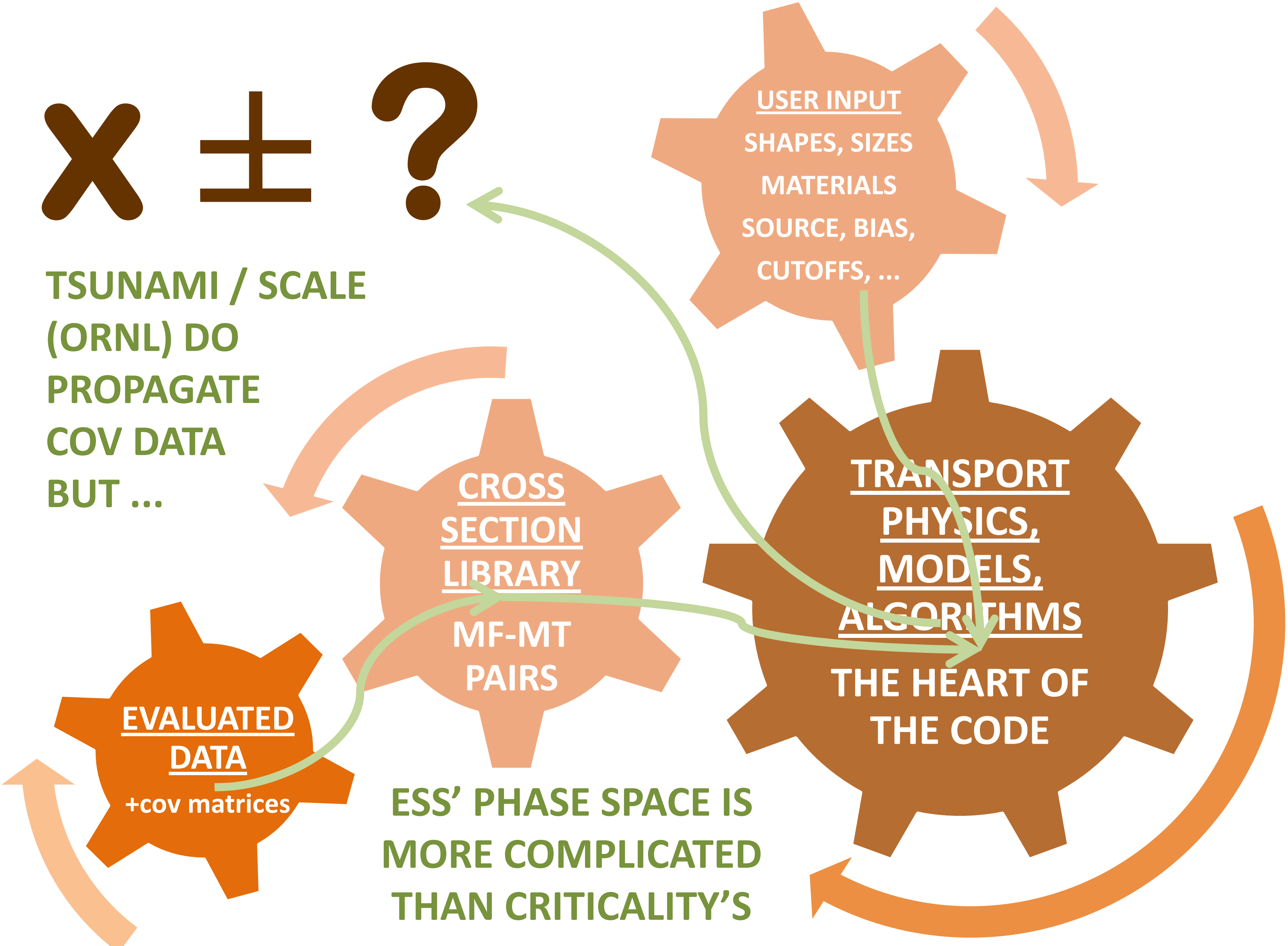
Use: Optional.

Note: Allows perturbations in cell material density, composition, or reaction cross-section data. Uses the first and second order differential operator technique. Perturbation estimates are made without actually changing the input material specifications. Multiple perturbations can be applied in the same run, each specified by a separate PERT card.

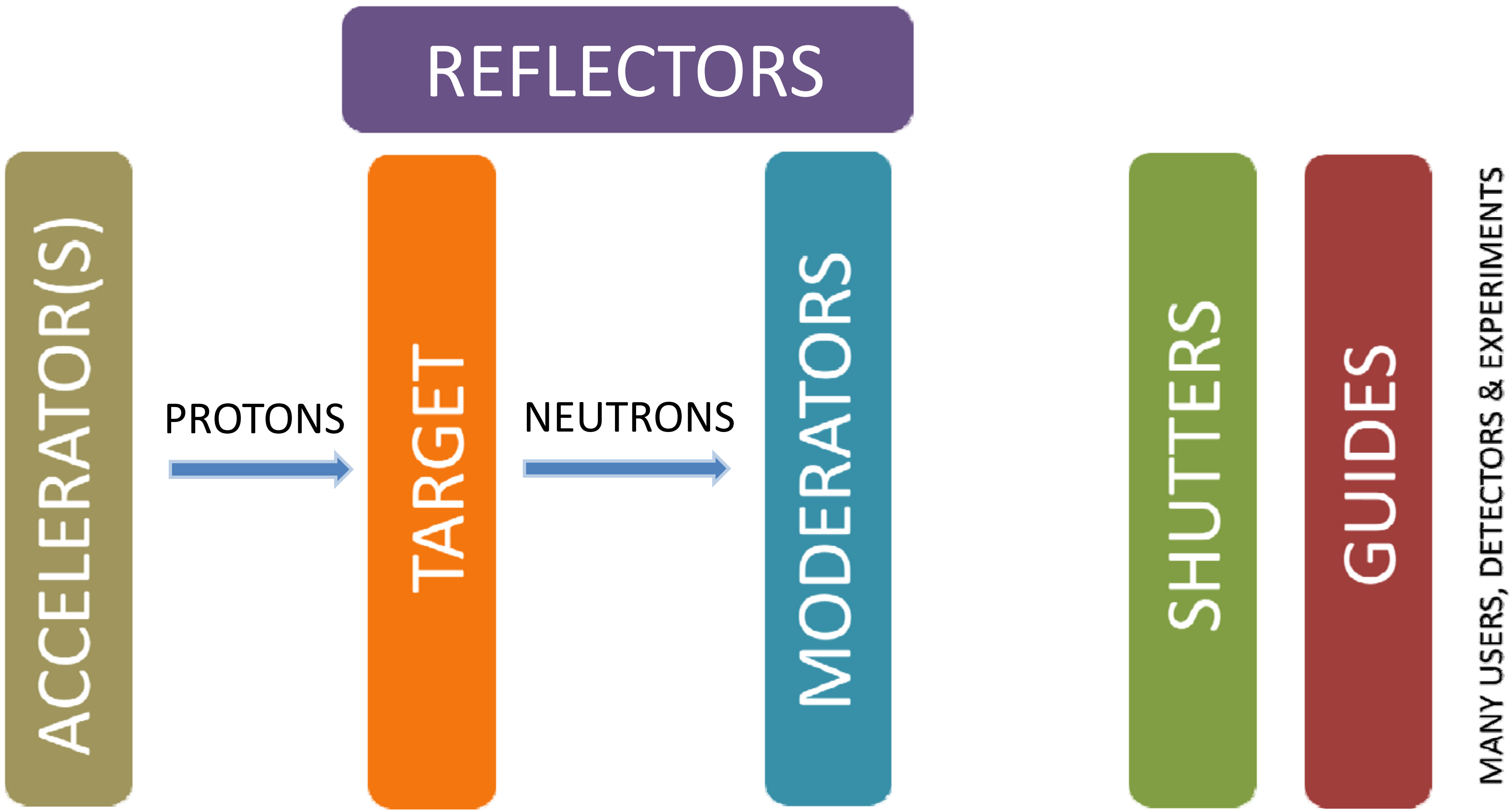
It only estimates perturbation if ZAID were replaced by another

The nuclide identification number with the form ZZZAAA.nnX
where
ZZZ is the atomic number,
AAA is the mass number (000 for elements),
nn is the unique table identification number, and
X=U for continuous-energy photonuclear tables.

A solo ZAID would have its own cov data, independent of another ZAID



X ± ?
TSUNAMI / SCALE (ORNL) DO PROPAGATE COV DATA BUT …
USER INPUT
SHAPES, SIZES
MATERIALS
SOURCE, BIAS,
CUTOFFS, …
CROSS SECTION LIBRARY
MF-MT PAIRS
TRANSPORT PHYSICS, MODELS, ALGORITHMS
THE HEART OF THE CODE
EVALUATED DATA
+cov matrices
ESS' PHASE SPACE IS MORE COMPLICATED THAN CRITICALITY'S

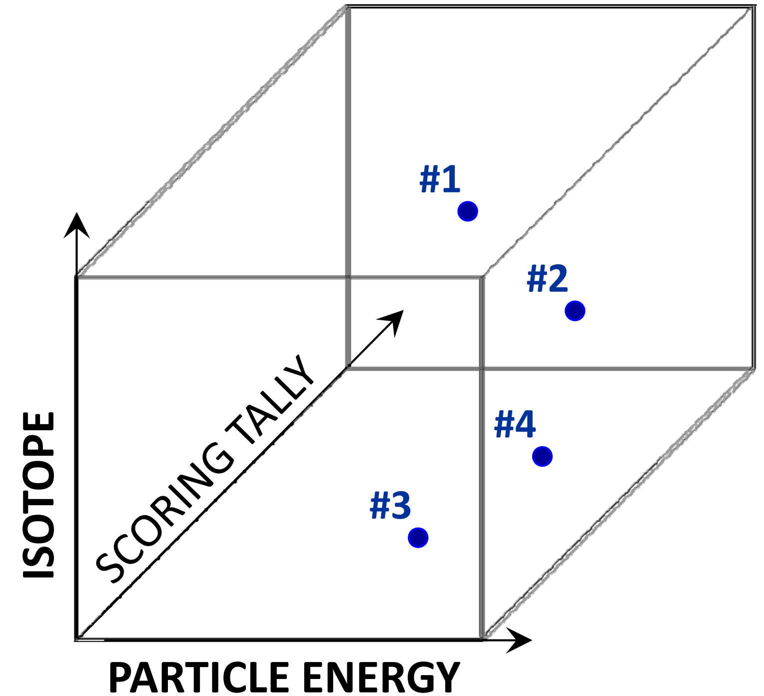


BROAD-RANGED SPECTRA OF:
ENERGY, PARTICLE TYPE,
TEMPERATURE, ISOTOPE

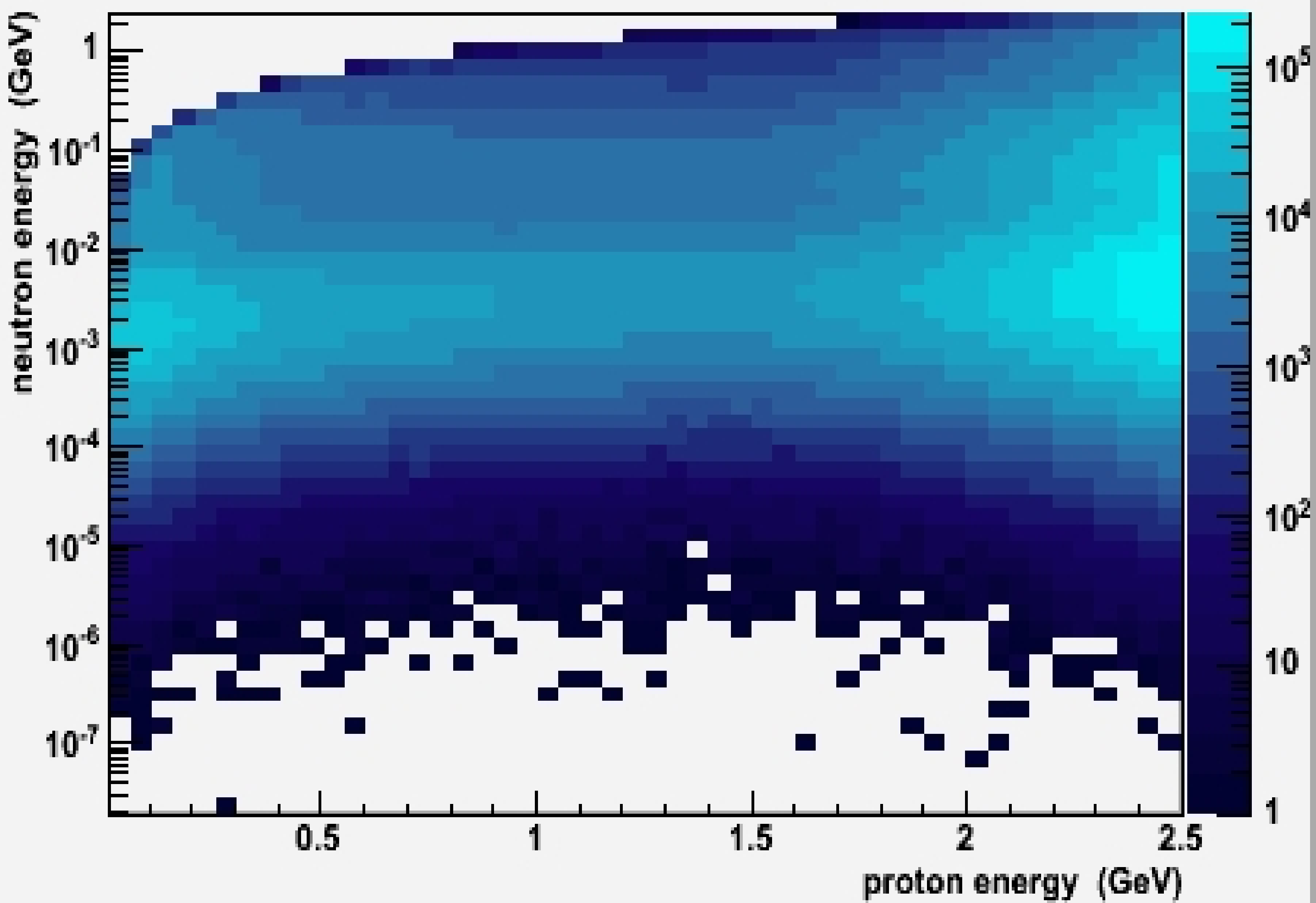
PHASE SPACE COMPLEXITY

NO CODE IS BENCHMARKED 100%

IT IS IMPOSSIBLE TO COVER EVERY POSSIBLE IRRADIATION CONDITION



BROAD-RANGED SPECTRA OF:
ENERGY, PARTICLE TYPE, TEMPERATURE, ISOTOPE

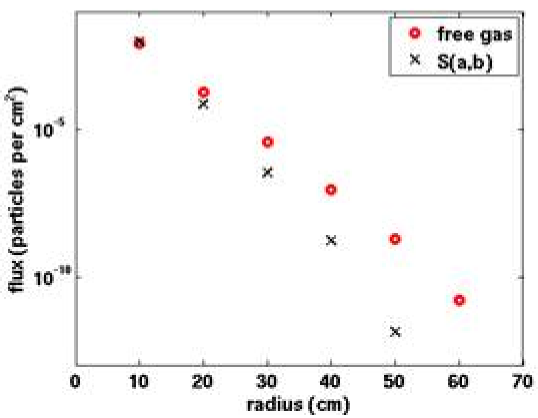


neutron energy (GeV)
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0.5
1
1.5
2
2.5
proton energy (GeV)
10^5
10^4
10^3
10^2
10
1

ENERGY RANGE
VULNERABLE AT BOTH ENDS

< meV → **2.5 GeV**

- **THERMAL MOTION**
- **CRYSTALINE STRUCTURE**[1]
- **CHEMICAL BINDING**[1]
- **LACK OF TABULATED NUCLEAR LEVELS**



Free gas vs **S(α,β)** thermal treatments. MCNPX2.5.0 simulations were started with 10^{6} 5 eV neutrons in concentric spheres of polyethylene, passing all 10 statistical tests. Thermal data at 300 K was taken from the tmccs library, which provides scattering data for ^{1}H only; ^{12}C was still represented by the default free-gas treatment.

- **LACK OF MEASURED DATA**
- **MANY REACTION CHANNELS OPEN UP**
- **MAINTAINING CORRELATION BETWEEN PARTICLES BECOMES TRICKY**

PARTICLES RECOGNISE NEITHER SIBLINGS NOR FOREPARENTS
eg. multiple 0.48 MeV gammas may emerge from a single $^{10}B(n,\alpha)^{7}Li$ collision[2]

1. Chin MPW et al 2009 *Variation of 3γ -to-2γ ratio from ^{18}F in haematological components measured using the GAMMASPHERE* Nucl Instrum Meth A 604 331-4
2. Chin MPW, Spyrou NM 2007 *Event-by-Event Monte Carlo Tracking of Neutron-Nucleus Collisions in Neutron Detectors* Trans Am Nucl Soc 97 288

ENDF/B-VII

Nuclear Data Sheets 107 (2006) 2931–3060

ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology

M.B. Chadwick,[1] P. Obložinský,[2*] M. Herman,[2] N.M. Greene,[6] R.D. McKnight,[3] D.L. Smith,[3]

TABLE II: Contents of the ENDF/B-VII.0 library, with ENDF/B-VI.8 shown for comparison. NSUB stands for the sublibrary number in the ENDF-6 format. Given in the last two columns are the number of materials (isotopes or elements).

No.	NSUB	Sublibrary name*	Short name	VII.0	VI.8
1	0	Photonuclear	g	163	-
2	3	Photo-atomic	photo	100	100
3	4	Radioactive decay	decay	3838	979
4	5	Spont. fis. yields	s/fpy	9	9
5	6	Atomic relaxation	ard	100	100
6	10	Neutron	n	393	328
7	11	Neutron fis.yields	n/fpy	31	31
8	12	Thermal scattering	tsl	20	15
9	19	Standards	std	8	8
10	113	Electro-atomic	e	100	100
11	10010	Proton	p	48	35
12	10020	Deuteron	d	5	2
13	10030	Triton	t	3	1
14	20030	^{3}He	he3	2	1

ESS

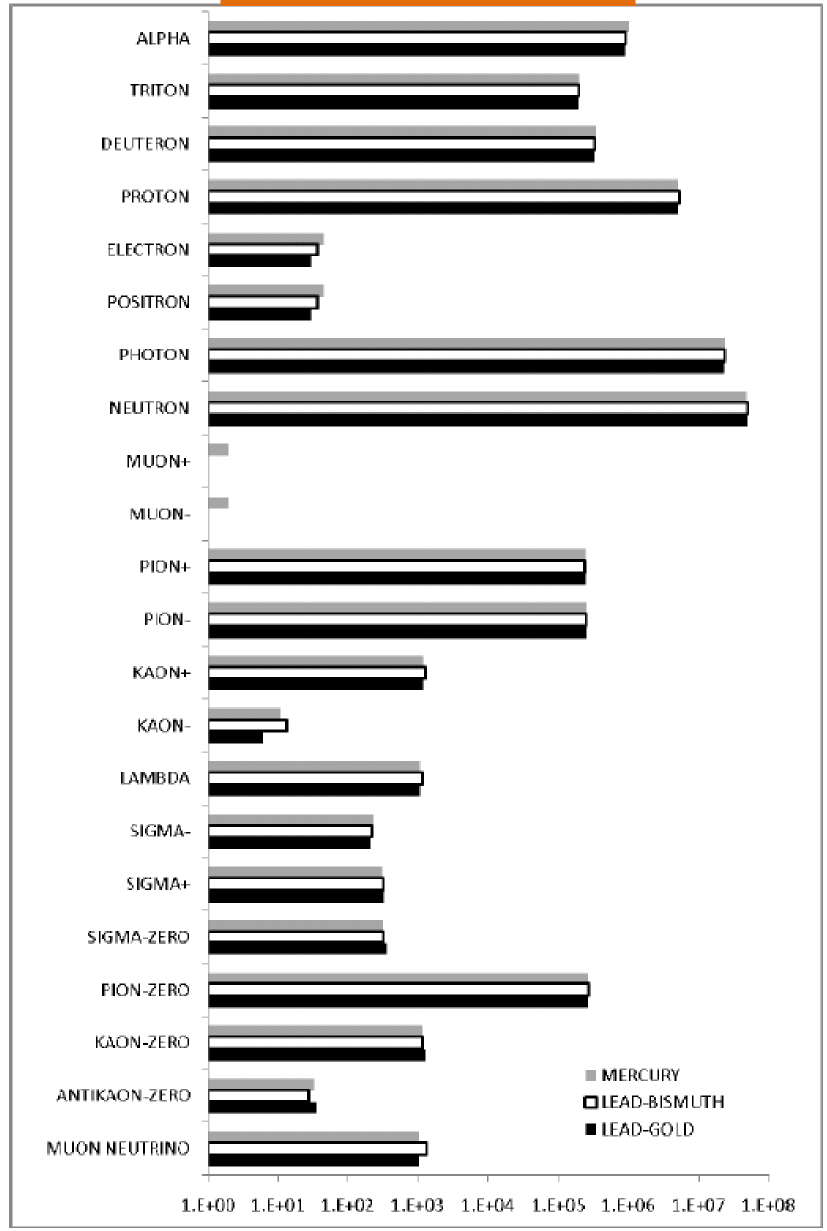


Fig. 1 Secondary particles produced in a FLUKA 2008.3b simulation of 5×10^5 2.5 GeV protons impinging an effectively infinite homogeneous slab: a count of various particle types.

ESS (cont'd)

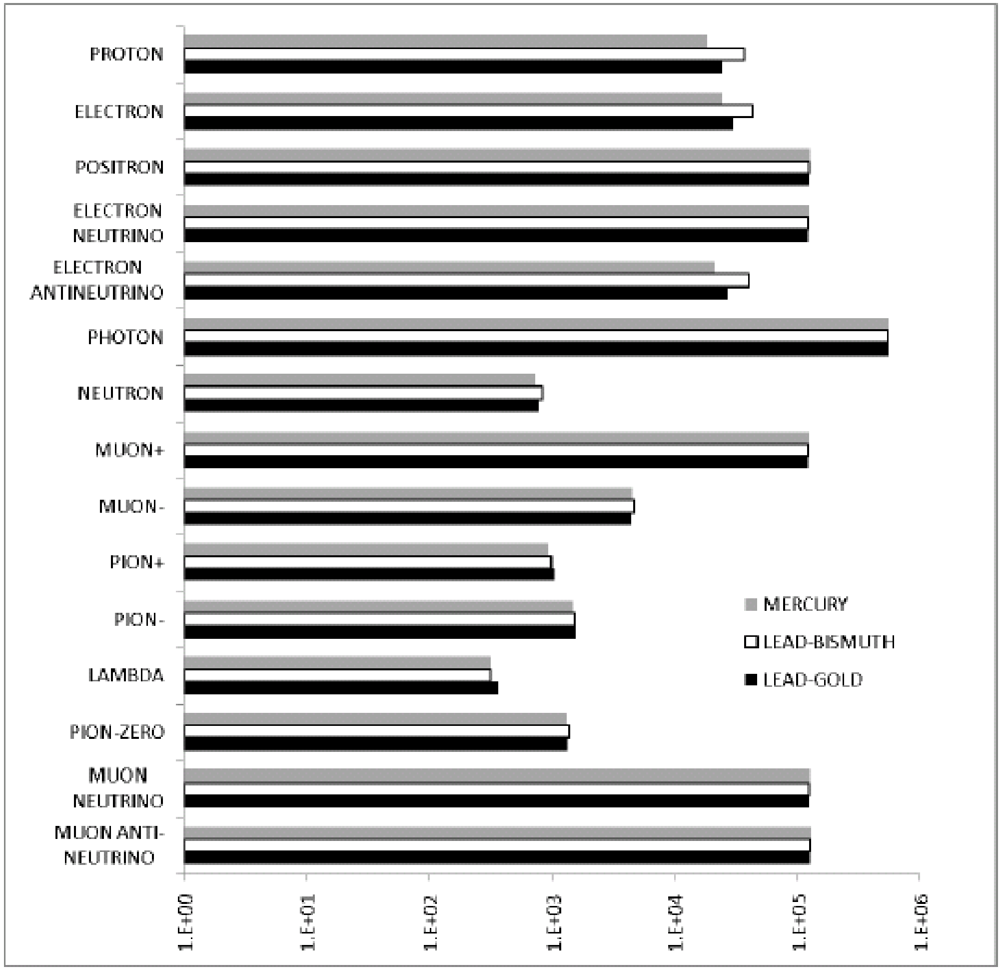


Fig. 2 Decayed products produced in a FLUKA 2008.3b simulation of 5×10^5 2.5 GeV protons impinging an effectively infinite homogeneous slab: a count of various particle types.

OLD-GENERATION REACTORS

MILITARY INTERESTS

<u>Some balancing is expected</u>

EMPHASIS / BIAS in terms of

ISOTOPES, ENERGY RANGE,

TEMPERATURE RANGE,

REACTIONS TYPES

ESS SHARES SOME

COMMON INTERESTS WITH

SISTER TECHNOLOGIES

ACCELERATOR DRIVEN SYSTEMS

FUSION TECHNOLOGIES

SPALLATION SOURCES

Major Libraries

- 1) ENDF/B-VII.0 (USA,2006)
- 2) JEFF-3.1.1 (Europe,2005-2009)
- 3) JENDL-3.3 (Japan,2002)
- 4) BROND-2.2 (Russia,1992)
- 5) CENDL-2 (China,1991)

Special Libraries

- 6) ROSFOND-2008: neutron library, 683 materials, Obninsk, Russia
- 7) TENDL-2008 (n,γ,p,d,t,he3,α) (Netherlands,NRG,2008)
- 8) FENDL-2.1 Fusion Evaluated Nuclear Data Library, 2004
- 9) ENDF/HE-VI (High Energy)
- 10) JEFF-3.1/A (Activation)
- 11) IRDF-2002 (Dosimetry)
- 12) INDL/TSL (Thermal Scattering Law)
- 13) IAEA-Medical (diagnostic radioisotopes prod.)
- 14) IAEA-Medical (therapeutical radioisotopes prod.)
- 15) IAEA-Standards, 2006
- 16) PADF-2007, Proton Activation Data File, 2007
- 17) IBA-EVAL Differential data for ion beam analysis
- 18) JENDL/AC-2008, JENDL Actinoid File 2008
- 19) JENDL/AN-2005, (alpha,n) Reaction Data File
- 20) JENDL/PD-2004, Photoreaction Data
- 21) JENDL/HE-2007, High Energy (neutron, proton)
- 22) MENDL-2, Medium Energy, 1995-1998
- 23) MINKS-ACT, Actinides Library (Maslov et al.)
- 24) Wind, U,Np,Pu (up to 100 MeV)
- 25) Yavshits (neutron, proton induced fission for Pb-Pu)

www-nds.iaea.org

BROAD TEMPERATURE RANGE

could be < 14 K

depending on the choice of moderator

could be > 600 K

depending on the choice of target

MCNPX2.5.0

- 293.6 and 300 K for most isotopes
- some isotopes have additional libraries for 0, 77.0, 587.2, 880.8, 3000.1 K
- extra libraries for the uraniums and plutoniums (which is not of ESS' special interest)

FLUKA

- 87 and 296 K for most isotopes
- additional 4K libraries for selected isotopes

	MELTING POINT (K)
LEAD	600.6
BISMUTH	544.4
LEAD-BISMUTH EUTECTIC	397.7
GOLD	1337.4
LEAD-GOLD EUTECTIC	485.2
MERCURY	234.3

MONTE CARLO CODES CAN'T DO TEMPERATURE CHANGES ON-THE-FLY

MODELS vs TABLES

MCNPX's advertising of its mix-and-match capability gives the impression that tables are always better

Models may be extremely dangerous

Chin MPW, Spyrou NM 2009 *Non-convergence of Geant4 hadronic models for 10 and 30 MeV protons in ^{18}O and ^{14}N* Appl Rad Isotop 67 3 406

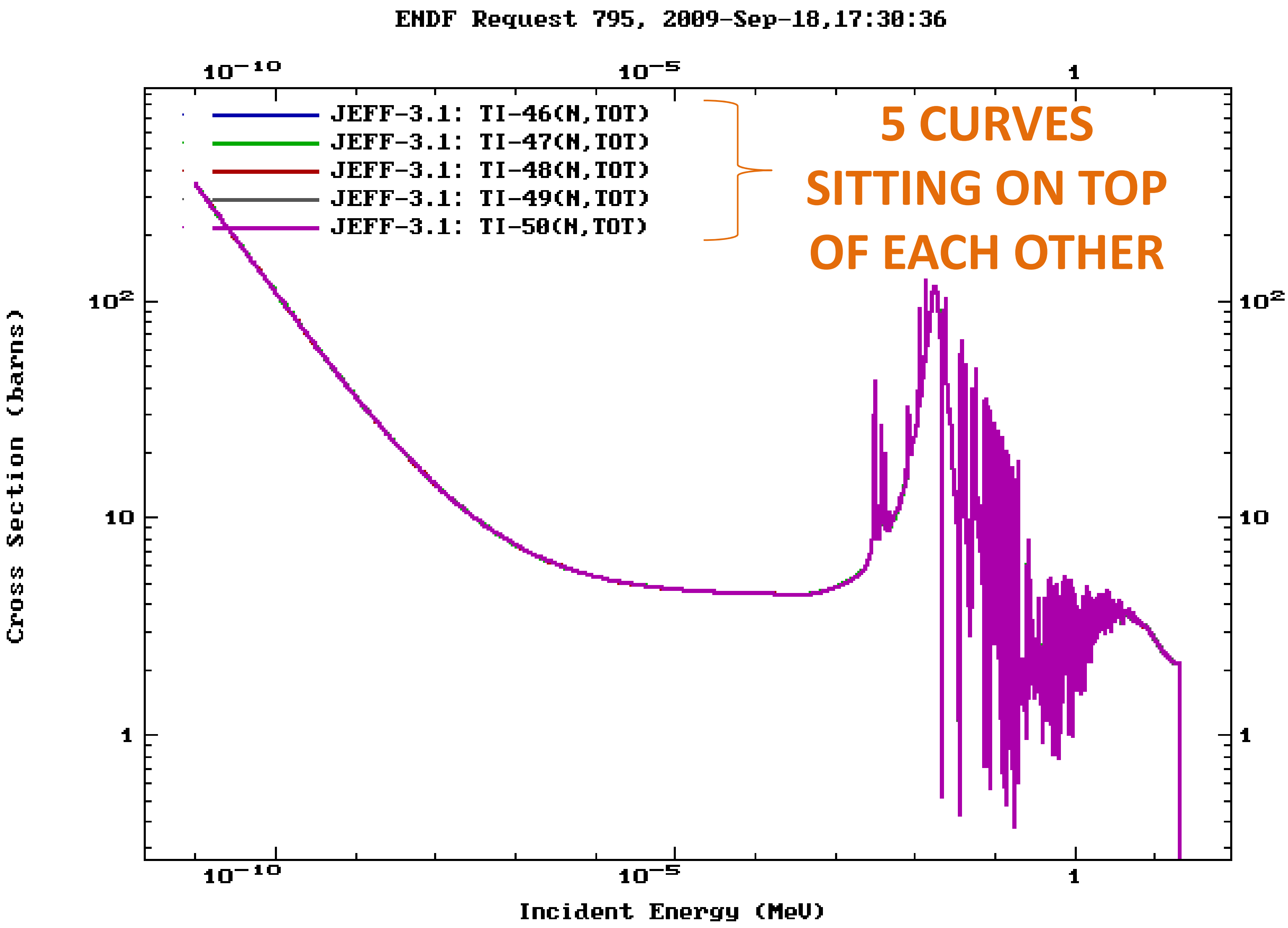
Models may even be more believable than measurements

Especially microscopic models built from bottom-up (instead of marcroscopic ones built top-down)

→ IAEA BENCHMARK OF SPALLATION MODELS

ESS' NUCLEAR DATA ACTIVITIES

- data pre-processing using NJOY and PREPRO
- preparation of non-ACE pointwise libraries
- data-checking: many errors still lurk behind publically available databases



some errors can only be discovered by accident

ROCK-SOLID FACILITIES + INFRASTRUCTURE

WE CAN DO EXPERIMENTS THERE

BUT WE CAN'T GO BACK IN TIME

TO DESIGN & BUILD CERN

SHALL BE AS GREEN AS IT CAN BE

CERTAINLY NOT AS GRAY

SHALL EMULATE THE

FREEDOM TO DO SCIENCE

ROCK-SOLID FACILITIES + INFRASTRUCTURE

WE CAN DO EXPERIMENTS THERE

BUT WE CAN'T GO BACK IN TIME

TO DESIGN & BUILD CERN