Geant 4

Ion and Neutron Transport in Geant4

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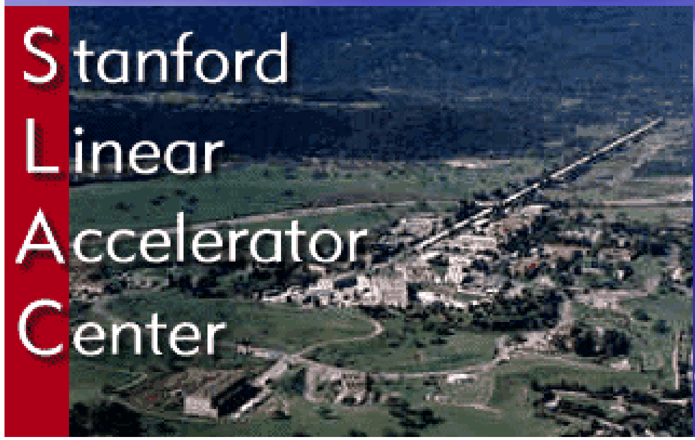
SLAC/SCCS

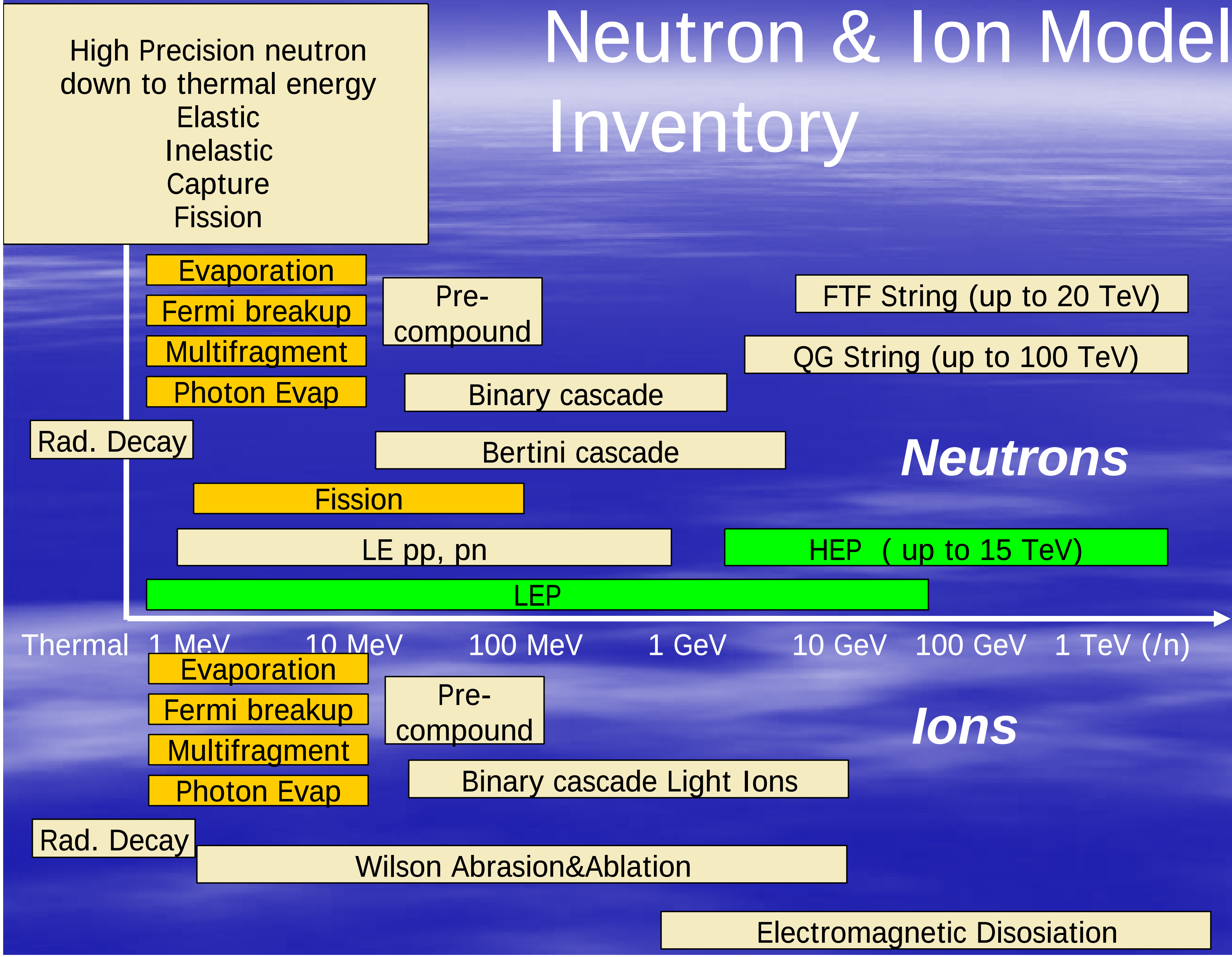
CALOR 2006



Outline

- Overview of Ion and Neutron Interaction in Geant4
- High energy neutrons interaction
- Low energy (<20 MeV) neutrons interaction
  - Neutron High Precision Models
- Ions inelastic interaction
  - Binary Cascade Light Ions
  - Wilson Abrasion & Ablation
- Ions electro magnetic dissociations
- Radio active decay

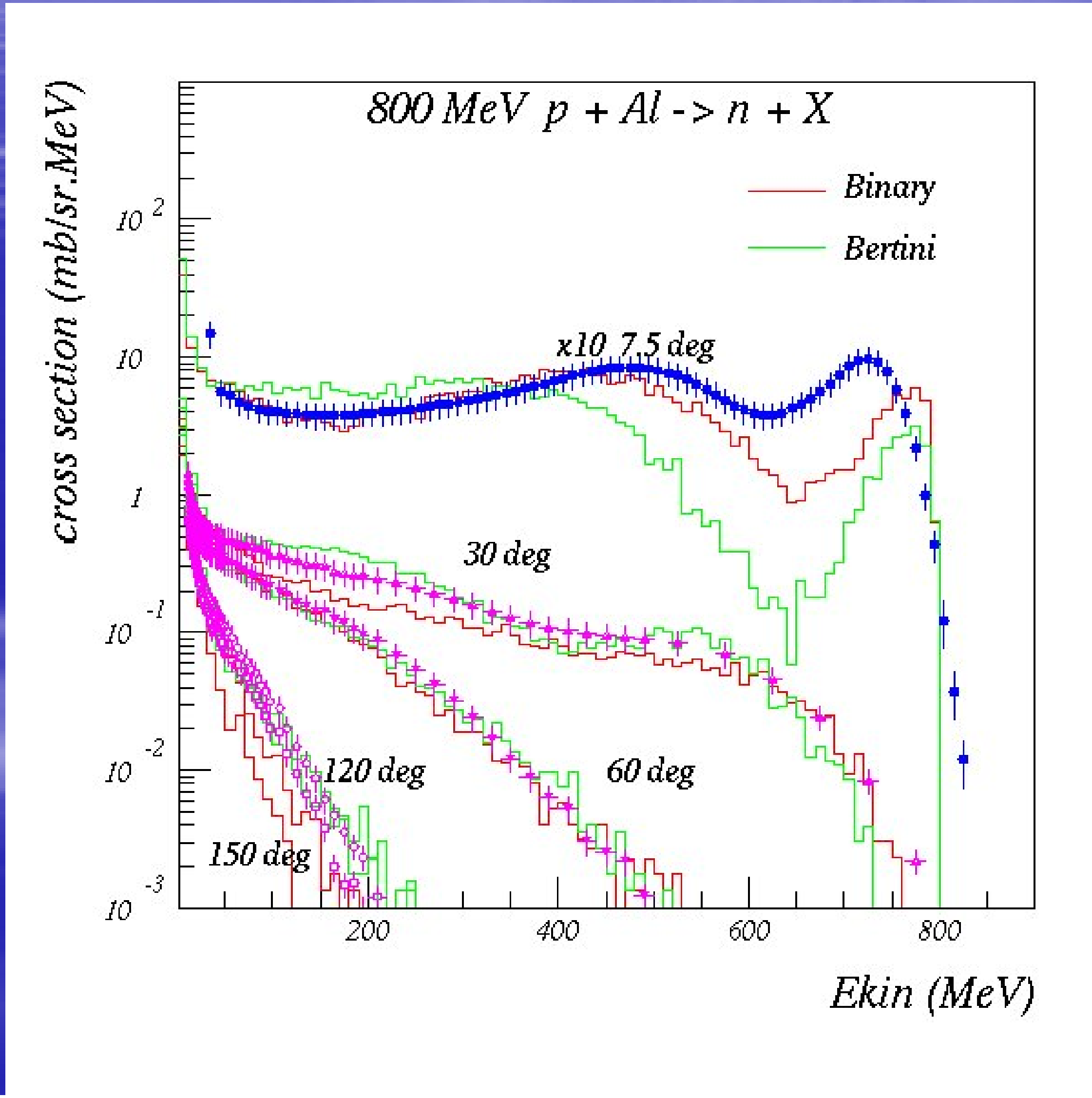
Neutron & Ion Models Inventory



High energy neutron physics

- Parameterized models
  - LEP 0~30 GeV
  - HEP ~15 GeV up to 15 TeV
  - a re-engineered version of GHEISHA
  - Elastic, Inelastic, Capture and Fission
- Theory driven models
  - Cascade Models
    - Binary Cascade < 3 GeV
    - Bertini Cascade < 10 GeV
  - High Energy Models ~15GeV < E < ~15 TeV
    - Quark-Gluon String (QGS)
    - Fritiof fragmentation (FTF)

Validation of Cascade Models



Low energy (< 20MeV) neutrons physics

- G4NDL (Geant4 Neutron Data Library)
- High Precision Neutron Models
  - Elastic
  - Inelastic
  - Capture
  - Fission
- NeutronHPorLEModel(s)
- Thermal neutron scattering S(α , β) Models

G4NDL (Geant4 Neutron Data Library)

- The neutron data files for High Precision Neutron models
- The data are including both cross sections and final states.
- The data are derived evaluations based on the following evaluated data libraries (in alphabetic order)
  - Brond-2.1
  - CENDL2.2
  - EFF-3
  - **ENDF**/B-VI.0, 1, 4
  - FENDL/E2.0
  - JEF2.2
  - JENDL-FF
  - JENDL-3.1,2
  - MENDL-2
- The data format is similar ENDF, however it is not equal to.
- After G4NDL3.8 we concentrated translation from **ENDF** library.
  - No more evaluation by ourselves.

Low Energy Neutron Transportation Elastic

- The final state of elastic scattering is described by sampling the differential scattering cross-sections
  - tabulation of the differential cross-section

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}(\cos\theta, E)$$

  - a series of legendre polynomials and the legendre coefficients

$$\frac{2\pi}{\sigma(E)}\frac{d\sigma}{d\Omega}(\cos\theta, E) = \sum_{l=0}^{n_l}\frac{2l+1}{2}a_l(E)P_l(\cos\theta)$$

Low Energy Neutron Transportation Inelastic

- Currently supported final states are (nA) n γ s (discrete and continuum), np, nd, nt, n 3He, n α , nd2 α , nt2 α , n2p, n2 α , np , n3 α , 2n α , 2np, 2nd, 2n α , 2n2 α , nX, 3n, 3np, 3n α , 4n, p, pd, p α , 2p d, d α , d2 α , dt, t, t2 α , 3He, α , 2 α , and 3 α .
  - 36 channels
- Secondary distribution probabilities are supported
  - isotropic emission
  - discrete two-body kinematics
  - N-body phase-space distribution
  - continuum energy-angle distributions
    - legendre polynomials and tabulation distribution
    - Kalbach-Mann systematic $A + a \rightarrow C \rightarrow B + b$, C:compound nucleus
  - continuum angle-energy distributions in the laboratory system

Low Energy Neutron Transportation Capture

- The final state of radiative capture is described by either photon multiplicities, or photon production cross-sections, and the discrete and continuous contributions to the photon energy spectra, along with the angular distributions of the emitted photons.
- For discrete photon emissions
  - the multiplicities or the cross-sections are given from data libraries
- For continuum contribution

$$f\left(E \rightarrow E_{\gamma}\right) = \sum_{i} p_i(E) g_i\left(E \rightarrow E_{\gamma}\right)$$

  - E neutron kinetic energy, E γ photon energies
  - pi and gi are given from data libraries
- If there is no final state data in ENDF files then Photon Evaporation model of Geant4, which uses Evaluated Nuclear Structure Data File (ENSDF) create final state products including Internal Conversion electrons

Low Energy Neutron Transportation Fission

- First chance, second chance, third chance and forth chance fission are into accounted.
- The neutron energy distributions are implemented in six different possibilities.
  - tabulated as a normalized function of the incoming and outgoing neutron energy $f(E \to E')$
  - Maxwell spectrum $f(E \to E') \propto \sqrt{E'} e^{E'/\Theta(E)}$
  - a general evaporation spectrum $f(E \to E') \propto E' e^{E'/\Theta(E)}$
  - evaporation spectrum $f(E \to E') = f\left(E' / \Theta(E) \right)$
  - the energy dependent Watt spectrum $f(E \to E') \propto e^{E'/a(E)} \sinh \sqrt{b(E) E'}$
  - the Madland Nix spectrum $f(E \to E') = \frac{1}{2}\left[g\left(E', \langle K_l \rangle\right) + g\left(E', \langle K_h \rangle\right) \right]$

Verification of High Precision Neutron models
Channel Cross Sections
20MeV neutron on Gd157

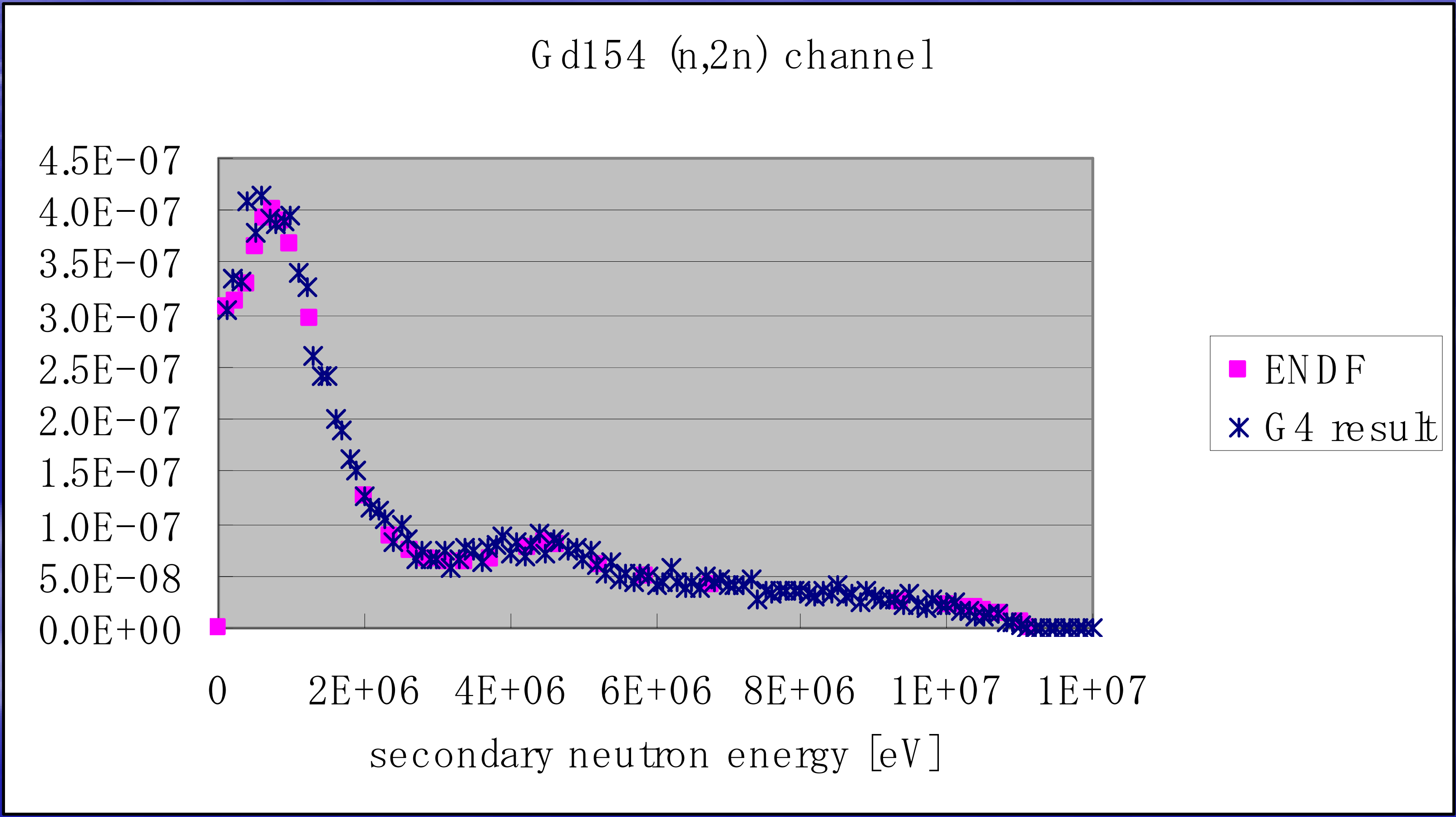
Geant4 results

- Ela XS 3.7104216 [barn]
- Inela XS 1.2508858
- Inela XS F01 0.99179298
- Inela XS F04 0.18413539
- Inela XS F06 0.020973994
- Inela XS F10 0.041302787
- Inela XS F23 0.009658162
- Inela XS F27 0.0030225183
- Cap XS 0.0017767842

ENDF data

- 3.708710+0 [barn]
- 9.940940E-1
- 1.836200E-1
- 2.126800E-2
- 4.064300E-2
- 9.717300E-3
- 3.306100E-3
- 1.646330E-3

Verification of High Precision Neutron Models
Energy Spectrum of Secondary Particles



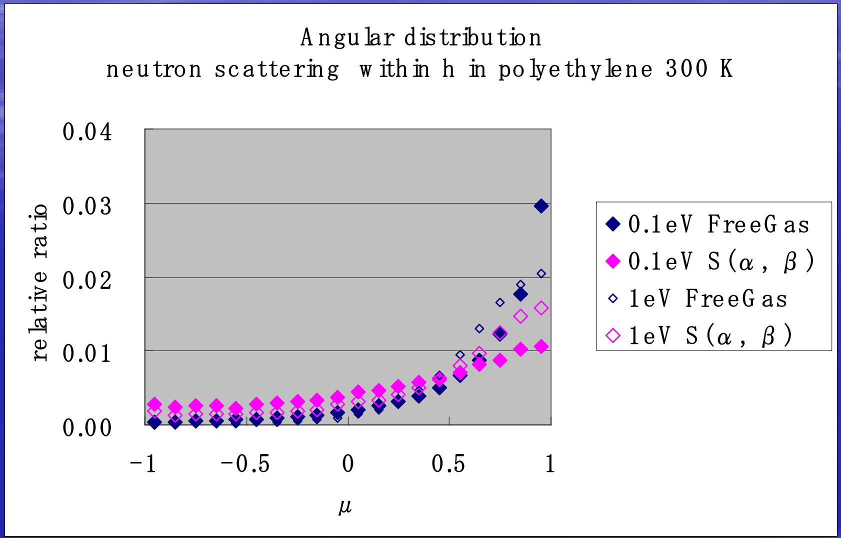
G4NeutornHPorLEModels

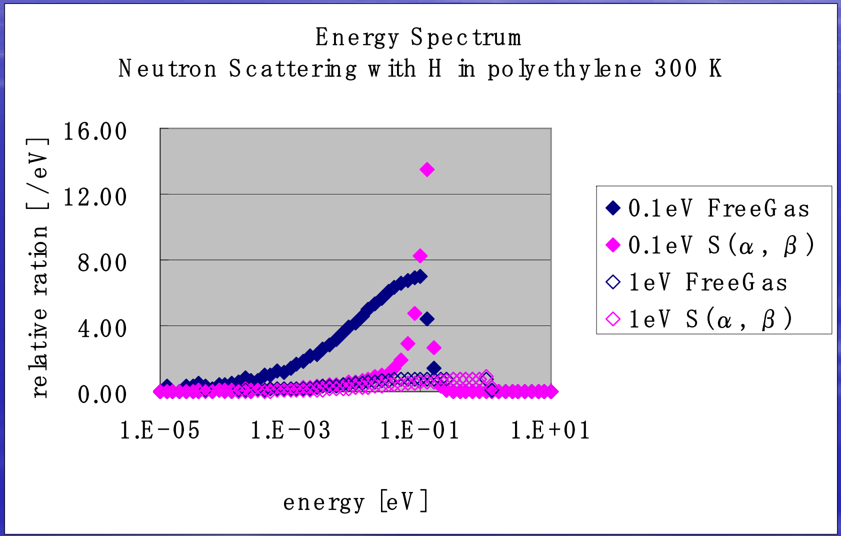
- Many elements remained without data for High Precision models.
- Those models make up for such data deficit.
- If the High Precision data are not available for a reaction, then Low Energy Parameterization Models will handle the reaction.
- Those can be used for not only for models (final state generator) but also for cross sections.
- Elastic, Inelastic, Capture and Fission models are prepared.

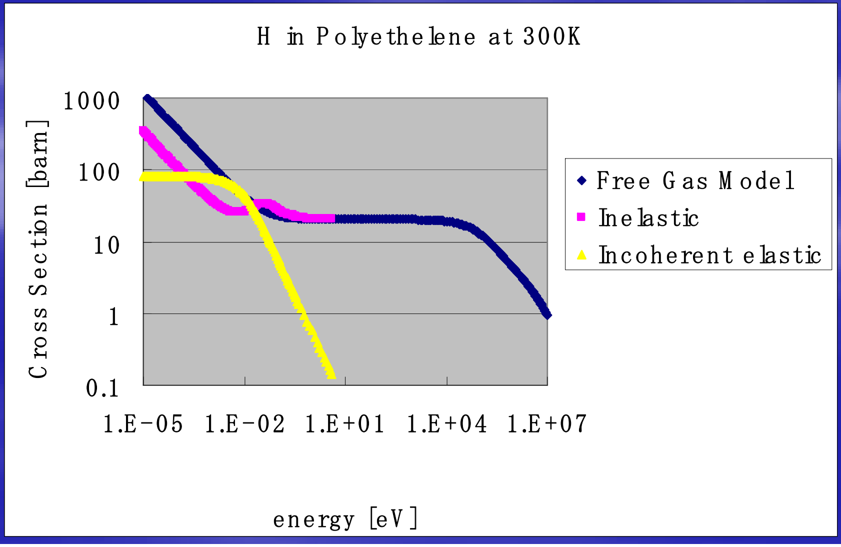
Thermal neutron scattering
S(α , β) Model

- For thermal neutron scattering from nuclei with chemically bonded atoms
- Based on thermal neutron scattering files from the evaluated nuclear data files ENDF/B-VI, Release2
- Coherent elastic, incoherent elastic and inelastic scattering are included
- Not Yet included latest release (v8.0.p01)

Cross section and Secondary Neutron Distributions of S(α , β) model







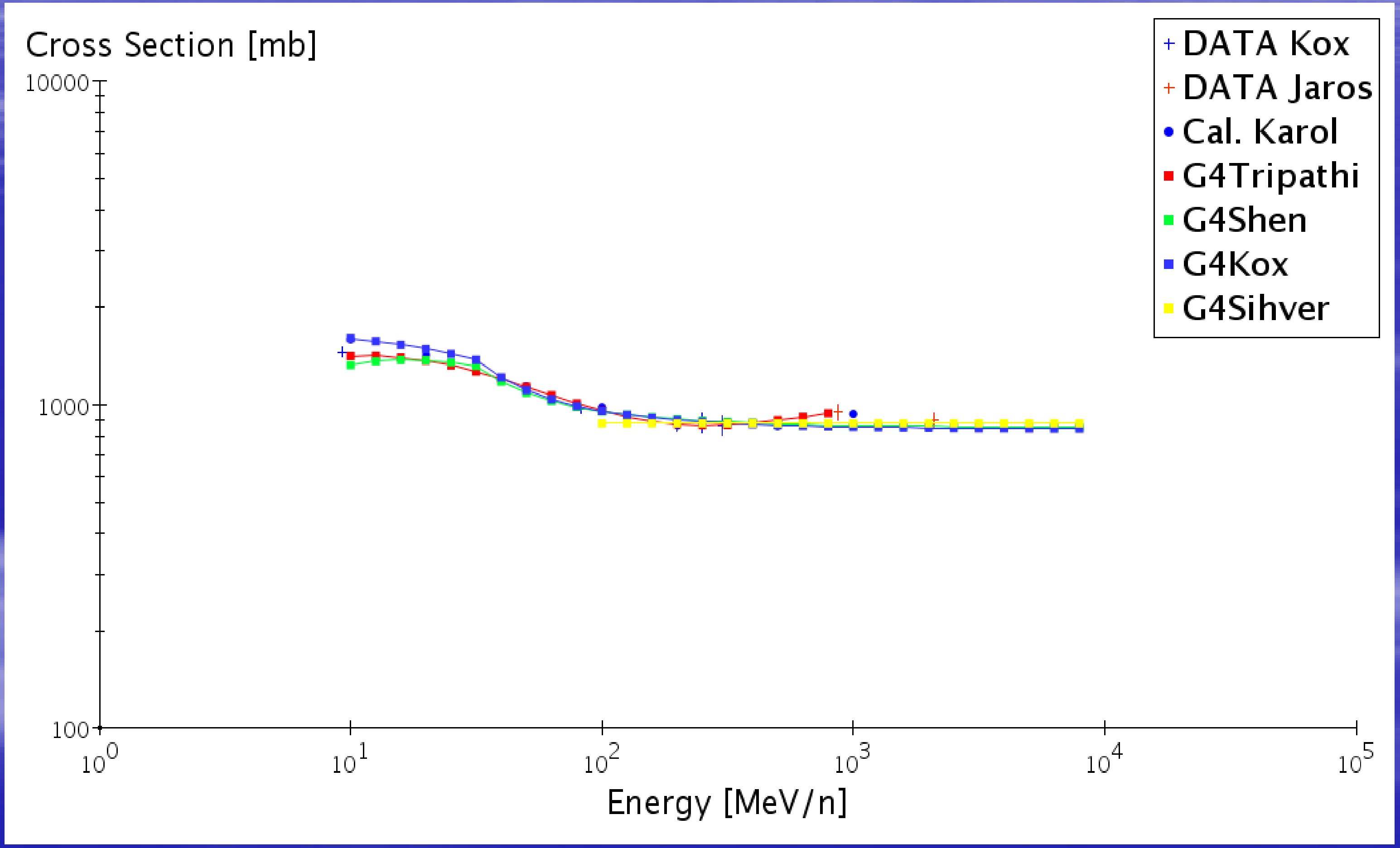
Ion Physics
Inelastic Reactions

- Cross Sections
  - Tripathi, Shen, Kox and Sihver Formula
- Model
  - G4BinaryLightIon
  - G4WilsonAbrasion

Cross Sections

- Many cross section formulae for NN collisions are included in Geant4
  - Tripathi Formula NASA Technical Paper TP-3621 (1997)
  - Tripathi Light System NASA Technical Paper TP-209726 (1999)
  - Kox Formula Phys. Rev. C 35 1678 (1987)
  - Shen Formula Nuclear Physics. A 49 1130 (1989)
  - Sihver Formula Phys. Rev. C 47 1225 (1993)
- These are empirical and parameterized formulae with theoretical insights.
- G4GeneralSpaceNNCrossSection was prepared to assist users in selecting the appropriate cross section formula.

Inelastic Cross Section C12 on C12



Binary Cascade
~Model Principals~

- In Binary Cascade, each participating nucleon is seen as a Gaussian wave packet, (like QMD)

$$\phi(x, q_i, p_i, t) = \left(2/(L\pi) \right)^{3/4} \exp\left(-2/L(x - q_i(t))^2 + ip_i(t)x \right)$$

- Total wave function of the nucleus is assumed to be direct product of these. (no anti-symmetrization)
- This wave form have same structure as the classical Hamilton equations and can be solved numerically.
- The Hamiltonian is calculated using simple time independent optical potential. (unlike QMD)

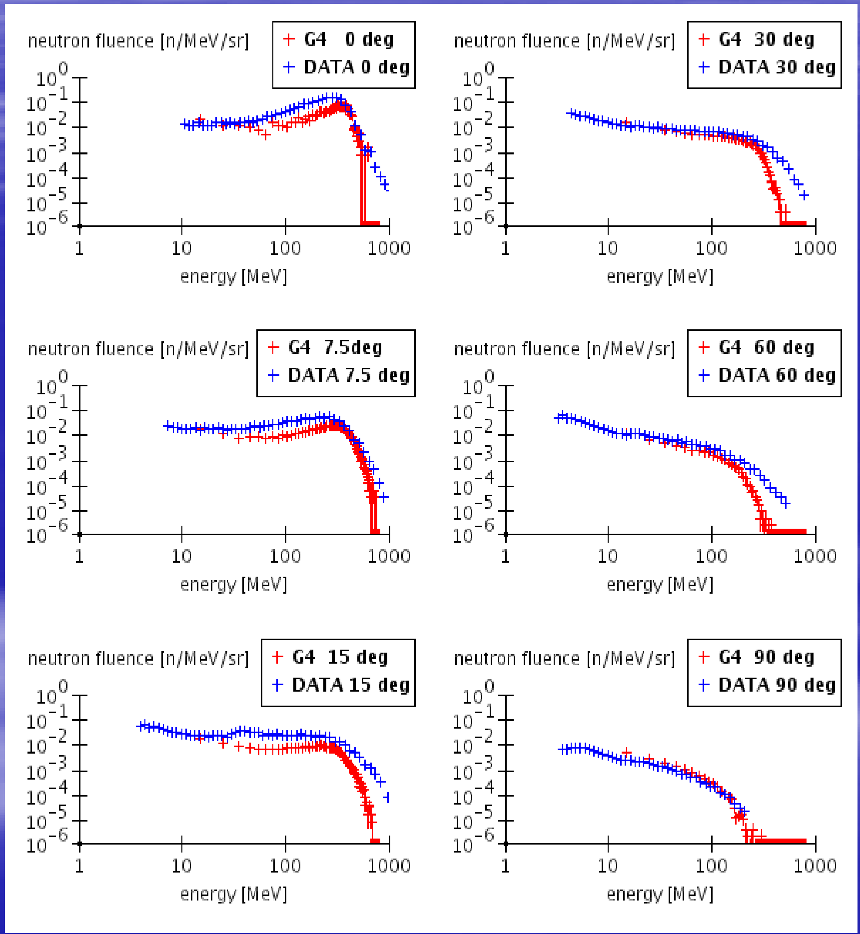
Binary Cascade ~nuclear model ~

- 3 dimensional model of the nucleus is constructed from A and Z.
- Nucleon distribution follows
  - A>16 Woods-Saxon model
  - Light nuclei harmonic-oscillator shell model
- Nucleon momenta are sampled from 0 to Fermi momentum and sum of these momenta is set to 0.
- time-invariant scalar optical potential is used.

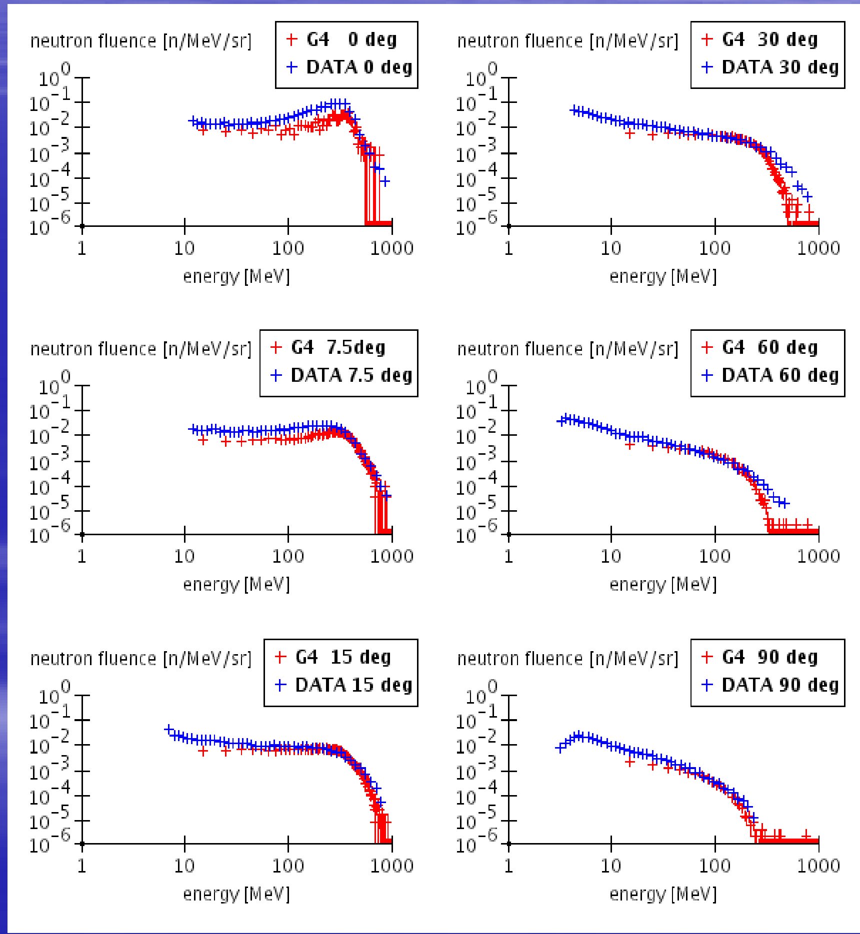
Binary Cascade
~ G4BinaryLightIonReaction ~

- Two nuclei are prepared according to this model (previous page).
- The lighter nucleus is selected to be projectile.
- Nucleons in the projectile are entered with position and momenta into the initial collision state.
- Until first collision of each nucleon, its Fermi motion is neglected in tracking.
- Fermi motion and the nuclear field are taken into account in collision probabilities and final states of the collisions.

Neutron Yield
Fe 400 MeV/n beams



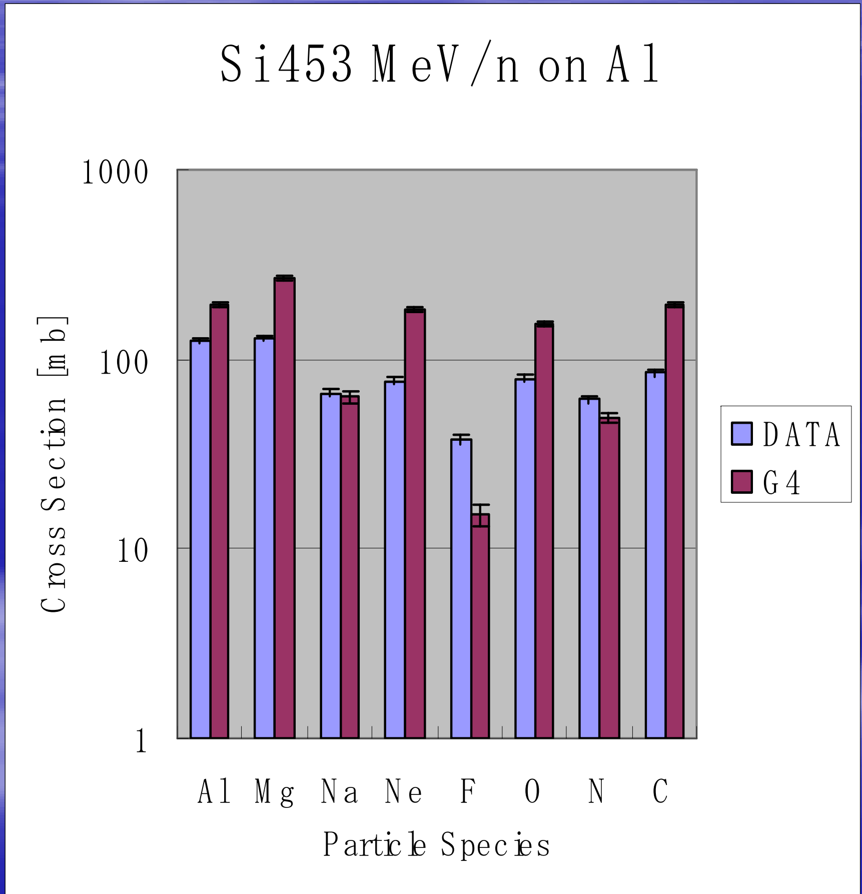
Copper

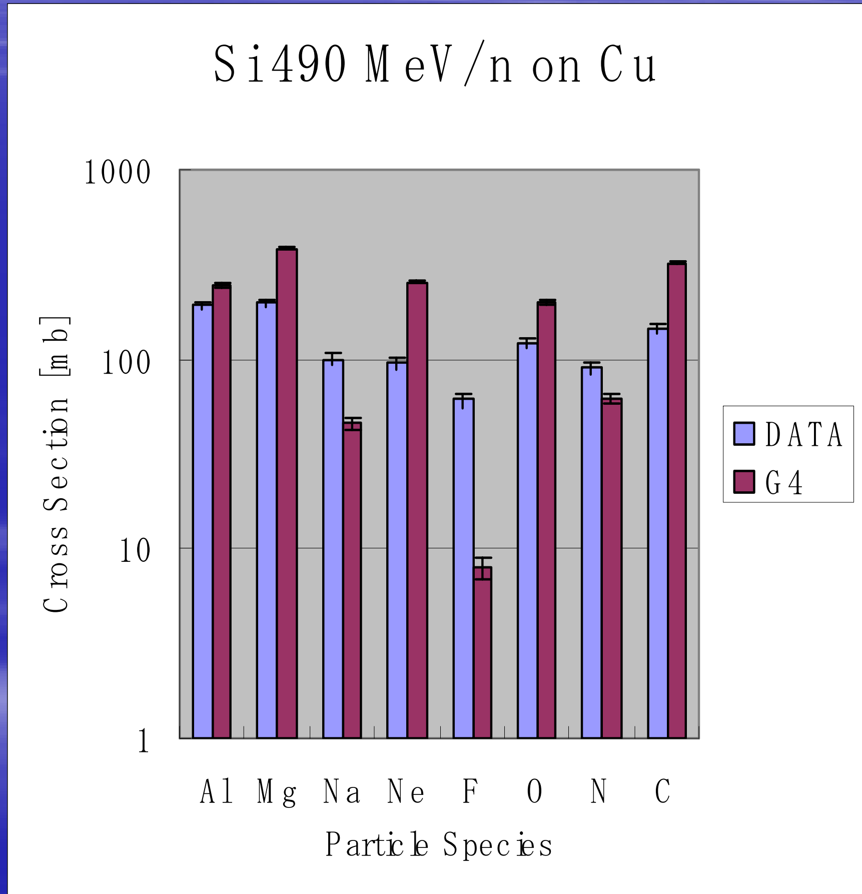


Lead

T. Kurosawa et al., *Phys. Rev.* **C62** pp. 04461501 (2000)

Fragment Production



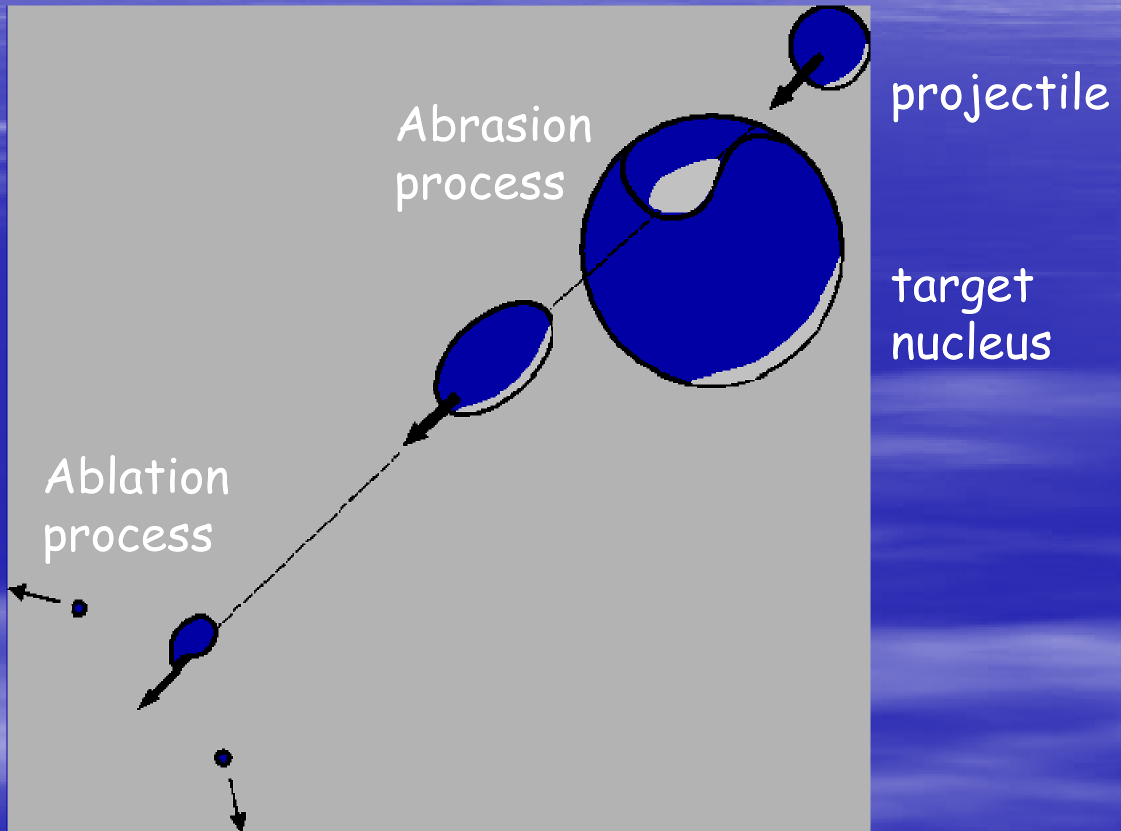


F. Flesch et al.,
J, RM, 34 237 2001

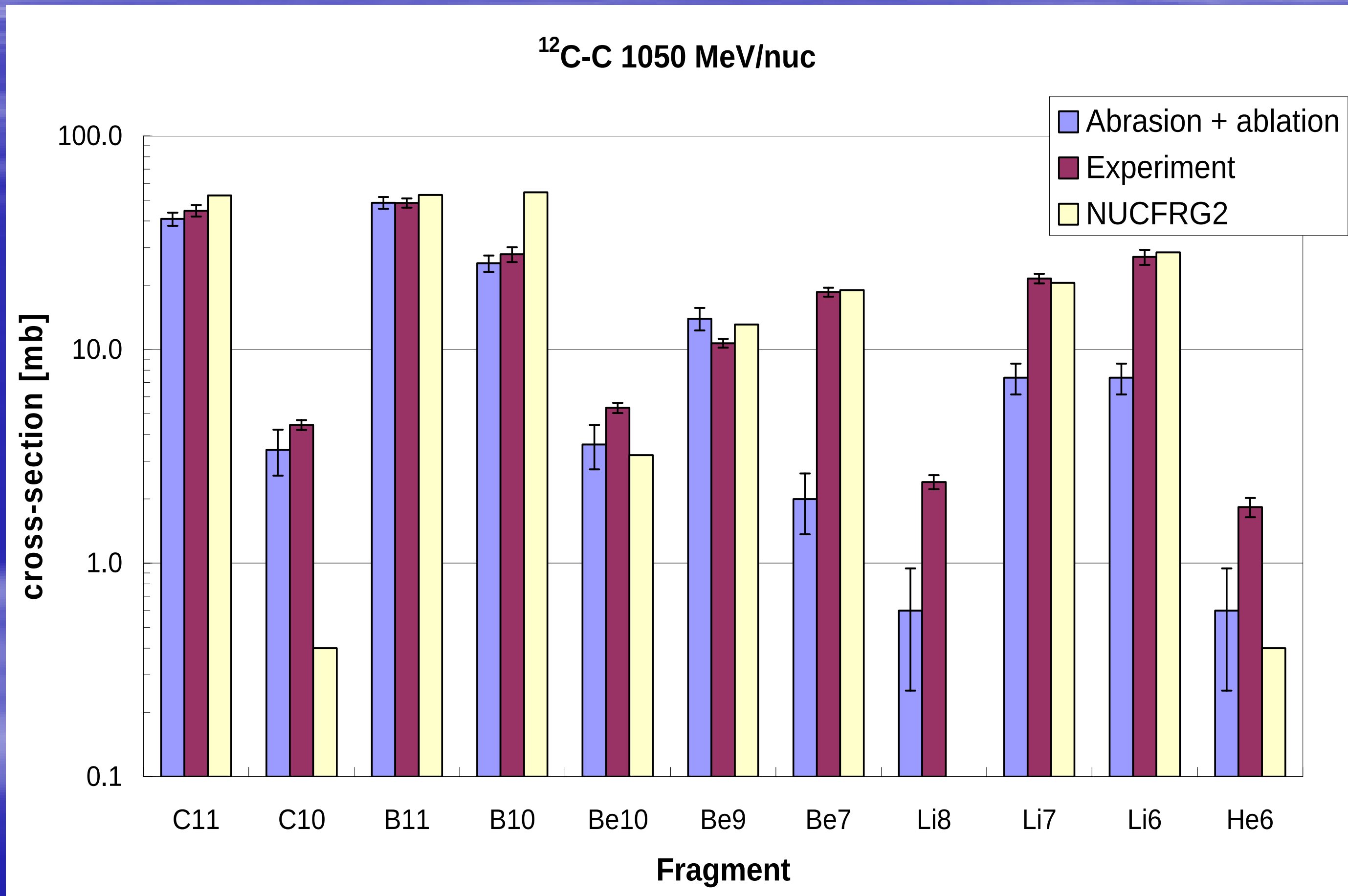
Wilson Abrasion & Ablation Model

- G4WilsonAbrasionModel is a simplified macroscopic model for nuclear-nuclear interactions based largely on geometric arguments
- The speed of the simulation is found to be faster than models such as G4BinaryCascade, but at the cost of accuracy.
- A nuclear ablation has been developed to provide a better approximation for the final nuclear fragment from an abrasion interaction.
- Performing an ablation process to simulate the de-excitation of the nuclear pre-fragments, nuclear de-excitation models within Geant4 (default).
- G4WilsonAblationModel also prepared and uses the same approach for selecting the final-state nucleus as NUCFRG2 (NASA TP 3533)

Abrasion & Ablation



Validation of G4WilsonAbrasionAblation model



Ion Physics
EelectroMagnetic Dissociation

- Electromagnetic dissociation is liberation of nucleons or nuclear fragments as a result of electromagnetic field by exchange of virtual photons, rather than the strong nuclear force
- It is important for relativistic nuclear-nuclear interaction, especially where the proton number of the nucleus is large
- G4EMDissociation model and cross section are an implementation of the NUCFRG2 (NASA TP 3533) physics and treats this electromagnetic dissociation (ED).

Validation of G4EMDissociaton Model and Cross Section

Projectile	Energy [GeV/nuc]	Product from ED	G4EM Dissociation [mbarn]	Experiment [mbarn]
Mg-24	3.7	Na-23 + p	124 ± 2	154 ± 31
Si-28	3.7	Al-27 + p	107 ± 1	186 ± 56
	14.5	Al-27 + p	216 ± 2	165 ± 24† 128 ± 33‡
O-16	200	N-15 + p	331 ± 2	293 ± 39† 342 ± 22*

Ion Physics
Radio Active Decay

- To simulate the decay of radioactive nuclei
- Empirical and data-driven model
- α , β +, β - decay and electron capture are implemented
- Data (RadioactiveDecay) derived from Evaluated Nuclear Structure Data File (ENSDF)
  - nuclear half-lives
  - nuclear level structure for the parent or daughter nuclide
  - decay branching ratios
  - the energy of the decay process.
- The data includes more than 2,200 isotopes
- If the daughter of a nuclear decay is an excited isomer, its prompt nuclear de-excitation is treated using the Photon Evapolation Model of Geant4

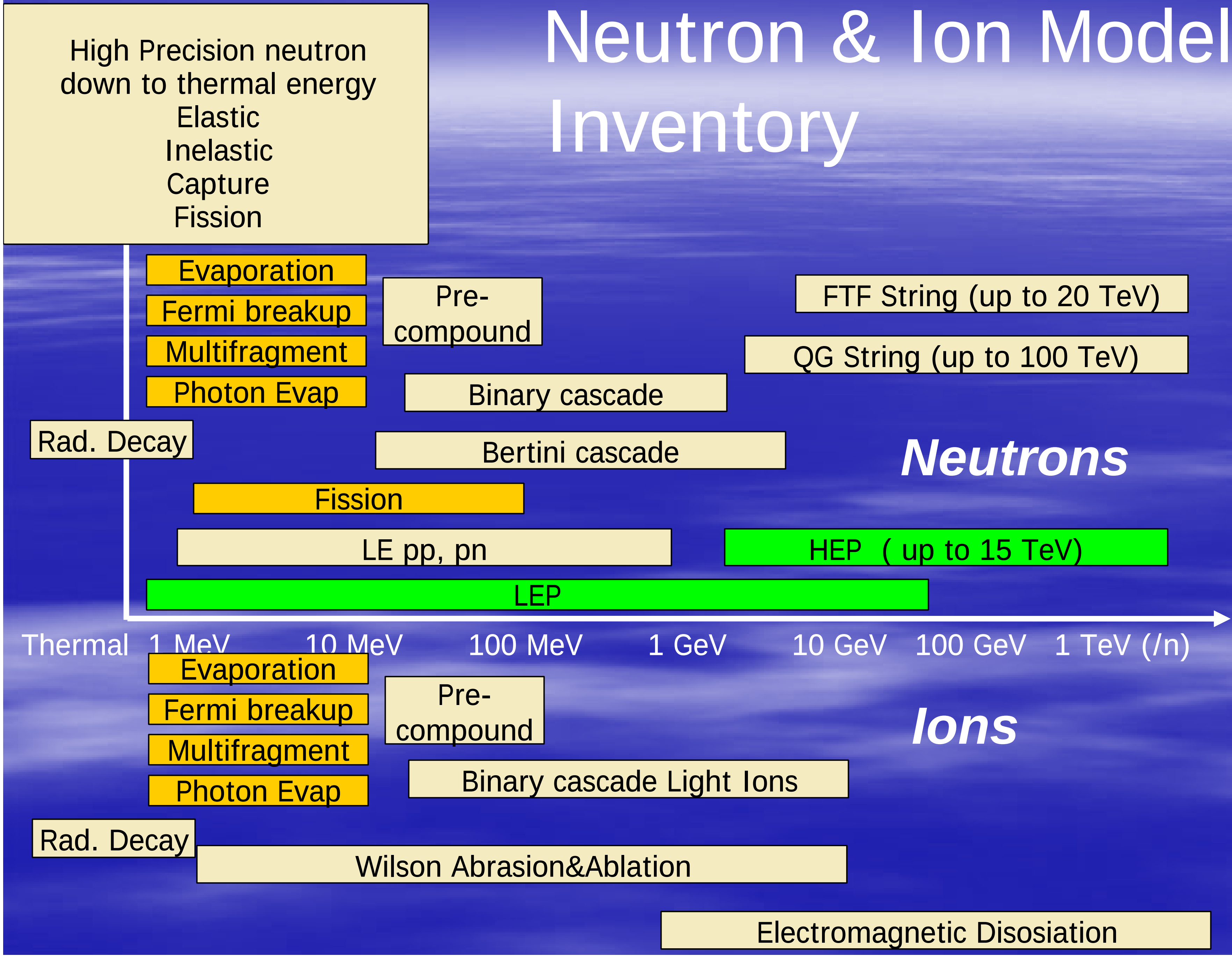
Other Ion related processes already implemented in Geant4

- Ionization Energy Loss
- Multiple Scattering
- Cerenkov Radiation
- Xray Transition
- All these processes work together for Ion transportation in Geant4

Geant4 Hadronic Contributors

- *Gunter Folger (CERN)*
- *Aatos Heikkinen (Helsinki)*
- *Vladimir Ivantchenko (CERN/ESA)*
- *Tatsumi Koi (SLAC)*
- *Mikhail Kossov (CERN)*
- *Fan Lei (QinetiQ)*
- *Nikolai Starkov (CERN)*
- *Pete Truscott (QinetiQ)*
- *Hans-Peter Wellisch*
- *Dennis Wright (SLAC)*

Neutron & Ion Models Inventory



Conclusions

- Now Geant4 has abundant processes for Ion and neutron interactions with matter from thermal energy to much above TeV energy.
- Without any extra modules, users may simulate ion transportation in the complex and realistic geometries of Geant4
- Validation and verification have begun and results show reasonable agreement with data. This work continues.
- The Geant4 toolkit contains a large variety of complementary and sometimes alternative physics models covering the physics of neutrons and ions.
- The development of new models will continue to be pursued in the future by the Geant4 Collaboration, in response to the evolving requirements of the wide experimental community using it.