A simulation tool for the calculation of NIEL in arbitrary materials using GEANT4

- Some new results -

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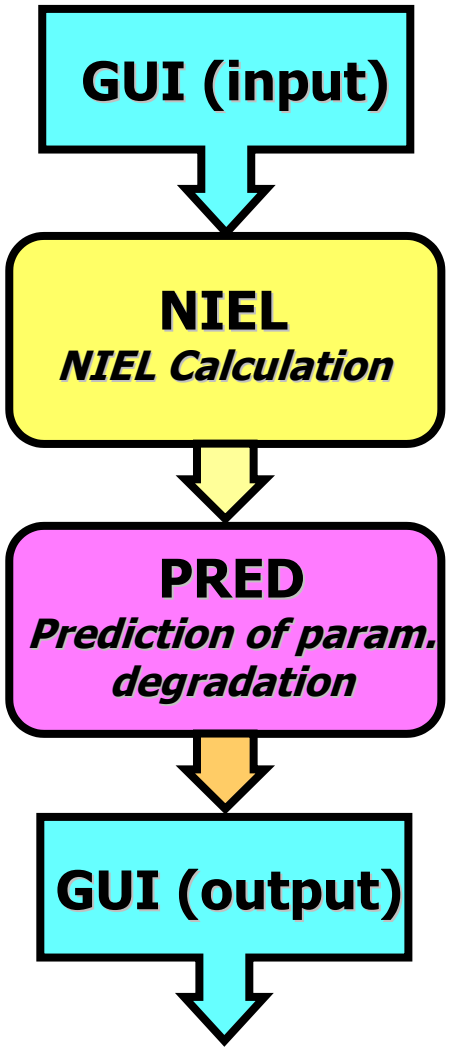
Overview

- **The Simulation Tool (ST)**
  - **Objectives**
  - **Main modules**
- **New results (*NIEL* data)**
- **Possible integration under SPENVIS**

Tool Objectives

- **Develop a S/W tool prototype allowing to**
  - **calculate displacement damage effects in semiconductors induced by non-ionising energy loss (NIEL) during a space mission**
  - **estimate the resulting performance degradation of electron. circuit components**
- **Aim**: ***Facilitate qualification procedure for new electronic devices used in space missions***

ST Main Modules



General Tool Features

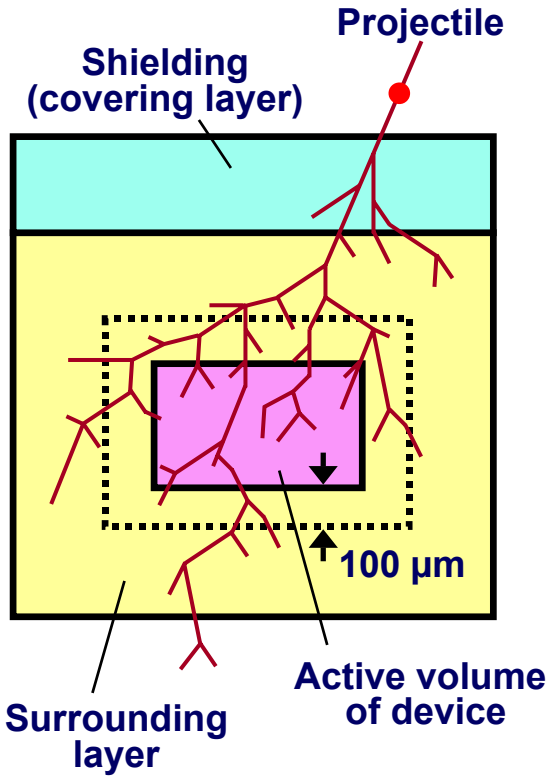
- **Modular structure**
  (easy maintenance)
- **Designed as internet application**
  (remote or local use of ST)
- **Modules NIEL and PRED partly use GEANT4**
- **Running under MS Windows**
  (portable to other platforms)

Tool Module "NIEL"

Two options of running module NIEL

(a) **NIEL calculation by applying the Lindhard partition function to the initial energy of the recoils** (not for high-energy projectiles, not for compounds with high ΔZ, no information about 3D defect distribution)

(b) **NIEL calculation by MC simulation of the damage cascade step by step in the vicinity of the active volume** (validity of algorithms and models in Geant4 limited at low energy; e.g. binary collision model rather should be replaced by a molecular dynamics code)



NIEL Calculation

Algorithmic basics for Lindhard approximation

- **Contribution of a given recoil type to NIEL:**

$$NIEL(E) = \frac{N_A}{A} \int_{T_{\min}}^{T_{\max}} dT\, Q(T)\, \xi(T)\, T \left(\frac{d\sigma}{dT} \right)_E$$

E	**Kinetic energy of impinging particle**
T	**Kinetic energy of recoil or fragment**
dσ/dT	**Differential partial cross section for recoil creation**
Q(T)	**Fraction of T being lost by non-ionising processes (Lindhard partition)**
ξ(T)	**Empirical efficiency function (optional)**
N_A/A	**Number of atoms per gram**

Tool Module "PRED"

Prediction of parameter degradation

Input: - *NIEL* curves (*NIEL* vs. particle energy)
- ground test data (experimental damage factors)

Algorithm:
- Extrapolation of ground test data over the required energy range using empirical power function scaling:

$$\boxed{\text{(parameter degradation)} \propto NIEL^{x}} \quad \text{(x=adjust. exponent)}$$

- *Alternative option*: Use a modified NIEL curve calculated by applying an efficiency function
- Fold particle spectra with the energy dependence of the damage factors

Output: Expected parameter degradation for a given mission radiation environment

NIEL Scaling Concept

Observation

- In many cases surprisingly good relationship between NIEL and device degradation (damage factor) of electronic components (e.g. max. power output of solar cells)
- For the same NIEL value, device degradation often is the same, independent of particle type and energy.

Missing Link

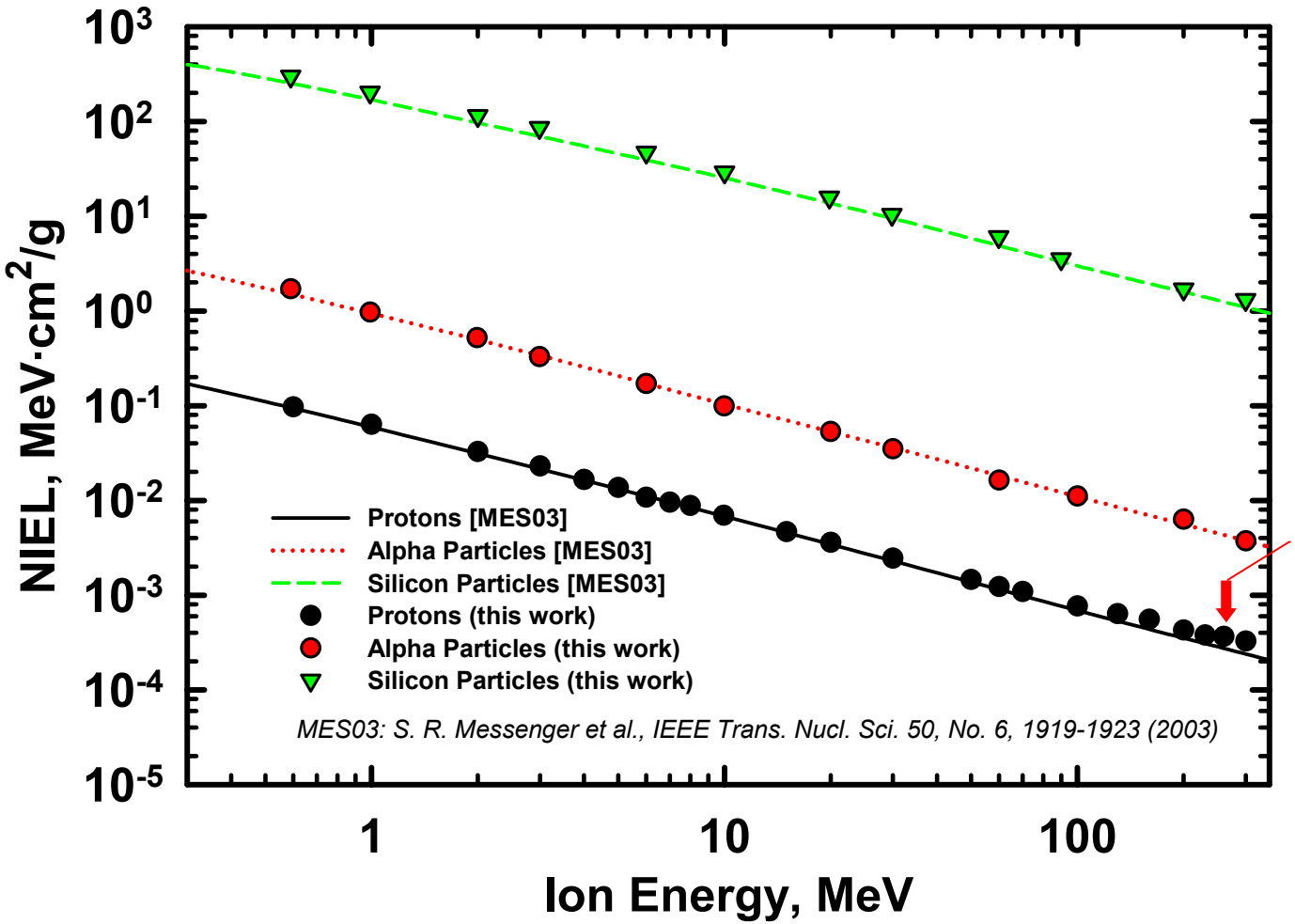
Implementation of screened Coulomb scattering

- **GEANT4 presently contains only algorithms for multiple Coulomb scattering without recoil generation**
- **To obtain the energy of the Coulomb recoils and to follow up single displacement events within the damage cascade, binary elastic Coulomb scattering had to be included in ST**
- **We decided to implement an algorithm developed at Vanderbilt University (by courtesy of the authors)*)**
  ***Advantage*: Already successfully validated**

***) M. H. Mendenhall, R. A. Weller, Nucl. Instr. Meth. B 227, Issue 3, 420-430 (2004)**

Validating Implementation

NIEL due to elastic Coulomb scattering of p, α and Si in silicon



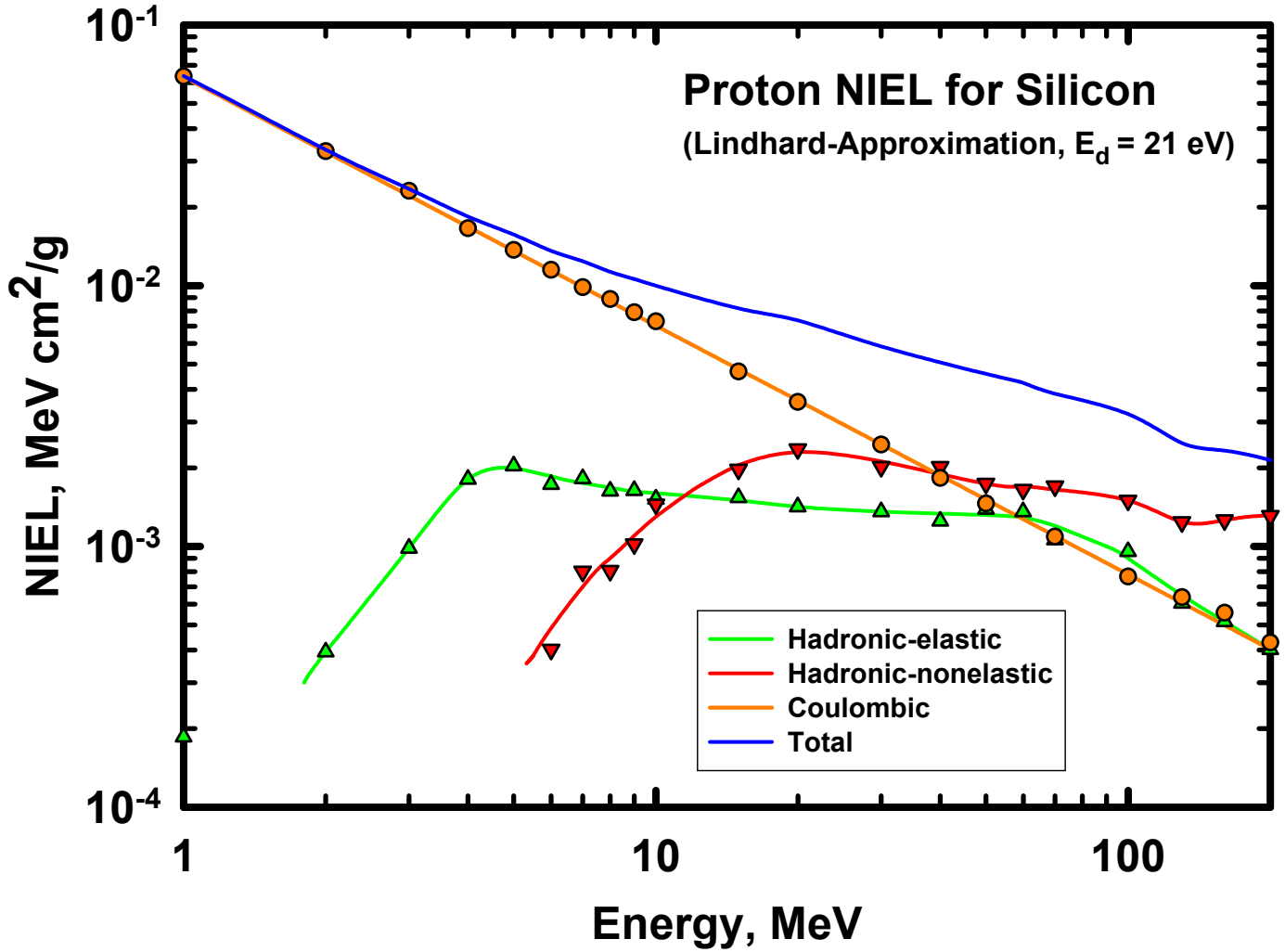
Dependency on projectile properties as expected

Symbols: Relativistic effects for E_p>100 MeV

Curves: Non-relativistic analytical method

Validating Module NIEL (1)

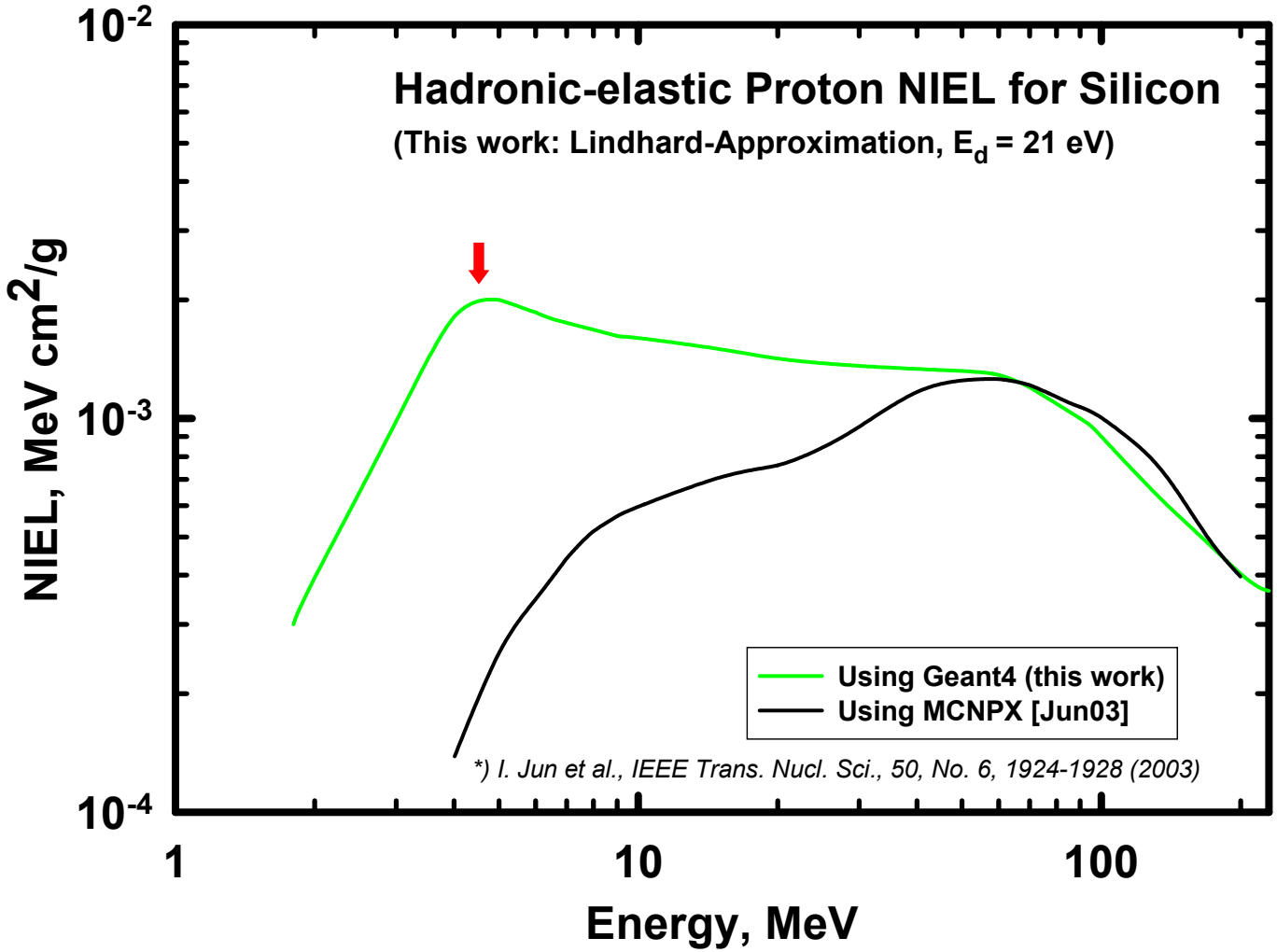
NIEL for p in silicon – Hadronic and Coulomb contribution



ST separately yields contributions of different types of interactions and recoils

Validating Module NIEL (2)

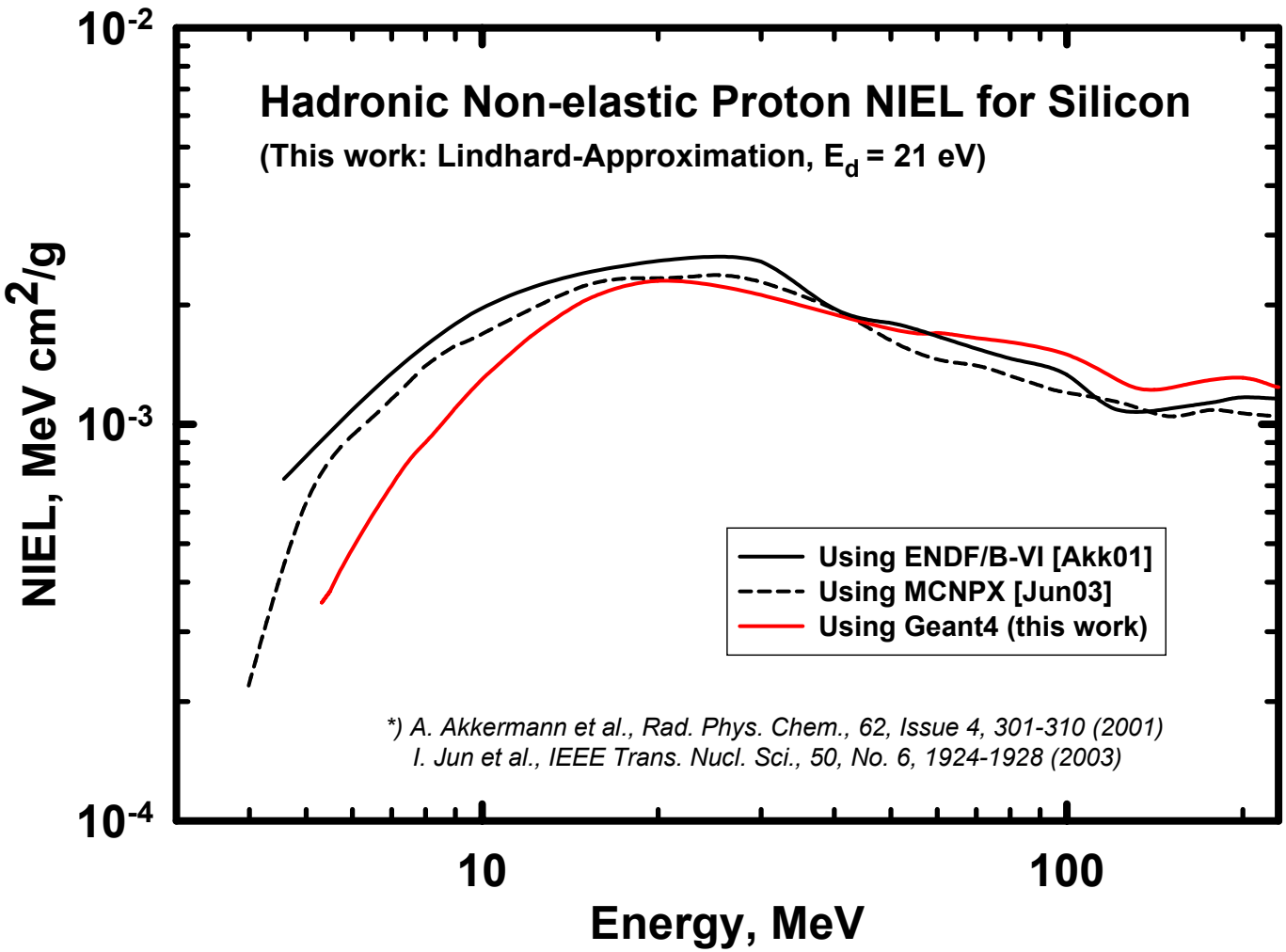
Hadronic elastic NIEL for p in silicon



Somewhat unexpected curve shape at low E. Underlying G4 process (*G4LELastic*) presently being revised (cf. bug reports #534 & #601). Lit. reference*)

Validating Module NIEL (3)

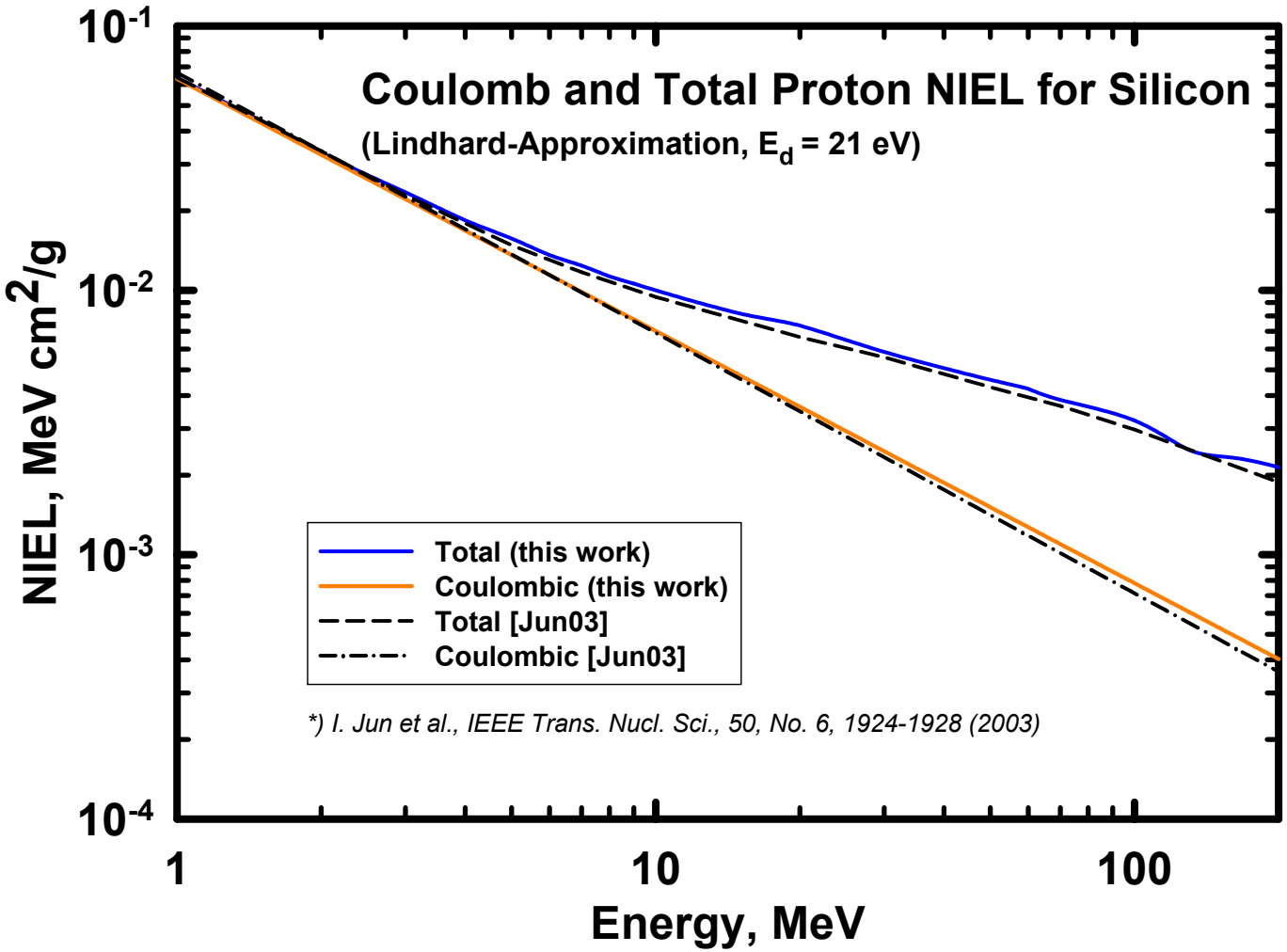
Hadronic non-elastic NIEL for p in silicon



Data & curve shape largely correspond to reference *)

Validating Module NIEL (4)

NIEL due to screened Coulomb elastic scattering of p in silicon

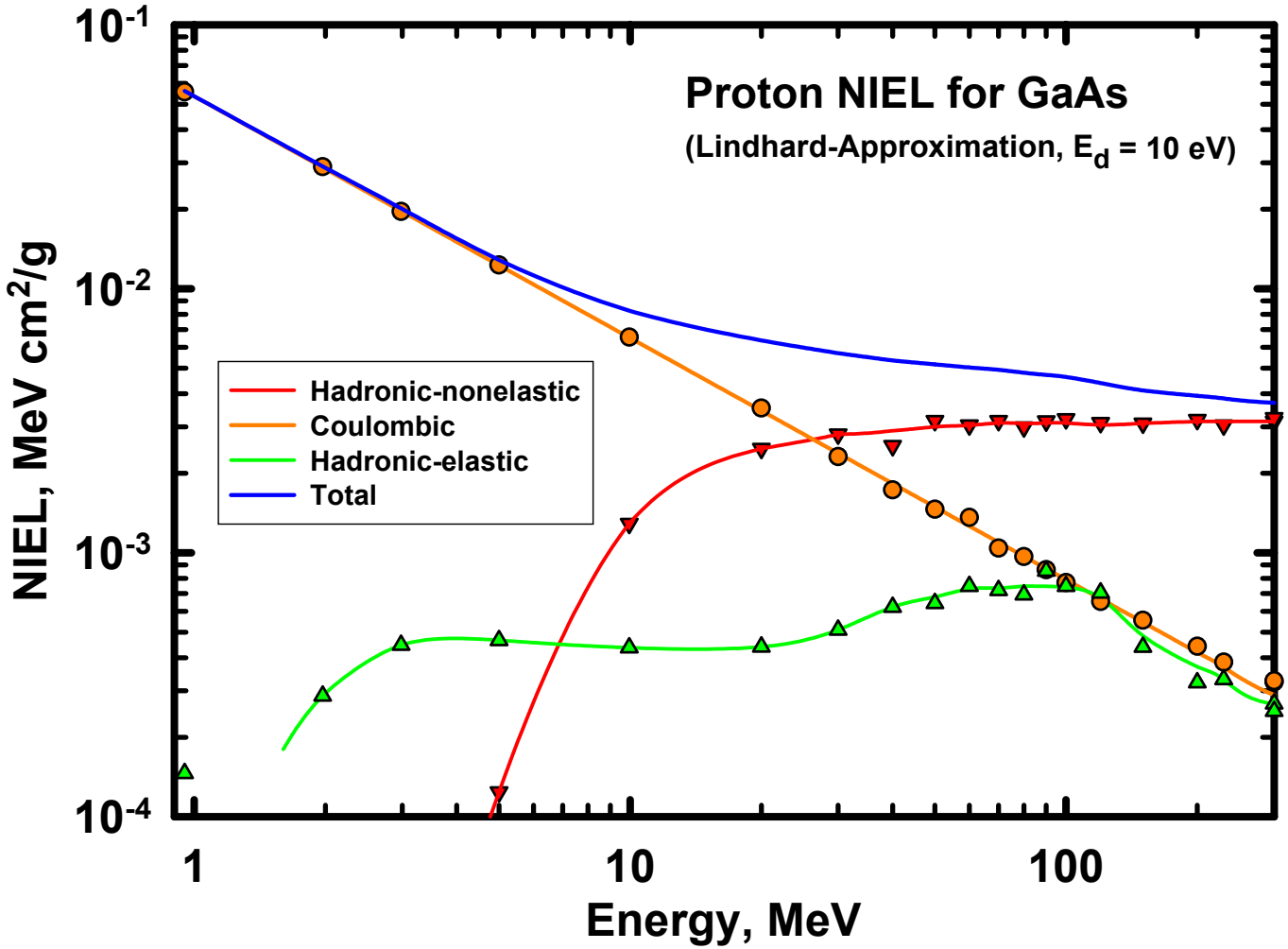


Coulomb contribution and total NIEL as expected

Lit. reference*)

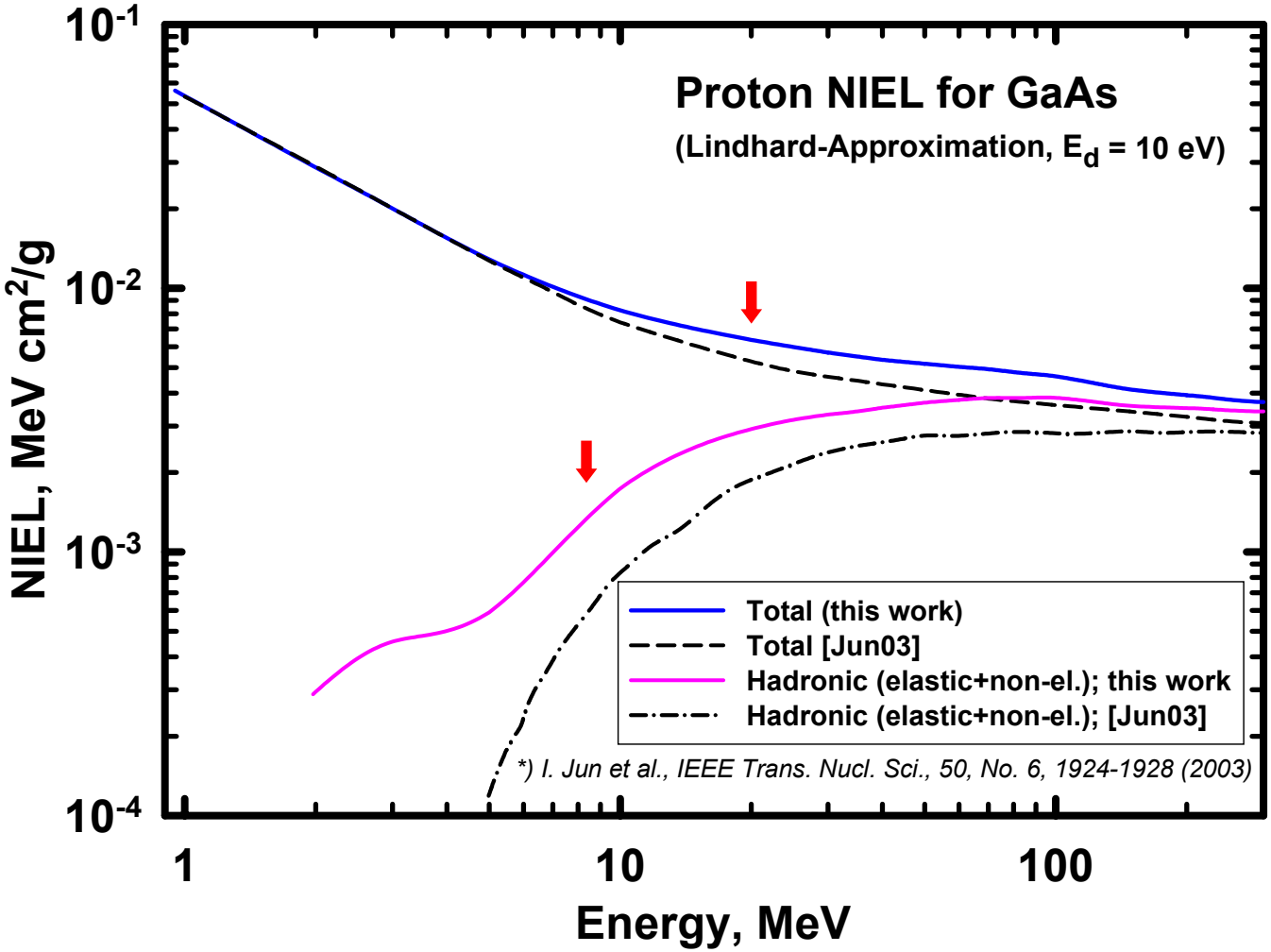
Using Module NIEL (1)

Total NIEL for p in GaAs – Hadronic and Coulomb contribution



Using Module NIEL (2)

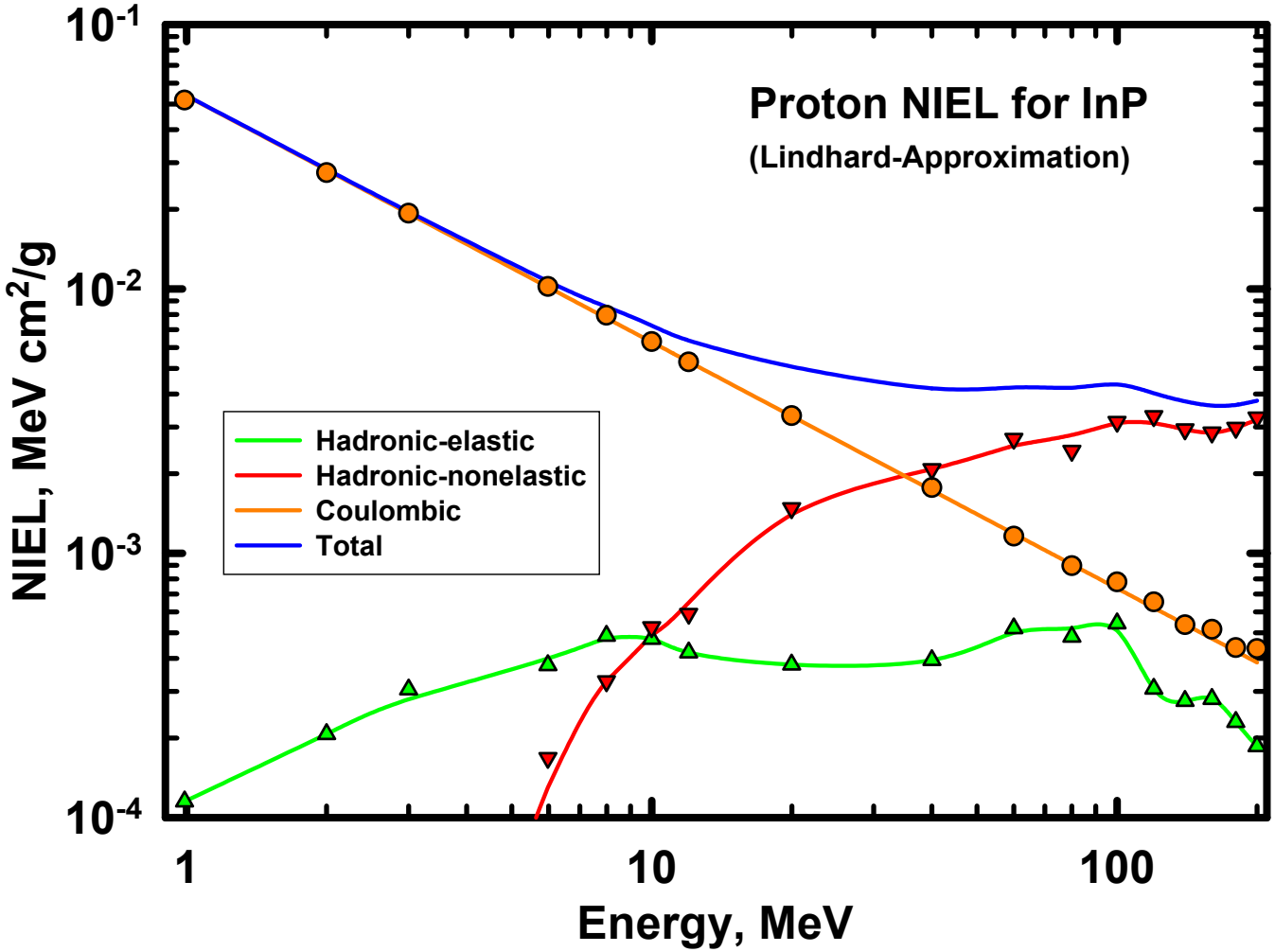
NIEL for p in GaAs – Hadronic contribution and total NIEL



Essentially in agreement with Lit. data. Hadronic contribution too high compared to Jun et al. Lit. reference*)

Using Module NIEL (3)

Total NIEL for p in InP – Hadronic and Coulomb contribution



ST under SPENVIS (1)

SPENVIS

- Orbit generator
- Radiation environment
- S/C shielding + MULASSIS

Mission particle spectra on device level

Ground Test Irrad.

- Irradiate device with one particle type and energy

Parameter degradation for one particle type & energy

Simulation Tool

NIEL calculation for each particle type

NIEL scaling of parameter degradation

Prediction of mission parameter degradation

ST under SPENVIS (2)

How to integrate ST under SPENVIS? – Some issues

- **The Simulation Tool (ST) and SPENVIS already worked successfully together by off-line data exchange**
- **Complete integration of ST under SPENVIS would be difficult**
- **Part of the ST functionality already exists in SPENVIS** (e.g. damage prediction using pre-calculated NIEL curves)
- **It would be feasible to**
  - **integrate only those algorithms of ST that are missing in SPENVIS**
  - **extend existing modules in SPENVIS (MULASSIS) to enable NIEL calculation in 1D geometry**
  - **extend modules that are planned to be integrated (e.g. GRAS) to enable NIEL calculation in 3D geometry**

Presently, a requirements document is worked out to integrate ST algorithms under SPENVIS

Summary

- **ST runs much more reliable with GEANT4 version 7.1 than with version 5.x** *(e.g. no longer problems with nucleus de-excitation; see bug report #540)*
- **Validity of hadron elastic scattering process in G4 still doubtful** *(routine G4LELastic)*
- **Choice and applicability of ionisation processes for hadrons at very low energies poorly documented in G4** *(options Standard/Low-Energy)*
- **Binary elastic Coulomb scattering code (needed for ST) still missing in G4 → Implementation of the Vanderbilt code in ST** *(turned out to be useful in ST and should be considered for G4)*
- **The Simulation Tool yields NIEL data for various projectiles and arbitrary targets in good agreement with literature data** *(as far as available)*