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An expert-assisted system for improving the quality of IBA simulations by SIMNRA

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Abstract. SIMNRA is a popular software suite for the simulation of ion beam analysis (IBA) spectra. SIMNRA 7.04 implements a new expert system supporting users in selecting the most accurate simulation settings for a given ion/target combination at a given energy and geometry. The expert system is a piece of artificial intelligence emulating the ability and knowledge of a human IBA expert. It points out potential problems with the current simulation parameters and recommends model settings with enhanced accuracy.

1. Introduction

Software for the simulation of ion beam analysis (IBA) energy spectra, such as Rutherford backscattering spectrometry (RBS), elastic recoil detection analysis (ERDA) non-resonant nuclear reaction analysis (NRA), or particle-induced Gamma ray emission (PIGE) is well developed [1], and popular codes such as SIMNRA [2, 3] or NDF [4] provide high numerical accuracy of simulations. In most cases, the accuracy of simulations is determined by the accuracy of basic input data (such as stopping powers, straggling models, or cross-section data) and not by implementation details of the codes [5, 6].

All codes provide a large number of different input data sets selectable by the user: SIMNRA for example provides six different stopping power models, three different straggling models, several models for the shape of straggling distributions, small and large angle scattering can be switched on or off, etc. This large number of possibilities renders it difficult to select the most accurate models for a given ion/target combination, ion energy and geometry - especially for inexperienced users. This problem cannot be overcome by appropriate default settings of simulation codes, because these are usually driven by programming or legal requirements, such as public availability of data or the permission to distribute additional third-party software: The default settings are therefore not necessarily the most accurate ones for a given setup, but the ones legally possible. Moreover, some settings (such as the dual scattering option in SIMNRA) increase accuracy, but at the cost of strongly increased computing time. The decision, if accuracy of simulations or a fast calculation is more important, cannot be made by software, but can be only made by the user.

The selection of the most accurate settings requires experience and understanding of the underlying physics models. These can be gained by reading the literature, by reading the software documentation, by training courses, or by discussions with experienced colleagues working in the same field. But in any case, this process is time consuming, and even for experienced users oversights of clumsy parameter settings sometimes happens.

This paper presents a new solution to this problem: An expert system that supports users in selecting the most accurate simulation settings for a given ion/target combination at a given energy and geometry. The expert system is a piece of artificial intelligence that emulates the ability and knowledge of a human IBA expert. It points out potential problems with the current simulation parameters and recommends model settings with enhanced accuracy for a given experiment in order to improve the quality and accuracy of IBA simulations and data analysis.

2. The SIMNRA expert system

The SIMNRA expert system is available in SIMNRA 7.04. It is implemented as system of If-Then rules emulating the knowledge of a human IBA expert. It points out potential problems with the current simulation setup through warnings and hints and recommends model settings with enhanced accuracy. The system output are recommendations. These can be observed, but without requirement. The final decision of parameter settings is always with the user, not the software.

The system has several levels of notifications:

- **Error:** An error is a setting that renders a calculation impossible. Usually these are formally incorrect parameter settings, for example incident ion energy below or equal to zero, no or impossible elements in the target, no selected cross-sections, etc. Error conditions must be solved before a simulation calculation can be performed.
- **Warning:** A warning is a setting that results in inaccuracies exceeding 2% over a larger energy range of the spectrum. Examples include the selection of an inaccurate stopping power model for the current ion/target combination, a difference of live and real times exceeding 2% while live time correction is switched off, etc.
- **Hint:** A hint is a setting that results in inaccuracies not exceeding 2% over a limited energy range of the spectrum. Typical examples are the selection of an inaccurate straggling model, multiple and/or plural scattering are switched off for targets containing high-Z elements, etc.
- **Ok:** A setting that is considered to have best possible accuracy, or that results in inaccuracies not exceeding 0.1%.
- **Disregard:** A setting that has no influence on the simulation, typically because that parameter is not used with the current settings. A typical example would be a live time below 0 s (which is formally incorrect and otherwise would cause an Error condition) if live time correction is switched off: In that case that parameter does not play any role as it is not used in calculations.

Due to computing time limitations the level of inaccuracy usually cannot be calculated precisely, but has to be estimated based on simplified models. The distinction between Hints and Warnings is sometimes subjective and may reflect some prejudice of the author.

A typical output of the system is shown in Fig. 1. Every output consists of two parts: A description of the detected problem, and a recipe how to solve it. Underlined text in light blue are direct links that open the respective forms.

3. Performed tests

3.1. Formal correctness of simulation parameters

All parameters are checked for formal correctness, i.e., energies, times, lengths etc. must be larger (or larger equal where appropriate) than zero, the target must contain at least one element, all elements in the target must be valid, at least one cross-section must be selected, etc. Formal correctness of pairs of parameters is checked where appropriate, i.e., the real time must be larger or equal to the live time, etc.

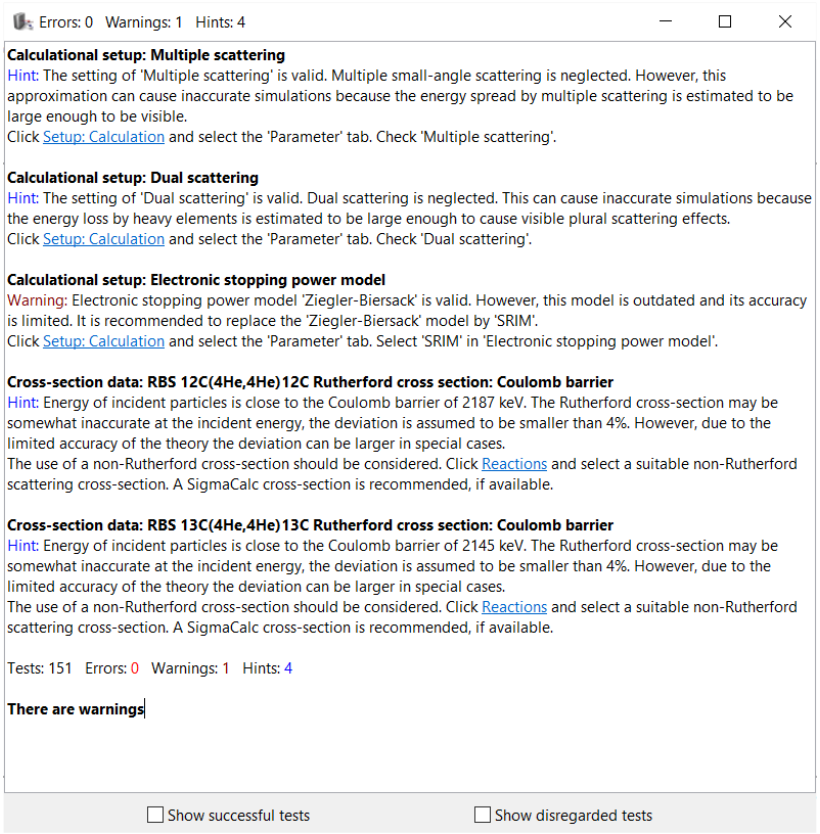

Fig. 1: Typical output of the expert system.

3.2. Geometry of the experiment

Incident angle α, exit angle β and scattering angle θ must be compatible with a conic section at the sample surface [7], otherwise a Warning is issued.

3.3. Metadata of a measurement

An experimental IBA spectrum is always accompanied by metadata, such as date and time of measurement, name of the raw data file, parameters of the data acquisition system, etc. While some metadata are important for traceability of measurements and quality assurance, some other metadata are important for improving the accuracy of simulation calculations. These are real and live times of a measurement (necessary for live time correction and pile-up calculation), the shaping time of the amplifier system and information about the use of a pile-up rejector (necessary for pile-up calculation). These parameters are stored in some data file formats for experimental data, but may be lacking in others. If an experimental spectrum is present, then the corresponding metadata should be also present: Values for live and real time should be given, otherwise a Hint is issued. The live time correction should be switched on, otherwise a Warning or Hint is issued. The pile-up calculation should be switched on, otherwise a Warning or Hint is issued.

Pure simulation calculations (without experimental spectrum) do not require metadata: In this case metadata are Disregarded.

3.4. Stopping power model

- SRIM 2003 [8] and later stopping powers are assumed to have good accuracy.
- Andersen-Ziegler (1977) [9, 10], Ziegler-Biersack (1985) [11], Konac et al. (1998) [12] stopping powers are assumed to be outdated, and a Warning is issued if these are used for simulation calculations.

- DPASS [13] stopping powers are assumed to have good accuracy for all ions heavier than He, and for all ions well below the stopping power-power maximum. DPASS stopping powers for H and He ions are assumed to have good accuracy at energies well above the stopping power maximum. However, a Hint is issued, that the spectrum may be less accurate at larger energy losses. DPASS stopping powers for H and He ions are assumed to be less accurate at energies in the vicinity of the stopping power maximum, and a Warning is issued if the incident energy is in this range.

3.5. Straggling model

- Bohr straggling [14] is assumed to have good accuracy only for incident H isotopes in lighter target elements at energies > 5000 keV/amu. In all other cases the accuracy is assumed to be limited and a Hint is issued.
- Chu straggling [15] neglects charge-state fluctuations and is assumed to have good accuracy only for incident H isotopes. In all other cases a Hint is issued.
- Yang straggling [16] is assumed to have good accuracy for all ion species.

3.6. Electronic screening to Rutherford cross-section

- The unscreened Rutherford cross-section [17] is assumed to be relatively inaccurate, and a Warning is issued.
- L'Ecuyer screening [18] is assumed to have good accuracy at backscattering angles > 90°. At smaller angles a Hint is issued.
- Andersen [19] and Universal [20] screening are assumed to have good accuracy at all angles and all energies.

3.7. Coulomb barrier

The Coulomb barrier, i.e., the energy where the cross-section deviates by more than 4% from its Rutherford value, is calculated according to [21] for ^{1}H, ^{2}H, ^{3}H, ^{3}He, ^{4}He, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{12}C, ^{14}N, ^{16}O ions. A Warning is issued if the Rutherford cross-section is used at energies above the Coulomb barrier.

As discussed in [22], the theory from [21] has only limited accuracy. Therefore already at energies in the range 90% to 100% of the Coulomb barrier a Hint is issued.

3.8. Multiple and plural scattering

- If multiple small-angle scattering [23] is switched off and the energy loss by heavy elements (with Z > 20) exceeds 2.5% of the incident energy, then a Hint is issued.
- If plural scattering [24] is switched off and the energy loss by heavy elements (with Z > 20) exceeds 10% of the incident energy, then a Hint is issued.
- SIMNRA uses Rutherford cross-sections for the calculation of plural scattering. This may result in inaccuracies, if plural scattering is switched on and the energy of incident particles is above the Coulomb barrier, see above. In this case a Warning is issued.

4. Conclusions

SIMNRA 7.04 implements a new expert system, that supports users in selecting the most accurate simulation settings for a given ion/target combination at a given energy and geometry. The expert system is a piece of artificial intelligence emulating the ability and knowledge of a human IBA expert. It points out potential problems with the current simulation parameters and recommends model settings with enhanced accuracy for a given experiment in order to improve the quality and accuracy of IBA simulations and data analysis. It also propels the use of metadata of measurements, such as live- and real times or pile-up parameters, which can improve simulation accuracy but are often disregarded.

Limitations of the expert system are its inability to detect incorrect experimental settings, such as incorrect incident energy or geometry. It cannot recommend cross-section data for non-Rutherford scattering or nuclear reactions, as in most cases the real accuracy of cross-section data sets is unknown. The expert system recommends SigmaCalc cross-sections [25] (if available for a given ion – target combination), as these are based on multiple measurements and a theoretical model and should have improved accuracy compared to individual measurements. The expert system also does not propose target structures based on a given experimental spectrum.

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