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Software aspects of the Geant4 validation repository

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Abstract. The Geant4, GeantV and GENIE collaborations regularly perform validation and regression tests for simulation results. DoSSiER (Database of Scientific Simulation and Experimental Results) is being developed as a central repository to store the simulation results as well as the experimental data used for validation. DoSSiER is easily accessible via a web application. In addition, a web service allows for programmatic access to the repository to extract records in JSON or XML exchange formats. In this article, we describe the functionality and the current status of various components of DoSSiER as well as the technology choices we made.

1. Introduction

Software collaborations in high energy physics regularly perform validation and regression tests for simulation results. This is the case for the Geant4 [1] collaboration and the developers of the GeantV [2] R&D project, toolkits for the simulation of radiation-matter interaction. It is also the case for GENIE [3], Monte Carlo event generator for neutrino interactions. A validation test compares simulation results with data obtained by various experiments while a regression test compares results of two or more versions of the software for an observable. As the areas of application expand, tests are improved and new tests are developed to insure that the physics processes are modeled correctly. As the number of regularly performed validation and regression tests increases and the collection of results grows, storing them and making them available to members of participating collaborations and the user community in general becomes a challenge. Therefore DoSSiER (Database of Scientific Simulation and Experimental Results) is being developed to collect and organize the materials in one central repository and to make this data easily available via a web application and web service. DoSSiER should be of general interest to collaborators and the user community. For example it should help experimenters to find answers to questions like:

- How well does the simulation describe the data of interest to the experiment?
- What data are actually used to validate the implemented physics?
- Which of the various models best describe the data of interest to the experiment?
- What are the benefits of switching to the latest improved version of the software?



2. Requirements

Below we briefly list the requirements and the desired functionality.

- It should be possible to store multidimensional experimental and simulation data used for validation in the form of arrays of data points and as histograms with meta-data. In addition, it should be possible to store complete plots with meta-data.
- Provide an API (Application Program Interface) to the database.
- Provide a web service which allows programmatic access. This allows the retrieval of records using any programming language that can handle HTTP requests and can parse the returned JSON/XML strings. A C++ API is of particular interest since it allows access to DoSSiER records directly from C++ validation jobs.
- The web application should provide an easy-to-use web-interface providing search engines and easy-to-navigate menus with default values, and should allow the user to select and overlay tests with experimental data. The actual plots are created on the fly.
- The web application and service should be based on modern Internet technologies and industry standards. It should also provide a fresh modern look and adhere to all security requirements set by the hosting laboratories.

We expect a relatively modest data-volume and number of requests to the system. The main users are the developers of the toolkits that will periodically provide updates with new simulation results. The update on the database with the new contributions will be centrally organized and we foresee monthly update campaigns (for example synchronized with the release of the Geant4 monthly releases). We expect that when the database will be populated with more results, experiment experts interested in performances of the simulation toolkits will regularly consult the webpages. In the case the number of requests increases substantially the web-portal could be scaled adding new instances of the web service. We do not expect that the usage of the system will impose scaling issue on the underlying database.

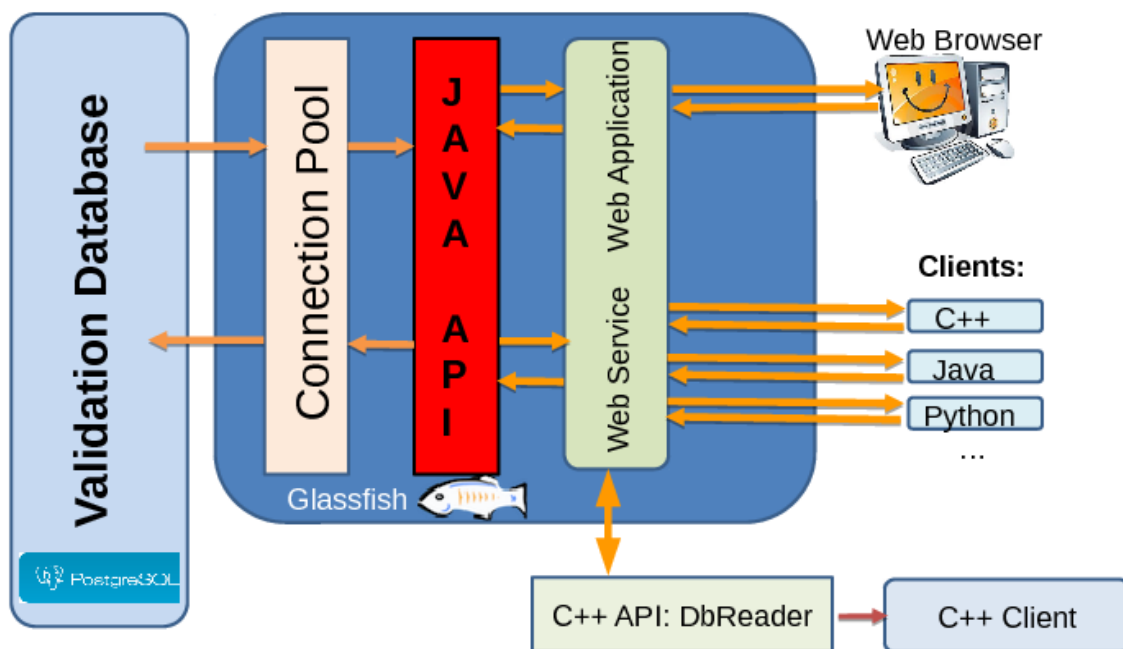


Figure 1. Software components of DoSSiER.

3. Software Components

DoSSiER is comprised of the software components shown in Figure 1. Each component will be described in detail in the following part of this section. All the technologies that we use are very well integrated in the IDE (integrated development environment) of our choice, NetBeans [4]. This greatly simplifies the development effort.

- **Validationdb** is a relational PostgreSQL database [5] that stores data in the form of images with meta-data, multidimensional histograms, and arrays of data points. Images of final plots (gif, jpeg, etc.) are stored as blobs (binary large objects) while histograms and data points are serialized into arrays in the database. The meta-data provides a description and lists literature references to the experimental data and other parameters that describe the test/experimental result (e.g. Geant4 version, beam particle, beam energy/momentum, reaction, target material, secondary particles etc.). Besides the mandatory parameters one can supply additional tags to provide more information. For literature references we make use of the INSPIRE High-Energy Physics Literature Database [6]. To facilitate fast access, we keep a copy of the relevant information of the referenced articles in DoSSiER, but a link to INSPIRE is provided in case that one wants to access additional information (e.g. retrieve a copy of the full article).
- **ValidationLib** is a multilayered Java API based on the data access object (DAO) [7] software design pattern. It provides an abstract interface to the database without exposing details of the database. To provide a format for data exchange and/or for uploading results into DoSSiER we use the Java Persistence API [8] or gson [9] which are Java libraries for serialization and deserialization of Java Objects into and from XML/JSON strings, respectively.
- **DoSSiER Web Application and Web Service** [10] offers menus that are easy to navigate, allow for interactive selection and overlay of compatible results. Data is compatible when observable and measurement variables reasonably agree. The application logic is such that only compatible data can be selected via the provided menus. The web application also provides security and authentication to grant access to groups of functions and data that are internal to the participating collaborations, e.g. viewing results from development releases, upload of new test results and modification of selected data. The Web Application is based on Java Platform, Enterprise Edition (Java EE) [11] and utilizes the PrimeFaces [12] open source JSF (Java Server Faces) component. This is part of the JavaEE Platform and it provides a Java specification for building component-based user interfaces for web applications [13]. The database is accessed using the classes provided by the Java API. It is deployed on a GlassFish application server [14] running on the FermiCloud service [15].
The DoSSiER Web Service is a RESTful [17] web service based on JAX-RS [18] that allows programmatic retrieval of data e.g. by validation jobs. Currently the functionality is relatively limited in that it only allows for retrieving results or the retrieval of the dictionaries describing the meta-data via their primary database key, but we plan to extend the API with e.g. search commands.
- **DbReader** is a C++ API providing access to data stored in DoSSiER directly from C++ clients. This is used by selected Geant4 validation jobs to directly retrieve the experimental data for comparison from DoSSiER.
- **Python tools** Not shown in Figure 1 are the Python-based ancillary tools that we are using to read and convert histograms and collections of data points from/to different data formats including ROOT, ASCII (CSV) and the JSON format used by DoSSiER. The files in JSON/XML format can then be used to download from and upload to DoSSiER. Other

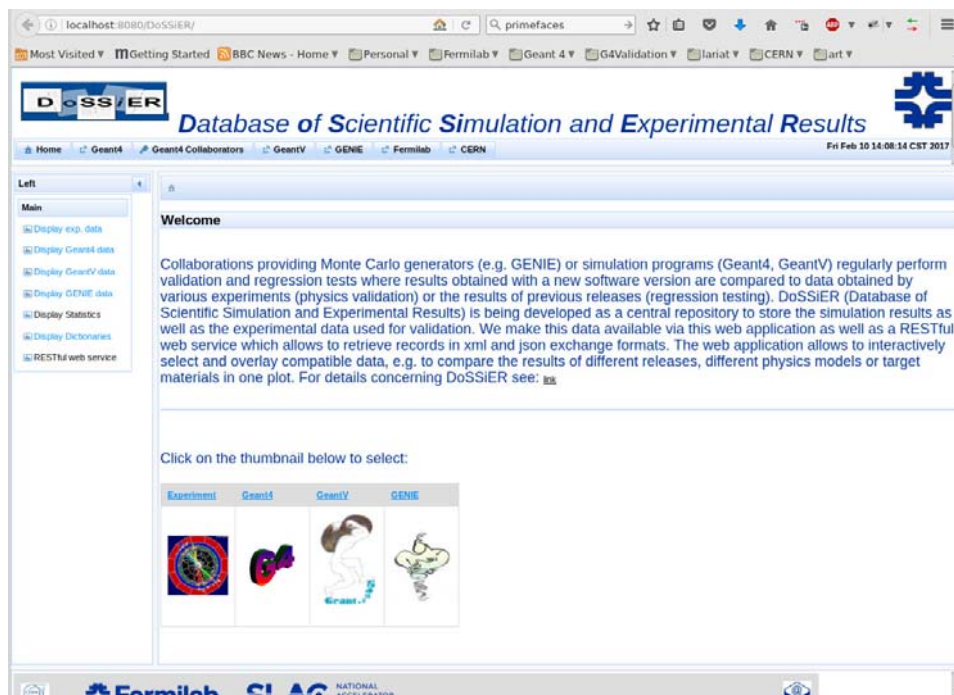


Figure 2. The DoSSiER entry page. It gives access to viewers of experimental data and Geant4 simulations. In addition the menu on the right allows access to database statistics, the dictionary browser and provides access to the RESTful web service. At the moment the GENIE and GeantV buttons are placeholders as adding data is still in progress.

functionality provided by this tool are the ability to inspect and interact with histograms (matplotlib) and script integration with the command line tools (CLI).

4. DoSSiER Views

In this section we highlight a few selected views currently provided by DoSSiER. Figure 2 shows the DoSSiER entry page. It gives access to viewers of experimental data and Geant4 simulations. At the moment the GENIE and GeantV buttons are placeholders as adding data is still in progress. In addition the menu on the right allows access to database statistics, the dictionary browser and provides access to the RESTful web service.

Figure 3 shows the DoSSiER dictionary browser which allows to navigate the references, test descriptions and the meta-data dictionaries used to describe the data stored in DoSSiER.

Figure 4 shows the display (blue squares) of a Geant4 simulation estimating the total cross section of π^- on a Carbon target as a function of kinetic energy. On the top of the view we find information describing the Geant4 test and the publications from which the data for physics validation was extracted. The menus on the top of the graph are automatically created based on the contents of the database. In this case, one can select results based on target material (Pb, Cu, S, C, Au, Ag, Sn, Ca, Fe) and beam particle (π^+ , π^-). If there are more variables to choose from, then additional menus will be created. Each test comes with a set of defaults and one automatically gets the default plot when initially selecting a test. When a user selects the pull down menu for a given variable, the fields of the preselected defaults are highlighted to guide further refinement of the selection. DoSSiER will search the database for any experimental results matching the meta-data of the test selection. In this case the search finds measurements

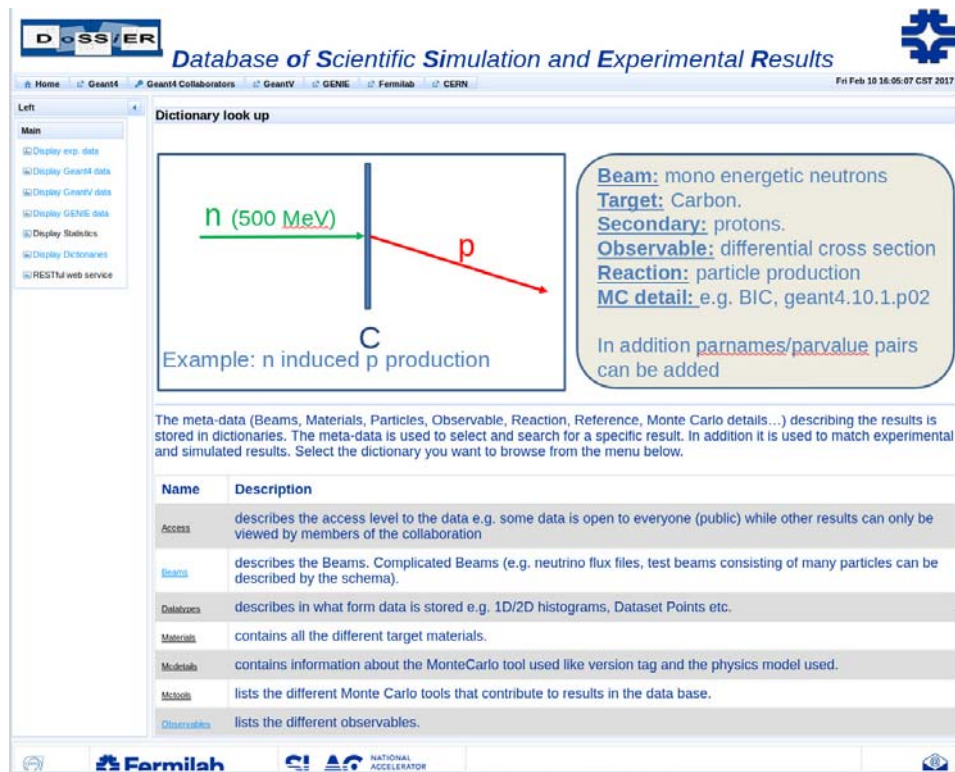


Figure 3. The DoSSiER dictionary browser allows to navigate the references, test descriptions and the meta-data dictionaries used to describe the data stored in DoSSiER.

from three different publications (orange, green, red curves) and overlays them on the simulation result. For plotting we use the plotly.js [16] JavaScript library.

Figure 5 shows a display of experimental data as a table, which shows values of the differential cross section of proton production induced by a neutron beam on a Cu target. The header of each table lists the meta-data (beam, reaction, target, secondary, observable, ...). DoSSiER allows the data to be downloaded in various formats (EXCEL, PDF, CSV, XML, JSON).

5. Conclusions and Outlook

DoSSiER provides a repository to collect and organize validation and regression test results and the experimental data used for physics validation tests. The web application component of DoSSiER allows easy access to the information for members of simulation collaborations and the general user community. The web service component allows for programmatic access to the data stored in DoSSiER. We are in the process of adding new tests and experimental data to the repository. Originally we concentrated on Geant4 tests of hadronic and electromagnetic physics that are of interest for high energy physics experiments, but in the future we plan to include tests that are of interest in other areas such as medical and space science. Also we are in the process of adding GEANTIE and GeantV data in cooperation with the respective collaborations. The website front-page (currently reachable at <http://g4devel.fnal.gov:8080/DoSSiER/>) is already available to the general public interested in providing feedback. Additional data-sets and simulation results are expected in the near future and we plan to improve the website based on the comments of the first users in the next few years, the current priority being the extension of included simulations and data. With the addition of more data we expect that this tool

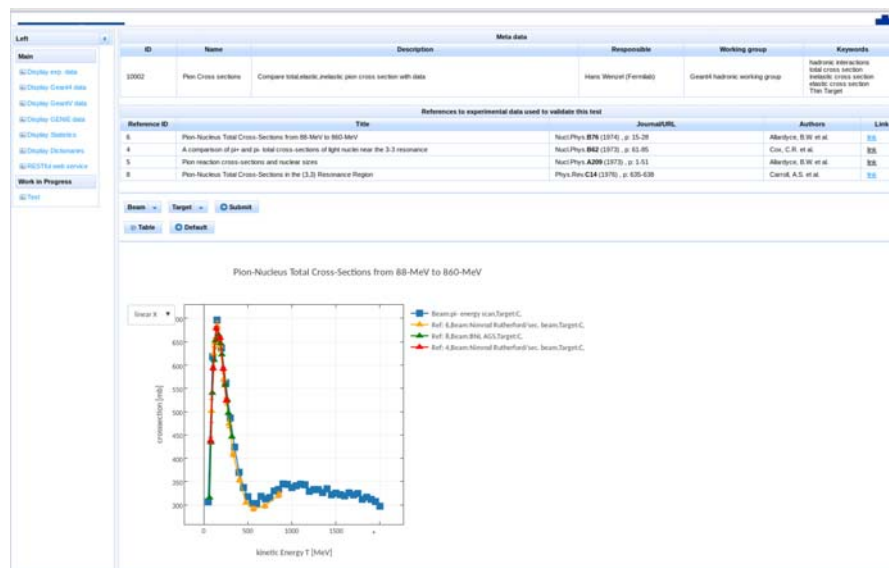


Figure 4. Display of a Geant4 simulation (blue squares) estimating the total cross section of π^- on a Carbon target as a function of kinetic energy. On the top we find information describing the Geant4 test and the publications from which the data for physics validation was extracted. The menus on the top of the graph are automatically created based on the contents of the database. In this case, one can select results based on target material (Pb, Cu, S, C, Au, Ag, Sn, Ca, Fe) and beam particle (π^+ , π^-). If there are more variables to choose from, then additional menus will be created. Each test comes with a set of defaults and one automatically gets the default plot when initially selecting a test. DoSSiER will search the database for any experimental results matching the meta-data of the test selection. In this case the search finds measurements from three different publications (orange, green, red curves) and overlays them on the simulation result.

Select Geant4 Test - Display selected Geant4 Test - Display selected Geant4 Test as table									
Beam: [particle(s)] [Energy] [Joule] 50N Neutron beam [542MeV] [1112] [142.0] [MeV]									
Reaction: particle production									
Target: Cu									
Secondary: proton									
Observable: differential cross section dσ/dΩ dE									
dtype: 1									
Parameters: [beta outgoing particle] [54]									
Min x of Bin E[MeV] (x) of sec.	Max x of Bin E[MeV] (x) of sec.	Value dσ/dΩ / dE	Error +	Error -					
0.0	4.0	1509.34			35.3116			35.3116	
4.0	8.0	9142.77			86.9087			86.9087	
8.0	12.0	4589.89			61.5785			61.5785	
12.0	16.0	2906.32			49.0			49.0	
16.0	20.0	2087.63			41.5289			41.5289	
20.0	24.0	1577.91			36.1048			36.1048	
24.0	28.0	1286.29			30.1081			30.1081	
28.0	32.0	1112.14			30.2977			30.2977	
32.0	36.0	1023.57			29.0793			29.0793	
36.0	40.0	944.266			27.93			27.93	
40.0	44.0	886.437			27.0613			27.0613	
44.0	48.0	799.693			25.7031			25.7031	
48.0	52.0	805.476			25.7959			25.7959	
52.0	56.0	788.129			25.5166			25.5166	
56.0	60.0	4765.322			255.2152			255.2152	

Figure 5. Display of Geant4 simulation data as a table. Shown are differential cross section values of proton production induced by a neutron beam on a Cu target. The header of each table lists the meta-data (beam, reaction, target, secondary, observable ...). DoSSiER allows to download the data in various formats (EXCEL, PDF, CSV, XML, JSON).

will become the main entry point to serve as result repository for both higher level (e.g. shower shapes in calorimeters) and microscopic (e.g. cross-sections, final state multiplicities) validations. To achieve this goal we are working in close collaboration with simulation experts.

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