

HepData reloaded: reinventing the HEP data archive

Andy Buckley

School of Physics and Astronomy

University of Edinburgh

E-mail: andy.buckley@ed.ac.uk

Mike Whalley

Institute of Particle Physics Phenomenology

Durham University

E-mail: m.r.whalley@cern.ch

James Monk*

Department of Physics and Astronomy

University College London

E-mail: jmonk@hep.ucl.ac.uk

We describe the status of the HepData database system, following a major re-development in time for the advent of LHC data. The new HepData system benefits from use of modern database and programming language technologies, as well as a variety of high-quality tools for interfacing the data sources and their presentation, primarily via the Web. The new back-end provides much more flexible and semantic data representations than before, on which new external applications can be built to respond to the data demands of the LHC experimental era. The HepData re-development was largely motivated by a desire to have a single source of reference data for Monte Carlo validation and tuning tools, whose status and connection to HepData we also briefly review.

13th International Workshop on Advanced Computing and Analysis Techniques in Physics Research,

ACAT2010

February 22-27, 2010

Jaipur, India

*Many thanks to James Monk who presented this material in our absence.

1. Introduction

The HepData “reaction database” is a repository of data from particle and nuclear physics experiments dating back to the 1960s, which has been hosted at Durham University since the 1970s. The emphasis of the database content is on published distributions – that is, it neither attempts to store raw experimental data nor particle properties such as branching fractions, which are the preserve of the complementary Particle Data Group [1]. Approximately 10000 papers are archived in HepData.

Historically, HepData was originally accessed via teletype, then interactive shell terminal. Finally, a Web interface built on CGI scripts was introduced in the early 1990s: this is the interface to which most users are accustomed. In this note, we describe a major upgrade effort from 2005–2009 which rebuilt the entire HepData infrastructure and migrated all existing data with significant improvements in functionality and data quality – in time for the LHC experimental era.

This upgrade was part of the CEDAR [2] e-Science project, and was largely motivated by the desire to programmatically obtain and synchronise reference data for HEP Monte Carlo generator tuning from HepData. The new HepData system provides the mechanisms for this and other uses of data from our community’s experimental legacy and for the LHC era.

We now describe the implementation of the new HepData system.

2. Object model

Database systems for complex data structures can rapidly become unmaintainable if all data access requires knowledge of the database table structure. Loose coupling of data storage and usage was adopted to avoid lock-in to either a single DB engine or a flawed initial DB schema design. A programmatic object model of HEP data structures was developed, with a persistency layer to translate between the objects and their database representation. The object model allows application code to concentrate on clearly expressing its data-handling logic, rather than the details of how the data is retrieved or stored.

The most important object in the HepData model is the `Paper`, representing an experimental publication and containing a collection of `Dataset` objects, each representing a plot or table in the publication. Each `Paper` also references a collection of metadata summarising its publication history, run conditions, featured reactions, principal authors, etc., which are used for database searches, in particular via the Web interface. Each `Dataset` contains at least one `XAxis` and at least one `YAxis` object, representing the combination of controlled variables and sets of measurements corresponding to those configurations respectively. Each `XAxis` contains several `Bin` objects and each `YAxis` contains several `Points`: these provide access to bin ranges, widths, foci, etc., and to various data uncertainties respectively. All numerical quantities are represented in a semantic units system, allowing consistent automatic unit conversions in applications while rendering the data in the units preferred by the authors of the source papers. Consistency through the object model is ensured by reciprocal parent–child contracts between objects, so that all object relationships can be traversed in both directions.

Java was chosen as the implementation language for the object model due to its object orientation and high-level standard and external libraries. The Maven 2 software control system was successfully

used to handle builds of all parts of the HepData system, including automatic management and retrieval of all third-party libraries.

The result of this development is that database searching can now be performed to the axis level rather than the paper, with numerical values decoupled from their textual representation by the units system. Combined with persistency layers to file and database storage, this structure is the core of new applications using the HepData information.

The main remaining restriction in the object model is its adherence to a model with a single data-type: binned distributions. Hence, it is not easy to meaningfully represent data where the x -values have no obvious bin edges, such as often is the case with collider energies, sets of data points where the x -errors do not correspond to bin widths, or data where there is no natural x axis at all¹. There is also no natural representation for more abstract data objects such as bin-error correlation matrices. Extension of the data types to handle several distinct types of data object would allow for semantically correct storage of a wider range of experimental data.

3. Object persistency

Hierarchical relationships such as those in HepData can be expressed in relational form for use by SQL databases such as MySQL or Oracle, by implementation of parent–child links – but maintaining consistency and navigating efficiently requires care. In HepData, this job is performed by the Java Hibernate [3] framework. Ownership relationships between objects are declared via an extended form of Java Persistency Annotations (JPA), which abstract most of the details of table representation. Hibernate also avoids object orphaning, ensures that db transactions are atomic, and helps to optimise database querying by judicious use of lazy and eager fetching strategies. The optimisation of these features must be done manually, but is at a much higher level than manually implementing the database accesses. The Envers [4] database versioning layer may be used in conjunction with Hibernate at some point, to allow for arbitrary roll-back of database contents.

File persistency is internally an important feature of the new HepData system, particularly since the migration of the 10000 papers from the legacy database was performed via intermediate files. Because of its ubiquity and natural hierarchical structure, an internal XML dialect – HepML – was developed for representation of HepData records, implemented via the external Castor marshalling framework [5]. This data format is not intended for external use, since the diversity of HepData records makes the format rather lengthy: it is instead intended for database backups, and as an intermediate format for data input and updates.

4. Migration

The migration of data records from the old HepData system to the new was a highly non-trivial task, largely due to the lack of strict structure in the legacy database. This was centered on the hierarchical Berkeley Database System, an unmaintained DBMS accessed programmatically from Fortran routines and without a concept of field type: all stored values are strings. Accordingly many records in the legacy database were found to be corrupted with typographical errors or unparseable

¹A dummy x -axis value and error, usually the collider energy with errors of ± 1 , is currently used as a work-around in this case.

spacing introduced for presentational purposes: these problems were too numerous for manual correction, and had to be resolved as part of the migration process to the new data structures.

This migration was performed by dumping the legacy database to a set of flat text files – one for each data type – via a combination of Fortran and Perl scripts. These files were then merged into one HepML file per logical paper using a Python script, `mkhepml`, which cross-references legacy papers to build complete data sets while heuristically correcting for the aforementioned misformattings, typos, and other improvable elements.

`mkhepml` makes substantial use of the BeautifulSoup [6] Python XML library – designed for tolerant screen-scraping, but used because of its powerful and flexible element-searching API. To speed up the system, lazy searching for object hierarchies was introduced, combined with pre-build sorting of the flat file entries: this step minimised the number of XML tag searches required. At this stage, most entries would take several seconds to build, but a substantial number of large papers would take many minutes or even several hours to migrate to HepML. This problem was obviated by introduction of a multi-threading layer so that slow papers would not delay the entire processing queue. In the final form, migration of the entire database could be performed overnight: necessary to keep up with the arrival of new papers in the legacy database, and fixes to corrupt records which were only discovered as a result of the migration process.

This phase of HepData re-development proceeded for several years, both because of the time taken to develop a fully-working object model and Web interface and because of the intrinsic scale of the migration process. All new records are now added, and updates made, directly on the new database and the migration process from the legacy database has been happily decommissioned.

5. Web interface

The new HepData Web interface, like the rest of the runtime system, is written in Java. The Tapestry 5 [7] framework is used rather than raw Java Servlets, since it combines a high-level approach to building Web applications with strong Hibernate and Maven 2 integration, and excellent scalability.

The resulting Web interface is designed around the idea that the URL should itself be a clean and predictable user interface: each area of the URL corresponds to a Java page-rendering class which interprets the rest of the URL as a set of arguments and produces a bytestream of HTML, XML, text or graphic as appropriate: multiple output formats are trivial to add, given a routine which constructs the desired representation from the object model – in fact, this can even be done by third-party applications via read-only access to the database.

Hence, URLs under the `view` page can be programmatically restricted to point to any (valid) combination of axes on any single dataset of a paper, and that data can be represented as e.g. HTML tables, HepML, plain text, ROOTCINT, or PyROOT macros. The `view` renderer also makes use of a `plot` renderer, which dynamically produces data plots of arbitrary size in PNG or PDF formats, with all combinations of log or linear axes – all programmatically accessible and bookmarkable via the predictable URL scheme. POST-type HTML form handling is specifically avoided for this reason. Internally, a simple templating markup language (TML) allows static HTML elements to be written as HTML, with substitutions delegated to Java classes, allowing re-use of common code components between pages.

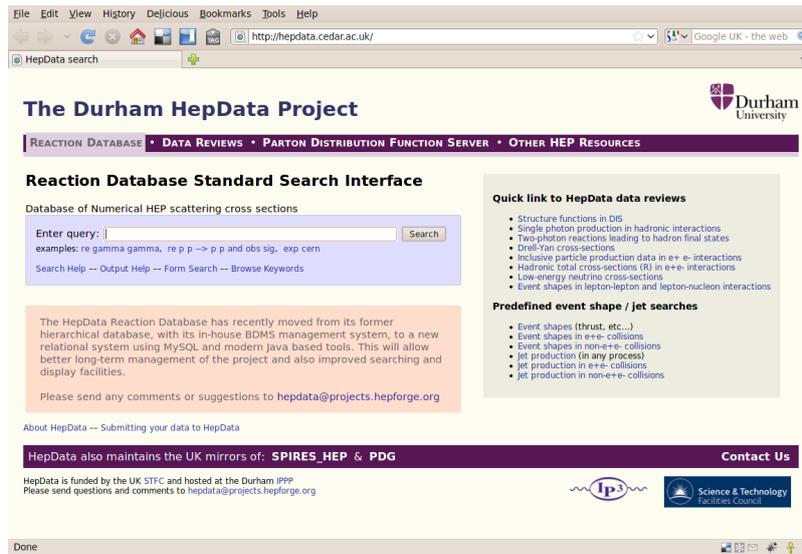


Figure 1: HepData main Web search page

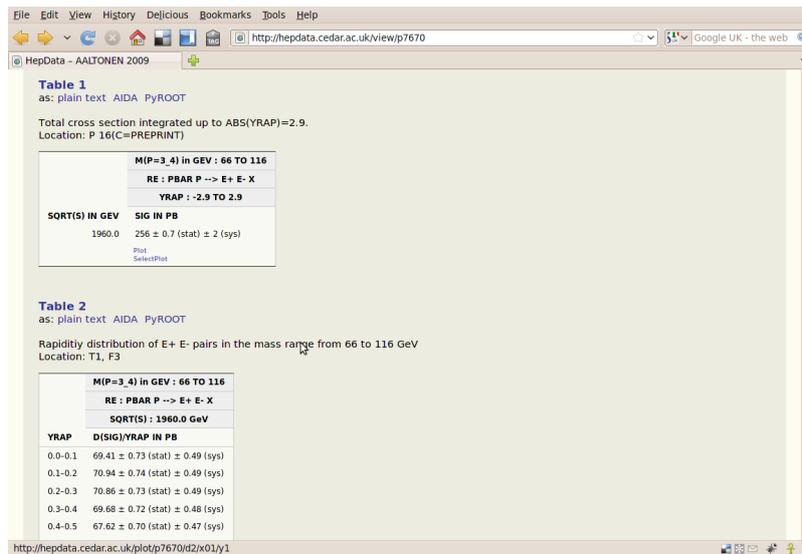


Figure 2: HepData paper display as HTML tables

The HepData server system consists of a Jetty Java servlet container and MySQL database sitting behind a firewall and exposed via a reverse proxy on an Apache 2 Web server. The system is shared with the popular HepForge [8] HEP code development system. The HepData system is live at <http://hepdata.cedar.ac.uk>, and screenshots of major interface elements are shown in Figures 1–3.

The first LHC data was successfully submitted to HepData after some discussion of submission formats: work is underway via LCG to provide tools for conversion of ROOT data objects to a suitable (simplified) input format for HepData and for pre-submission validation of the generated data files.

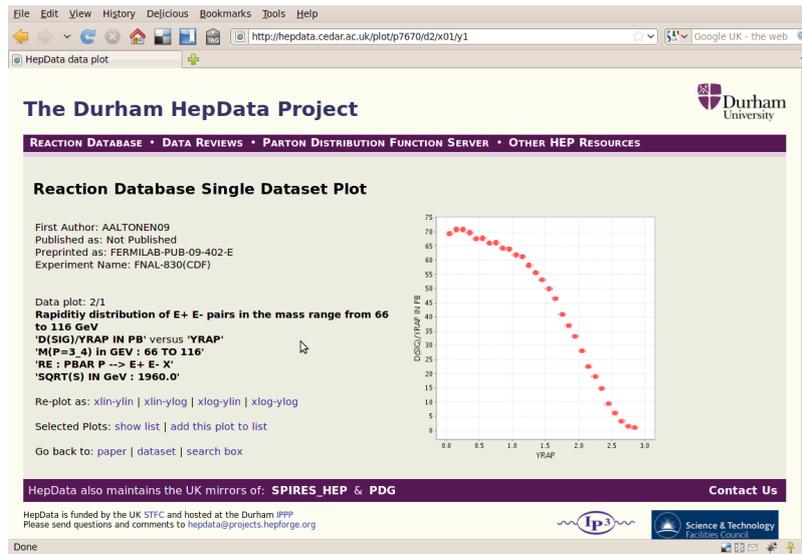


Figure 3: HepData plot display via dynamic rendering

6. HepData in MC generator validation and tuning

The re-development of HepData was largely driven by the requirements of the MC generator community for validation and optimisation infrastructure. Reliable reference data is required for quality generator tuning, and a perennial problem has been the translation errors during transcription of tabulated data into arrays in validation code, exacerbated by the lack of any synchronisation between the reference data hard-coded into the analyses and the paper itself, which may receive post-publication updates. The development of a more flexible HepData interface means that this data synchronisation can now be far more direct, exemplified by the Rivet [9] validation system.

Rivet is a generator-agnostic analysis framework, intended as a re-engineering of the FORTRAN HZTool library with the benefits of hindsight and a more expressive application programming language. Rivet has two main rôles:

- to provide a collection of physics utility routines, such as jet algorithms and event shapes;
- to collect a set of analyses which produce data comparable with experimental results.

Rivet is implemented in object oriented C++ and specifically only accesses event data via the HepMC event record [10] – it is hence generator-independent by design. Other features ensure the scalability and robustness of the system.

The reference data in Rivet are bundled with the package as AIDA XML files, one for each paper. These files can be directly imported from HepData by an automated URL query using the paper’s SPIRES identifier as a unique key. Inside the Rivet package, the HepData records are used to automatically choose the binnings for histogrammed observables – this makes the Rivet analysis code far more compact and readable than its predecessors, and reference data fixes and updates can be applied without code changes.

Rivet is currently being used by Genser and LHC experiments as a validation tool, and by the Professor [11] tuning framework as the main source of data for event generator tuning. Professor performs MC parameter optimisations by first parameterising generator responses to parameter variations as a large set of analytic functions, and then numerically minimising a goodness-of-fit measure – again, the reference data in this goodness of fit is provided automatically by HepData. Professor is a joint project between Edinburgh University, Durham University (IPPP), Lund University, and Berlin Humboldt University as part of the MCnet research network, and is used by phenomenologists and by the LHC experiments for their internal MC tuning efforts.

Acknowledgements

We would like to thank James Monk for presenting this material in our absence. HepData development has been supported by a long-term grant from the UK Science and Technology Facilities Council, and its re-development by the CEDAR e-Science project, also supported by STFC. A. Buckley additionally acknowledges support from an STFC Special Project Grant, from the Scottish Universities Physics Alliance (SUPA), and from the EU MCnet Marie Curie Research Training Network (funded under Framework Programme 6 contract MRTN-CT-2006-035606) for both financial support and for many useful discussions and collaborations with its members.

References

- [1] Particle Data Group Collaboration, C. Amsler *et al.*, Phys. Lett. **B667**, 1 (2008).
- [2] A. Buckley, PoS **ACAT2007**, 050 (2007), 0708.2655.
- [3] Hibernate website, <http://hibernate.org>.
- [4] Envers website, <http://www.jboss.org/envers>.
- [5] Castor website, <http://www.castor.org>.
- [6] Beautifulsoup website, <http://crummy.org/beautifulsoup/>.
- [7] Tapestry 5 website, <http://tapestry.apache.org>.
- [8] Hepforge, <http://www.hepforge.org>.
- [9] A. Buckley *et al.*, (2010), 1003.0694.
- [10] M. Dobbs and J. B. Hansen, Comput. Phys. Commun. **134**, 41 (2001).
- [11] A. Buckley, H. Hoeth, H. Lacker, H. Schulz, and J. E. von Seggern, Eur. Phys. J. **C65**, 331 (2010), 0907.2973.