Modernizing GooFit: A Case Study

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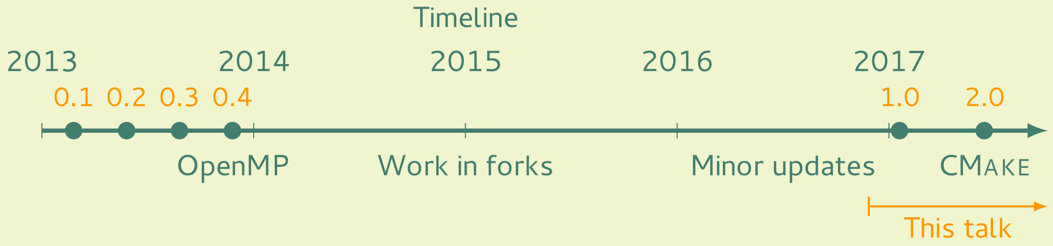
goofit.github.io/pearc17.pdf

PEARC17

UNIVERSITY OF Cincinnati

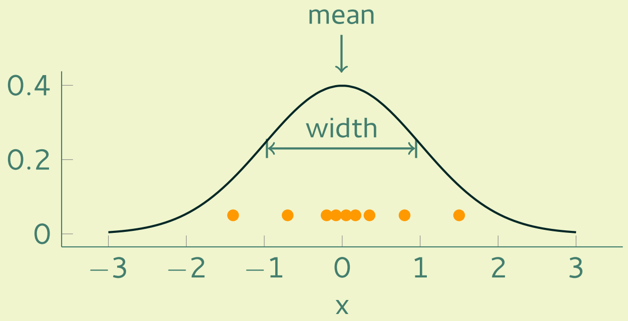
History of GooFit



/GooFit/GooFit

- Developed by Rolf Andreassen in 2013
- A lot of duplicated work in 2014-2016
- We will cover the 2016-2017 modernization

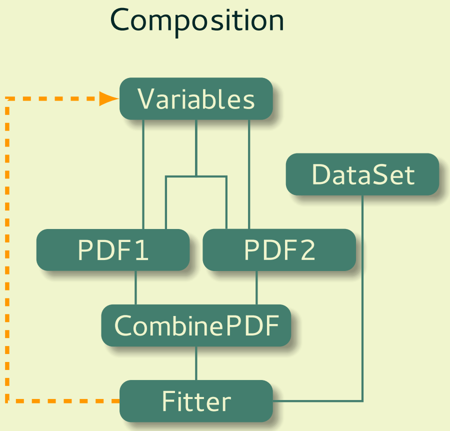
GooFit: Probability Density Function (PDF) Fitting



Design

- Resembles the popular RooFit package in ROOT
- Built with CUDA/OpenMP using Thrust
- Includes 30+ High Energy Physics (HEP) PDFs and examples

Features of a Fit



Composition

- Changed often
- 100+ Variables possible

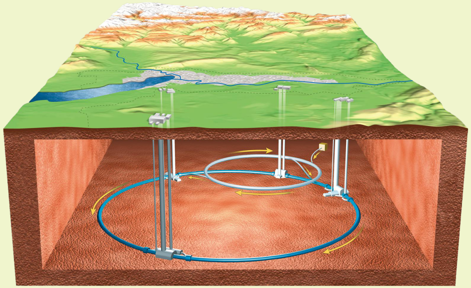
PDFs

- Many provided
- Users may add more

Backend

- Managed by core team

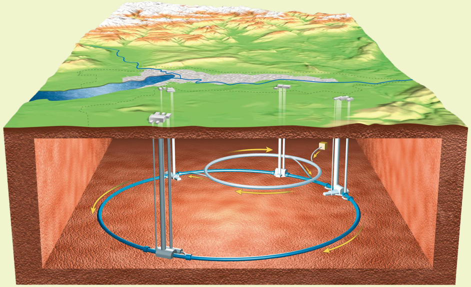
Why GooFit?



Charm Physics at CERN's LHCb experiment

- 1,000,000+ events in dataset
- 5 or more independent variables common
- 20+ PDFs with complex coefficients
- Some analyses run 1,000+ fits

Why GooFit?



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GooFit transforms fitting with 950x speedup over single-core RooFit

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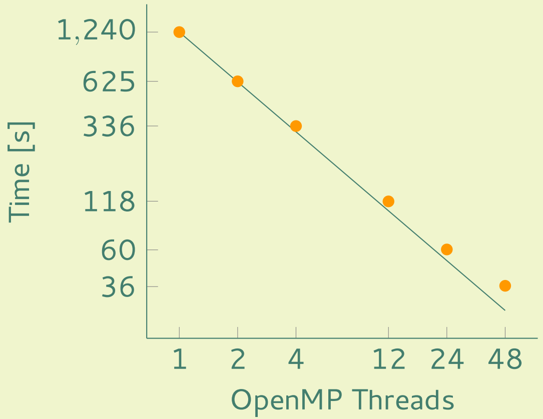
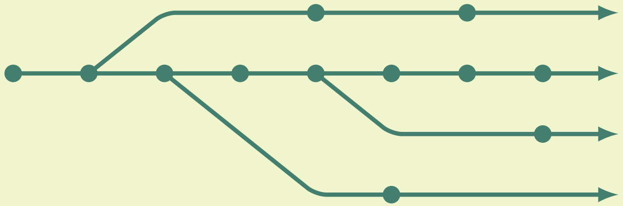


GooFit is fast

- 142576 events
- Unbinned fit
- 24 physical Xeon cores

K40	96.6 seconds
P100	23.5 seconds

GooFit 0.4: A State of Disrepair



Research level code

- Written for CUDA 4.0 and Compute Architecture 2.0
- Hardcoded paths in Makefiles
- Little file organization
- Forked 10+ times, new features not in master
- Cludges: fake `nvcc`, globbing, fake ROOT, ...

Build system updates

Iterative Approach

1. Makefile cleanup and consolidation
2. Organization of file structure
   - `ModernizeGooFit.py` script
3. Adding CMake
   - Coexisted with makefiles for a while

```
#include "CompositePdf.hh"
abortWithCudaPrintFlush(__FILE__, __LINE__, "Failed");
```

`ModernizeGooFit.py` ↓ Uses regular expressions and Plumbum

```
#include <goofit/PDFs/combine/CompositePdf.h>
GooFit::abort(__FILE__, __LINE__, "Failed");
```

CMake

CMake CUDA support

- Require CMake 3.4+
- Backported FindCUDA from CMake 3.7
- Keyword vs. standard targets
- CUDA in 3.8 massively improved

Features

- IDE support (Xcode, QtCreator)
- Library discovery / configuration
- Multiple compiler support
- Integration with other tools
- Download datafiles from GitHub releases

Git Submodules

- Libraries as submodules
- Automatic checkout by CMake build
- Separate CMake folder (`/CLIUtils/cmake`) and external libraries

Automation and Testing

Travis CI

- Verify OpenMP build
- Verify PRs
- Upload coverage reports
- Upload documentation

Challenges

C++11 • ROOT • Docs

Tests

- Run all examples with script
- Slowly added verification
- Unit-tests added with GoogleTest (evaluating Catch)

(NVIDIA-)Docker

- Added images with ROOT+Utils
- From scratch install

Modernization

C++11

- Limited to CUDA 7.0+
- Reduced # of lines / simplified
- Used CLANG-TIDY to convert (CMAKE 3.6+ integration)

Major updates

`nullptr` ● `foreach` ● `override`
Variadic templates ● Initializer lists

Cleanup

- Readability: CLANG-FORMAT
- Moved all code to namespace
- Compile-time logging choice
  `/fmtlib/fmt`
- Smart color output
  `/agauniyal/rang`
- Removed custom classes and iterators (complex, etc)

Command line parsing

```
./MyAnalysis generate_toy
        --params=file.ini
        --release_K892_mass
        --A12=0.3
        --plot
```

Recurring theme

- Analyses require 40+ options and multiple procedures
- Found a lot of duplicated code for argument parsing
- Many bugs related to parsing (usually segfaults)
- Needed powerful solution, with direct access to values

CLI11

/CLIUtils/CLI11

- No dependencies
- Compiles to single header file

Features

- Nested subcommands
- Configuration files
- 100% test coverage
- CI tests on macOS/Linux/Windows
- + GooFit's features

Use in GooFit

- Testbed for new build features

`GooFit::Application`

- Auto logging
- Optimization warnings
- GPU switches
- MPI support
- Completely optional

Improvements

Expanded physics tools

- Three body time-dependent amplitude analyses
- Four body time-integrated and time-dependent amplitude analyses
- Toy Monte Carlo generation using MCBooster

Caching: `/bryancatanzaro/generics`

- Support for LDG caching
- LDG generalized form
- Performance boost for mid-age cards

MPI

- Available for `Application`
- Supports multiple GPUs

`/MultithreadCorner/MCBooster` is deprecated
in favor of `/MultithreadCorner/Hydra`

MINUIT 2

MINUIT in HEP

- MINUIT is a standard HEP parameter search algorithm (CPU)
- MINUIT 1 and 2 available in ROOT
- Old copy of MINUIT 2 was available stand-alone

Status in GOOFIT 0.4

- Internal MINUIT1 copy
- Required manual upkeep

/GooFit/Minuit2

- Newly forked from ROOT 6.08
- CMAKE build, no other changes
- Already being used outside GOOFIT

PYTHON Bindings (GOOFIT 2.1 feature)

Pre-release syntax

```
from goofit import *
xvar = Variable("xvar", 0, 10)
xdata = UnbinnedDataSet(xvar)
xdata.from_numpy(np.random.exponential(size=100000))

alpha = Variable("alpha", -2, 0.1, -10, 10)
exppdf = ExpPdf("exppdf", xvar, alpha)
exppdf.fitTo(data)
```

/pybind/pybind11

- Only uses advanced C++11
- Full working example in GOOFIT 2.0
- Expanding for GOOFIT 2.1
- pip install with SCIKIT-BUILD

Current Challenges

- CUDA vs. C++
- Pythonic syntax
- Example conversion

GooFit Future

GooFit
CUDA/OpenMP
Fitting Framework

/GooFit/GooFit

GooFit 2.0: Released

- Source code and docs on GitHub

GooFit 2.1: Coming soon

- Drastically expanded Python bindings by Himadri Pandey

Plans

- Hydra integration
- Use in $D^0 \rightarrow K^- \pi^- \pi^+ \pi^+$ amplitude analysis
- GooFit 2torial under development at henryiii.gitbook.io/goofit

Build it yourself

```
docker run -it alpine
apk add --no-cache make cmake g++ git
git clone --branch=stable https://github.com/GooFit/GooFit.git
cd GooFit
make
```

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CERN image from project-hl-lhc-industry.web.cern.ch.

goofit.github.io

Questions?

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