RooFit's new heterogeneous computing backend

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ROOT
Data Analysis Framework
https://root.cern

Introduction

- **RooFit**: C++ library for statistical data analysis in ROOT
  - provides tools for model building, fitting and statistical tests
- Recent development focused on:
  - **Performance** boost (preparing for larger datasets of **HL-LHC**)
  - More **user friendly** interfaces and high-level tools
- Today: **20th anniversary** of RooFit first presented at a conference (CHEP 2003)

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In **this presentation**:

- Report on new **vectorized RooFit** interface with **GPU support** (aka *BatchMode*)
- Follow-up on ACAT 2021 talk with preliminary prototype results
- Today's benchmark results obtained with **ROOT *6.28.04*!**

Other RooFit presentations to follow:

- **Garimas Singhs** presentation on applying **automatic differentiation** to RooFit
- **Zef Wolffs** presentation on **configurable parallelization** in RooFit

Computation graphs in RooFit

RooFit evaluates expression trees many times for different parameter values to find NLL minima.

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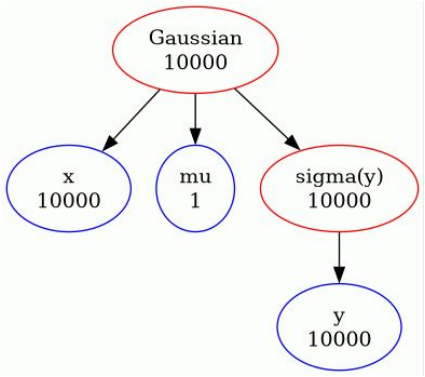
Expression tree with observables x and y for 10000 data points:
Gaussian(x|mu,sigma(y))

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RooGaussian gauss{"gauss", "gauss", x, mu, sigma};
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Why rewriting RooFit NLL evaluation backend:

- Old RooFit computation: re-evaluate expression tree of *for each event*
- Lots of function calls, **no vectorization possible**

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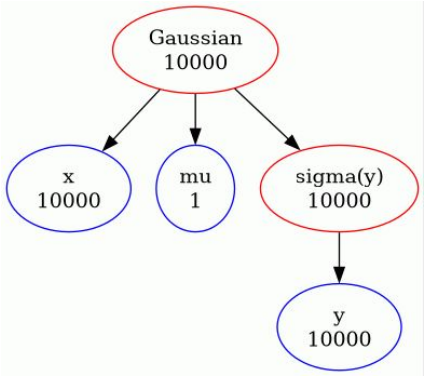


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Should have been easy to improve and do on GPU?!

1. Allocate memory for results
2. Call vectorized function/CUDA kernel for each node[1] in topological order if values of children have changed

[1] `RooAbsArg` in RooFit

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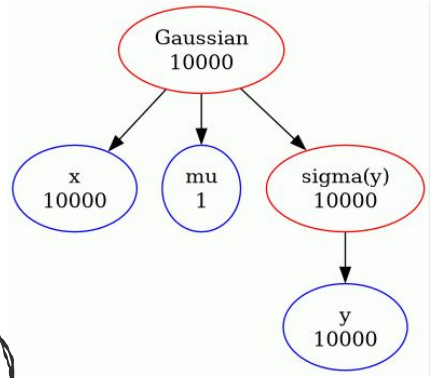

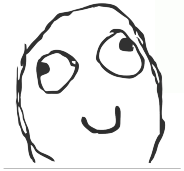

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Typical example: **normalization integrals**
(still harmless compared to other cases, but good for illustration)

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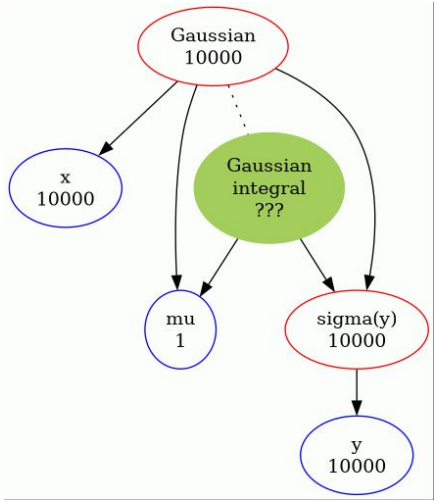


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Dynamic nature of computation graphs in RooFit makes organizing data flow and computations in a heterogeneous computing environment a challenge.

In other words: data structure for model *building* not completely suitable for *evaluation*.

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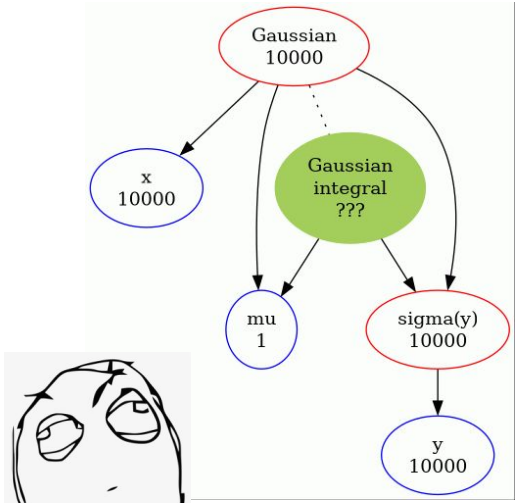


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If your RooFit classes don't fulfill this yet, you should consider overriding:
`RooAbsArg::compileForNormSet()`

- Function called recursively in NLL creation when using `BatchMode()`
- Result is ready for heterogeneous eval.
- Mechanism also used for the C++ code generation from RooFit models that enables automatic differentiation *(see next talk by Garima Singh)*

This function can also be used to hook in graph **optimizations**.

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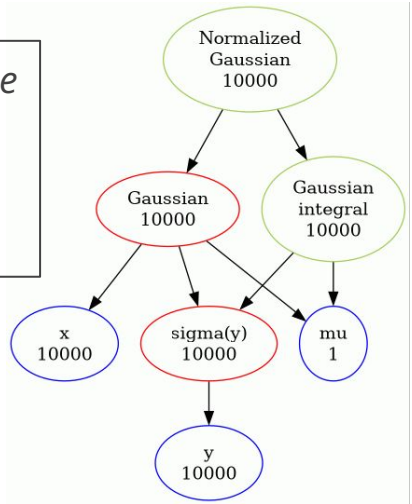

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```
auto nll = gauss.createNLL(
    *data,
    ConditionalObservables(y),
    BatchMode("cpu")
); // create NLL object

nll->Print("v"); // get some info on the graph evaluation order
```

```
--------------------------------------------------------------------------------
| Idx | Name                    | Class            | Size    | From Data |
--------------------------------------------------------------------------------
| 1   | y                       | RooRealVar       | 10000   | 1         |
| 2   | sigma                   | RooFormulaVar    | 10000   | 0         |
| 3   | mu                      | RooRealVar       | 1       | 0         |
| 4   | x                       | RooRealVar       | 10000   | 1         |
| 5   | gauss                   | RooGaussian      | 10000   | 0         |
| 6   | gauss_Int[x]            | RooRealIntegral  | 10000   | 0         |
| 7   | gauss_over_gauss_Int[x] | RooNormalizedPdf | 10000   | 0         |
| 8   | nll                     | RooNLLVar        | 1       | 0         |
--------------------------------------------------------------------------------
```

The vectorized evaluation functions

- The BatchMode backend uses **new functions** in RooAbsReal that you can **override** to add support for CPU and GPU of your class:
  - `RooAbsReal::canComputeWithCuda()`
  - `RooAbsReal::computeBatch()`

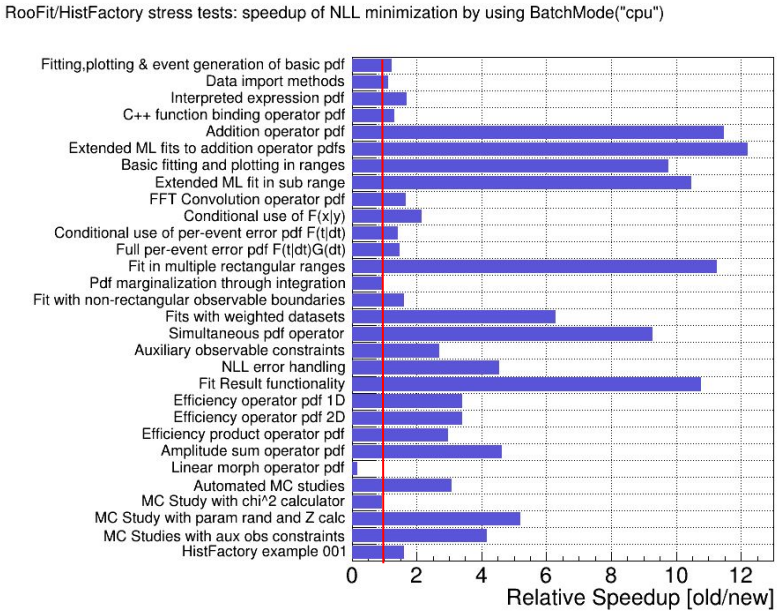
- Implementation of RooFit classes in ROOT uses `RooBatchCompute` library to implement `computeBatch()`:
  - **Architecture-specific accelerator libraries** for key functions
  - **Optimal one loaded at runtime**, given current architecture
  - More details in the ACAT 2021 talk

- Add the FastEvaluations stream to the RooMsgService the get **info printouts when** your RooAbsArgs **don't support** the **new backend**:

```
RooMsgService::instance().addStream(
        RooFit::Info, Topic(RooFit::FastEvaluations)
);
```

Benchmarking the RooFit test suite

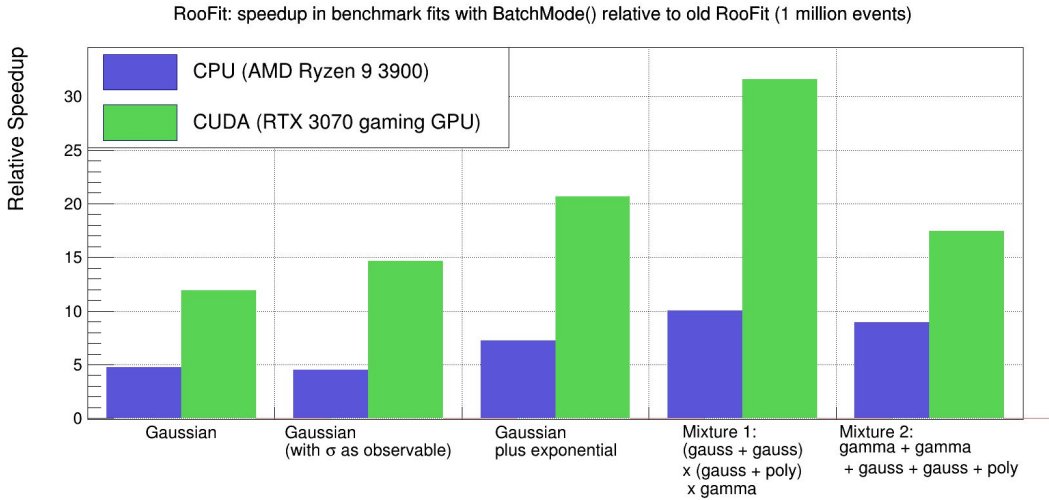
- Plot shows relative time spent for minimizations in [stressRooFit tests] for `BatchMode("cpu")` and `"off"`
- Significant speedup for almost all tests from a combination of:
  a. **Vectorized** evaluation
  b. Optimized computation graphs
  c. Less function calls
- Average speedup of **4.4x**



Results obtained with ROOT 6.28.04
Compare also to [ICHEP 2022] results, showing less drastic speedups in the middle of ROOT 6.28 development

Benchmarking basic unbinned fits

- Benchmarking unbinned bit with 1 million events
- The CPU BatchMode runs on a single thread
- The CUDA kernels are launched with **128 thread blocks** with 1024 threads each
- Plot shows speedup relative to the old scalar evaluation interface

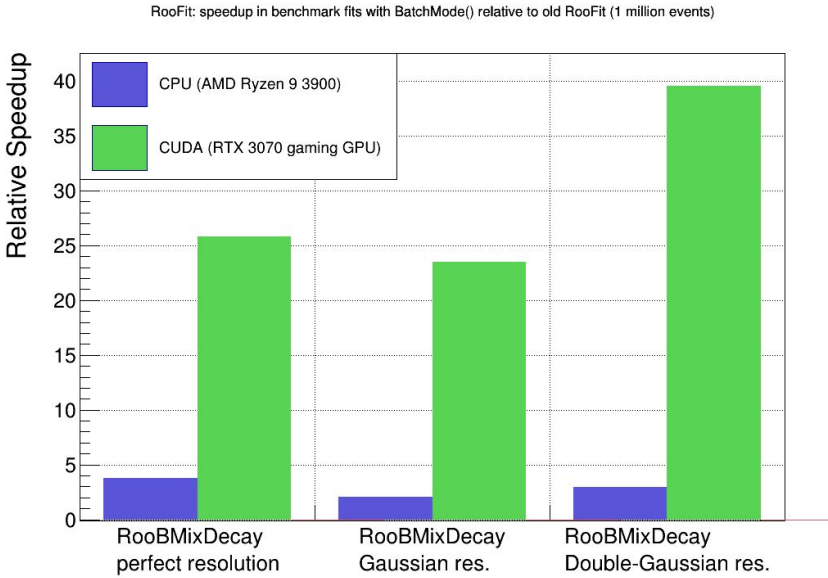


benchRooFitBackends in rootbench repo, plotting script is in same directory. Try it yourself with ROOT 6.28.04! Remember to use a ROOT build with -Dcuda=ON

New benchmarks for analytical convolution fits

- New benchmarks based on analytical convolutions of [RooBMixDecay] with resolution functions
  - With **perfect resolution** (`RooTruthModel`)
  - **Gaussian resolution** (`RooGaussModel`)
  - **Double-Gaussian** resolution (`RooAddModel` of `RooGaussModel`s)
- Describes the decay of B mesons with the effects of B0/B0bar mixing
- Quite an involved fit:
  double-Gauss fit takes 1 min with old backend
- GPU speedup **up to 40x**!
  - Larger speedups than for previously benchmarked simple models

Plan to also **do numeric integrals on GPU in the future** to support more B-physics usecases, i.e. amplitude fits.



RooFitUnBinnedBenchmarks in rootbench repo, plotting script is in same directory. Try it yourself with ROOT 6.28.04! Remember to use a ROOT build with -Dcuda=ON

How to use the new NLL evaluation backend

- Try it out by passing `"cpu"` or `"cuda"` to the `BatchMode()` argument of `RooAbsPdf::fitTo()` / `RooAbsPdf::createNLL()`:
  - `pdf.fitTo(data, RooFit::BatchMode("cuda"))`

It's a **one-line change**!

See also the RooAbsPdf documentation.

Conclusions and next steps

- RooFits new vectorized NLL evaluation backend (aka. BatchMode) is now production ready
  - **All RooFit tests pass** if enabled by default, which might happen in next ROOT release
  - If your model doesn't benefit from speedup yet, please open a bug report
  - Average speedup of about **4x** compared the old RooFit evaluation backed
- Revised CUDA backend in **ROOT 6.28.04**!
  - Gives you great speedup for wide range of unbinned fits with many events
  - Average speedup of **25x** (up to **40x!**) in fits with 1M events on **GeForce RTX 3070**
- The new backend relies on mechanism to fix computation graph that you might need to implement in custom RooFit classes
- **Next steps** *(CERN openlab summer student project)*:
  - Support even more PDFs with CUDA backend
  - **Numeric integration** also on the GPU