RooFit's new heterogeneous computing backend

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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
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(\( x | \mu, \sigma(y) \))

\[
\begin{align*}
\text{RooRealVar } x &\{"x", "x", 0.0, -20.0, 20.0\}; \\
\text{RooRealVar } y &\{"y", "y", 0.0, 0.0, 1.0\}; \\
\text{RooRealVar } \mu &\{"\mu", "\mu", 0.0, -20.0, 20.0\}; \\
\text{RooFormulaVar } \sigma &\{"\sigma", "1.0 + 2.0 * y", \{y\}\}; \\
\text{RooGaussian } \text{gauss} &\{"\text{gauss}", "\text{gauss}", x, mu, sigma\};
\end{align*}
\]
RooFit evaluates expression trees many times for different parameter values to find NLL minima.

Why rewriting RooFit NLL evaluation backend:

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

```cpp
RooRealVar x("x", "x", 0.0, -20.0, 20.0);
RooRealVar y("y", "y", 0.0, 0.0, 1.0);
RooRealVar mu("mu", "mu", 0.0, -20.0, 20.0);
RooFormulaVar sigma("sigma", "1.0 + 2.0 * y", \{y\});
RooGaussian gauss("gauss", "gauss", x, mu, sigma);
```
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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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RooFit model evaluation is not straight forward:

- Nodes often own other nodes that they evaluate
- These *internal nodes* are not registered in the graph
- Sometimes these nodes are even clones of entire subgraphs
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Typical example: **normalization integrals**
(still harmless compared to other cases, but good for illustration)
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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**.

gauss.getVal(/*normSet=*/x);
New mechanism to “compile” the graph for a given normalization set to fulfill condition

Each RooAbsArg involved in the evaluation must be connected to the top node via RooFits client-server relations.
**New mechanism** to “compile” the graph for a given normalization set to fulfill condition

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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auto nll = gauss.createNLL(
  *data,
  ConditionalObservables(y),
  BatchMode("cpu")
); // create NLL object
nll->Print("v"); // get some info on the graph evaluation order
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](https://example.com/)

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

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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 RooGaussModels`)
- 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.

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**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