Towards a framework for GPU event generation

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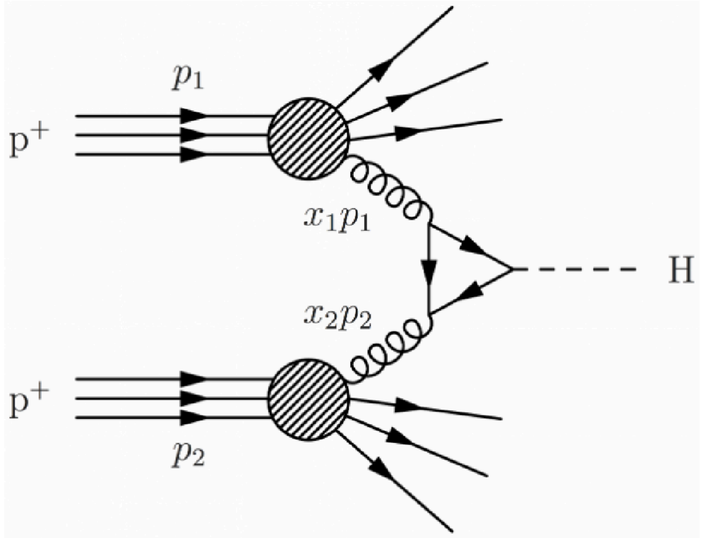
The ingredients of a Monte Carlo generator



- Filling interpolation grids
- Loop integrals and special functions
- PDF uncertainties
- Scale variations
- Infrared subtractions
- ....

histogramming / analysis

$$\mathcal{O} = \int d\Phi_n dx_1 dx_2 f_1(x_1, \mu_F^2) f_2(x_2, \mu_F^2) \, |M(\{p_n\}, \mu_R)|^2 \, \mathcal{J}_m^n(\{p_n\})$$

integrator

phase space

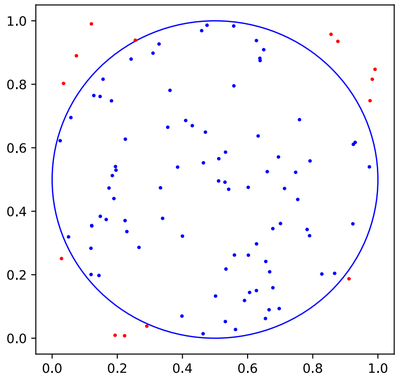
Parton Distribution Functions

matrix element

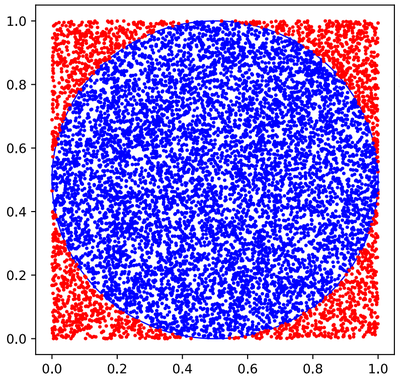
cuts

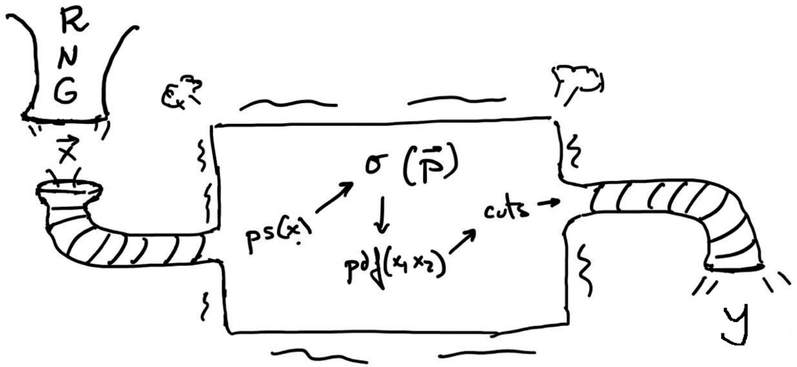
Monte Carlo integrals are highly parallelizable

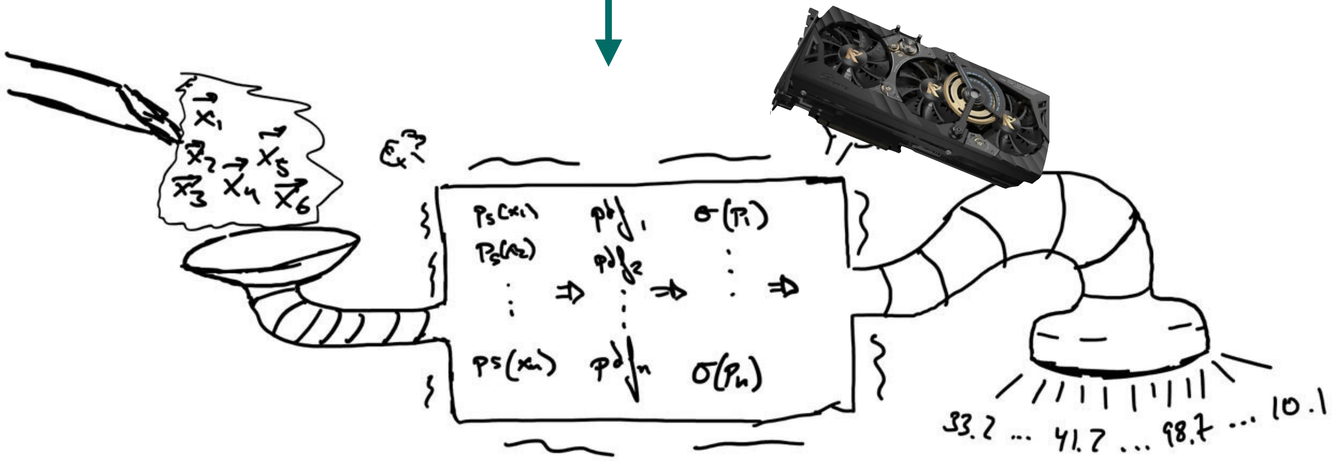
$\pi \simeq 3.2$

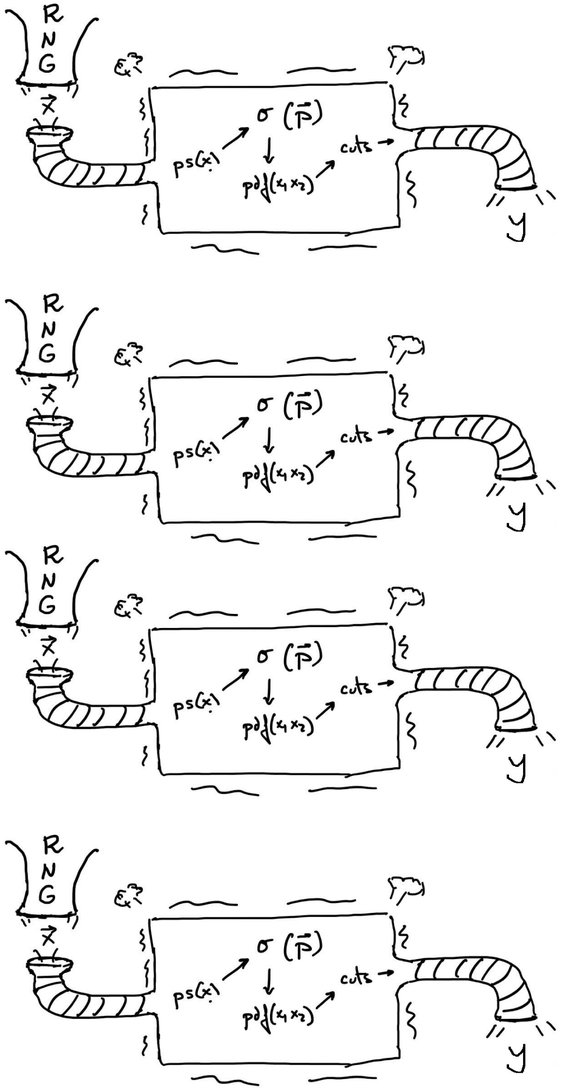


$\pi \simeq 3.16$



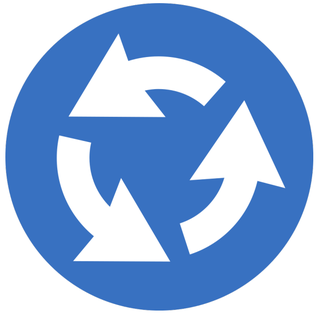






If they are so good, why are we not using them?

1. Lack of expertise? motivation? and (mostly) **time**
   - Huge codebases optimized for running on CPU clusters, not necessarily in GPU-friendly languages
   - Papers are needed, porting code is “wasted time”
   - Existing expertise not always translate cleanly to a completely different architecture/language
   - It’s a catch-22 situation!
2. Lack of tools
   - There are many tools to help you with your MC calculation… as long as it is running on a CPU…



So you extend your current code, which allows you to get a paper out, which makes you more proficient in whatever language that code was written in, which in turns makes the codebase even larger and with it the barrier to implement it on a GPU has also grown.

The phenomenologist (CPU-based) toolbox

integrator → myriad of Vegas implementations / cuba

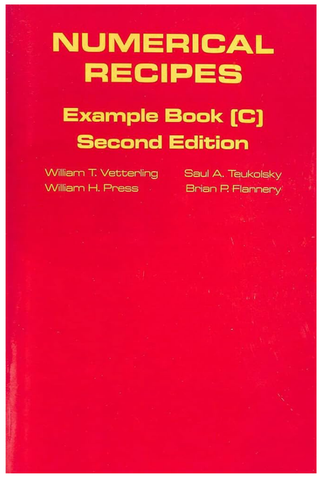
phase space → RAMBO / many algorithms available

matrix element → Madgraph / Comix / OpenLops

Parton Distribution Functions → LHAPDF

cuts → Fastjet

histogramming / analysis → Thousands of ROOT scripts



The phenomenologist (GPU-based) lack thereof

integrator → ?????

phase space → ?????

matrix element → ?????

Parton Distribution Functions → ?????

cuts → ?????

histogramming / analysis → ?????

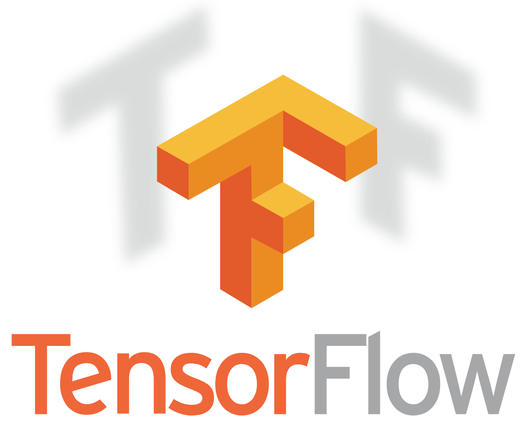
pepper

pdfflow / lhapdf…?

In the next few slides I'll try to motivate how having some kind of framework can make this jump much easier even if it is far from perfect.

Filling up the box with some new tools

In order to create an environment in which we could start moving forward we have written some of these tools using TensorFlow



Our goals:

- ☑ Exactly the same code base for CPU and GPU (no matter the brand!)
- ☑ A lot of mathematical functions already available
- ☑ Not adding extra dependencies to our existing codebase (mostly python and, yes, TF)
- ☑ Easily extensible and **interfaceable with other languages (C++, Cuda, Fortran, Rust)**

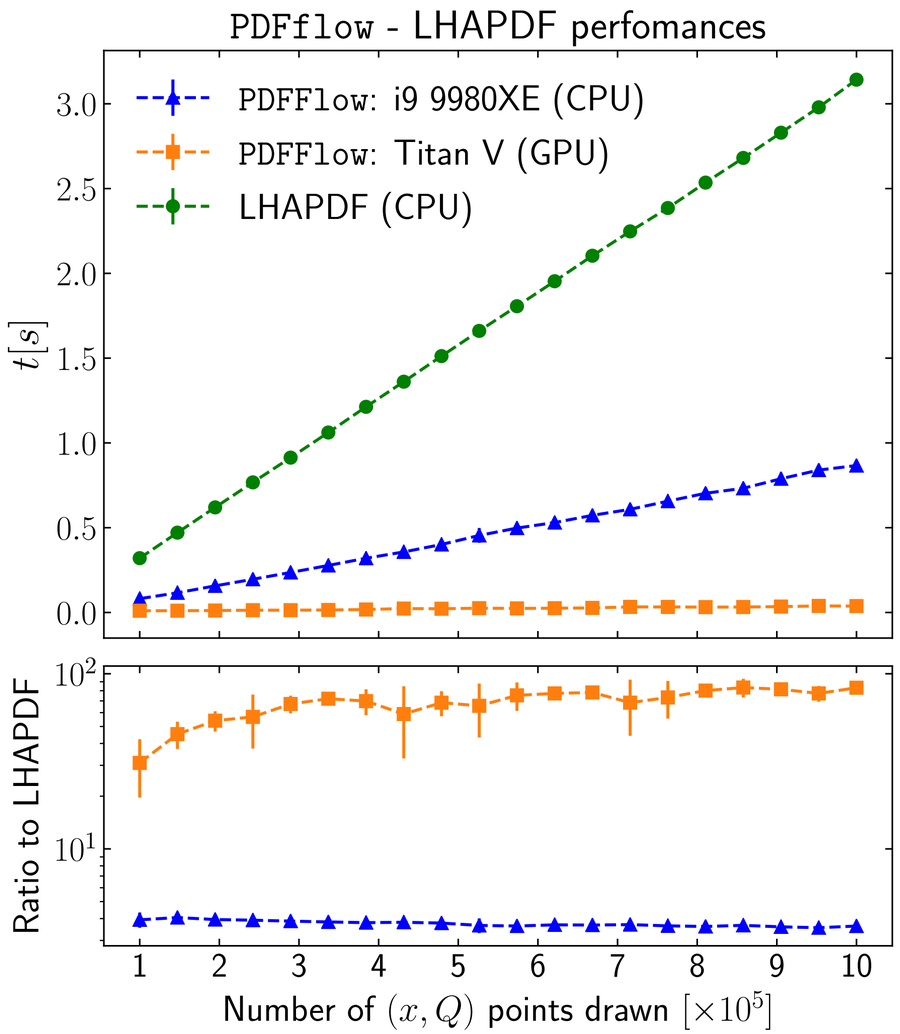
Some caveats and disadvantages:

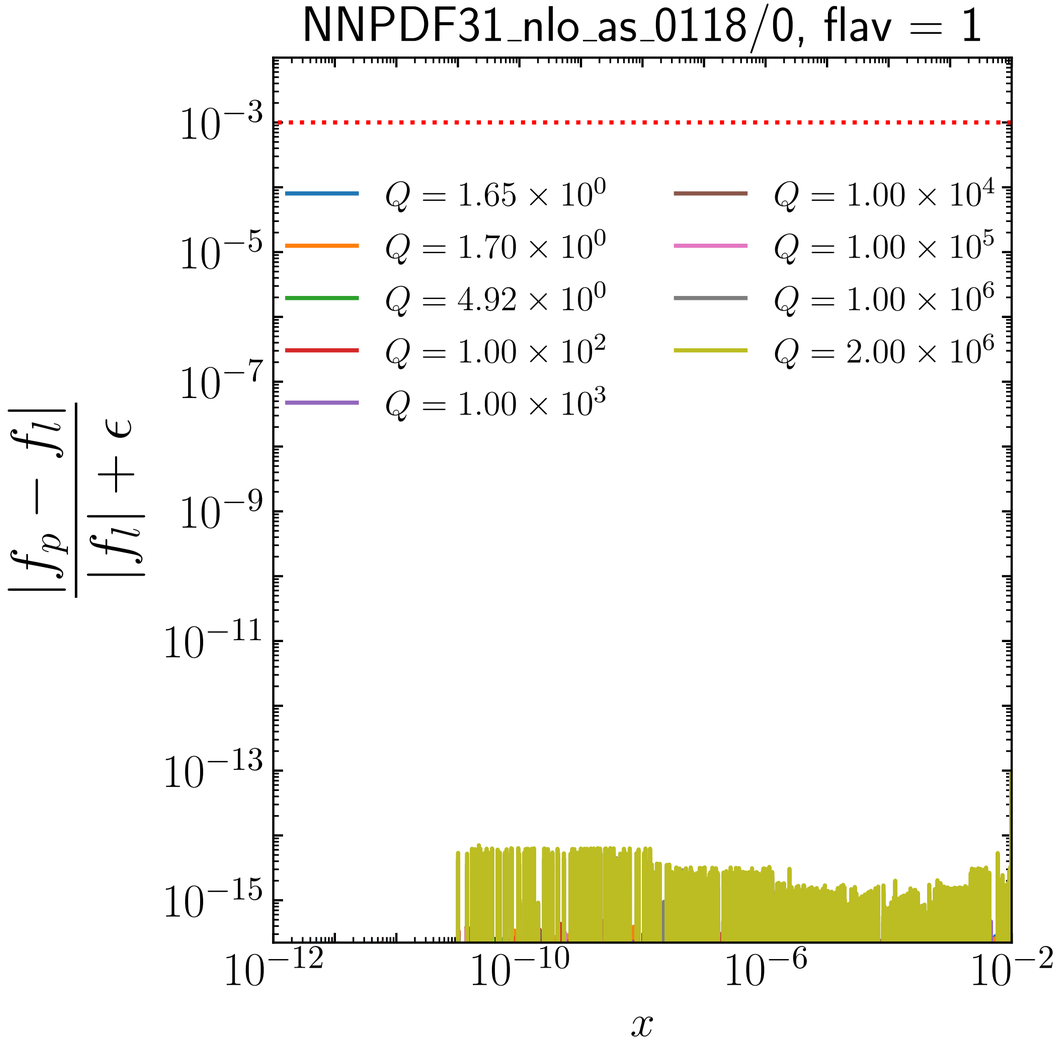
- ☐ It's an external Machine Learning library, their goals are not always aligned with ours
- ☐ The above is most obvious on some overheads in (mostly) memory and execution time]
- ☐ The *easily* in "easily extensible" is subject to opinion

PDF Interpolation Library: PDFFlow

[hep-ph] 2009.06635

github.com/N3PDF/pdfflow





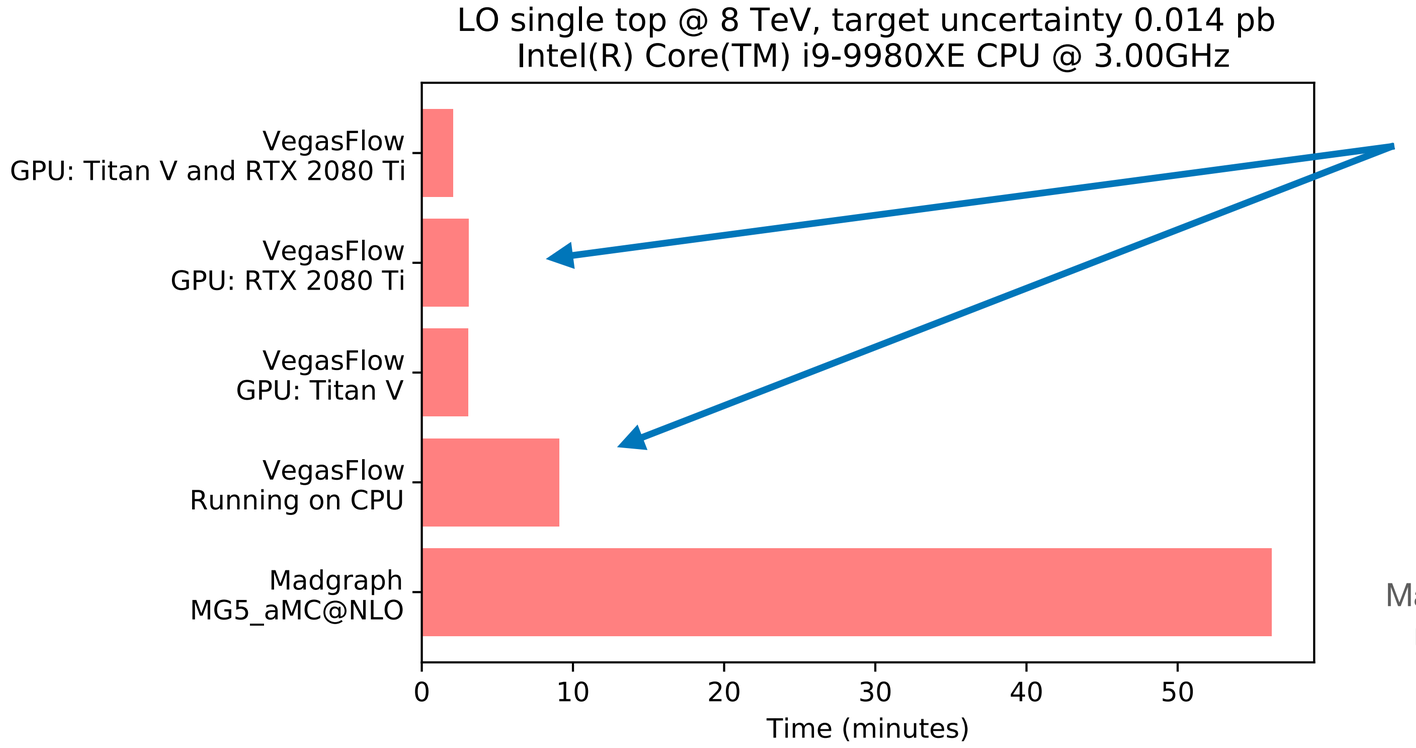
GPU-aware integration wrapper: VegasFlow

[hep-ph] 2002.12921

github.com/N3PDF/vegasflow

VegasFlow implements some widely used importance sampling algorithms and knows how to dispatch integrands to one (or multiple) GPUs.

The first real-life test we can do is a simple Leading Order process with easy expressions and a not too complicated phase space



At this point we have a framework which we can use to run in different kind of hardware with relatively little added effort.

We can start building from here!

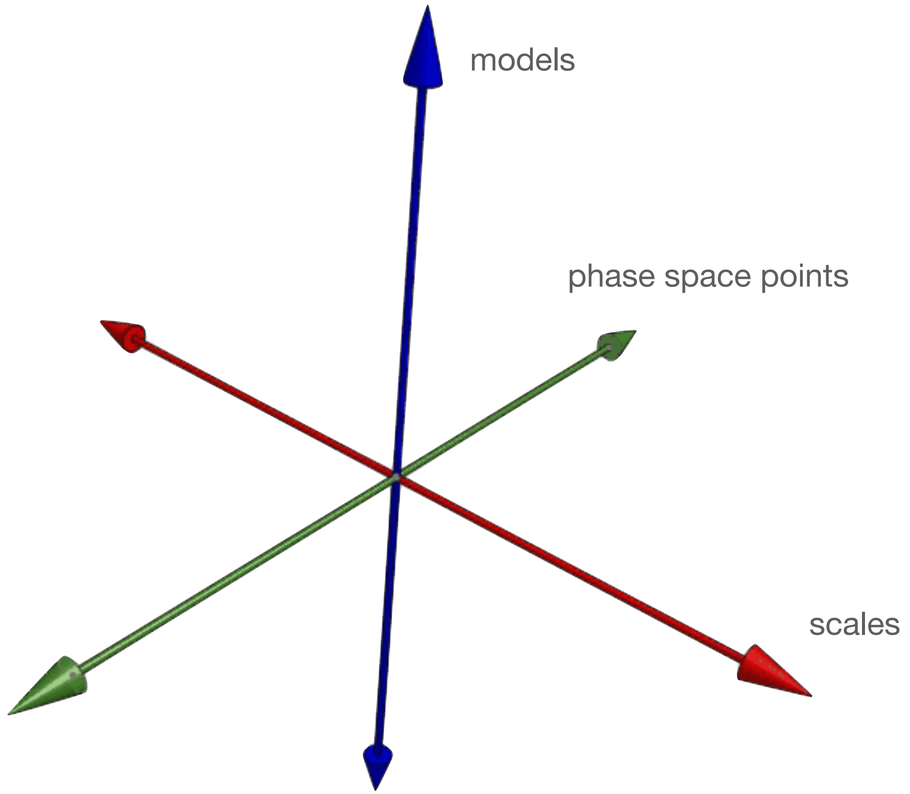
Madgraph timing here for reference, it's not an apple-to-apples comparison

Parallelising outside the box

While we are often thinking about vectorising in the “event-axis”, that’s only one of the options

Maybe -for whatever reason- the strategy doesn’t allow for non-sequential running.

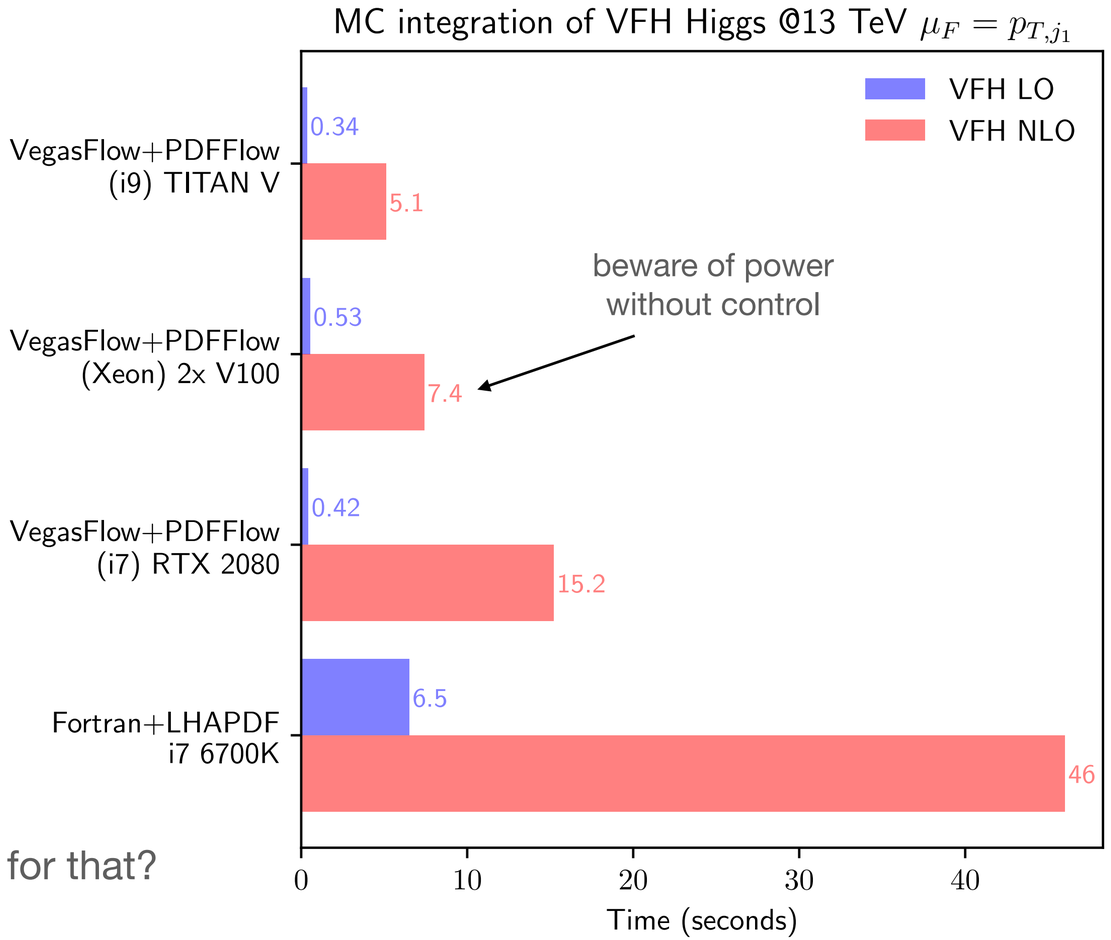
* Running different models at once
* The goal of the game is to keep as much of the calculation along the parallelisation axis constant (luminosity channels, for instance, are probably not a good candidate for this)
* Maybe thinking about a more general tensorization instead of vectorization



Beyond Leading Order

Let's introduce a more realistic scenario: a NLO calculation with non trivial cuts and 4 particles in the final state

- Infrared subtraction are subtracted locally with antenna subtraction.
- The Phase Space was manually written with this process in mind.
- The whole batch of events is generated and cuts immediately applied before continuing the calculation.
- Phase Space points are then reorganized to eliminate any kind of branching in the more expensive parts of the calculation
- For this process, at NLO the cancellation of infrared divergences works very decently, otherwise care needs to be put on that as well.
- We kept an index of each event, its phase space and its weight in order to fill histograms at the end, in this case we were trading memory for performance

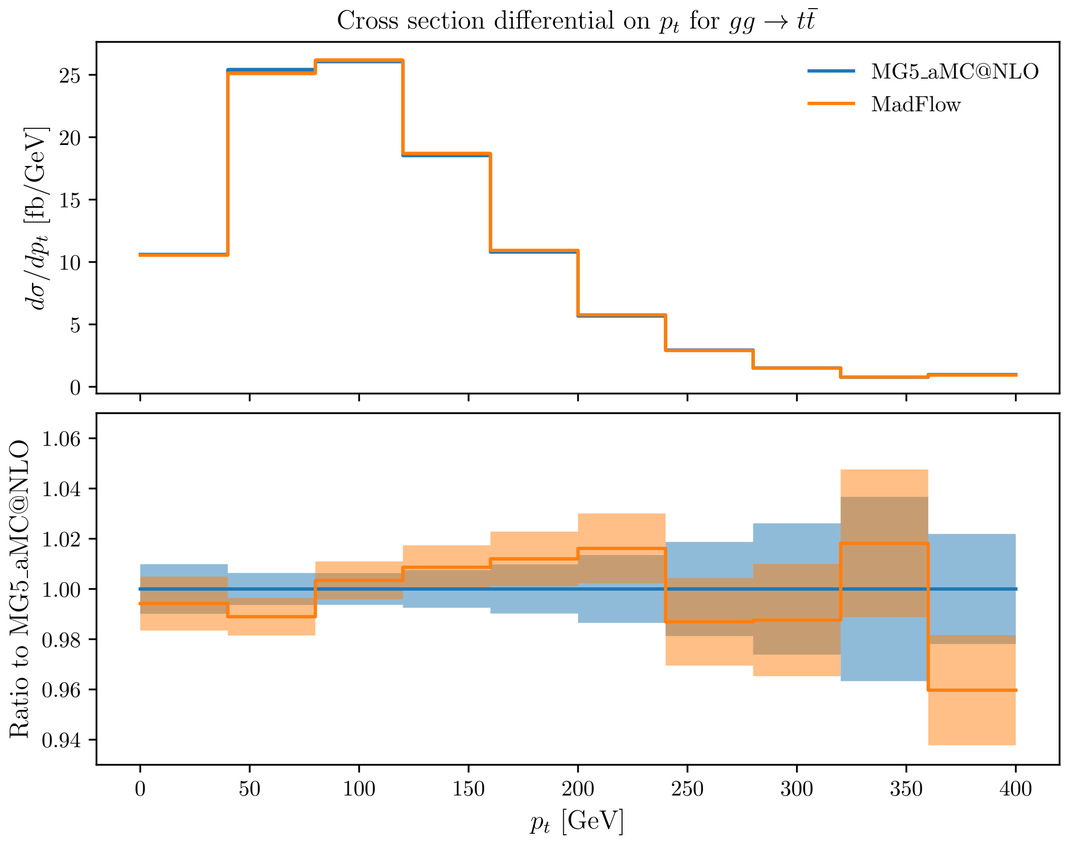


Can we generalize this to any process? What would we need for that?

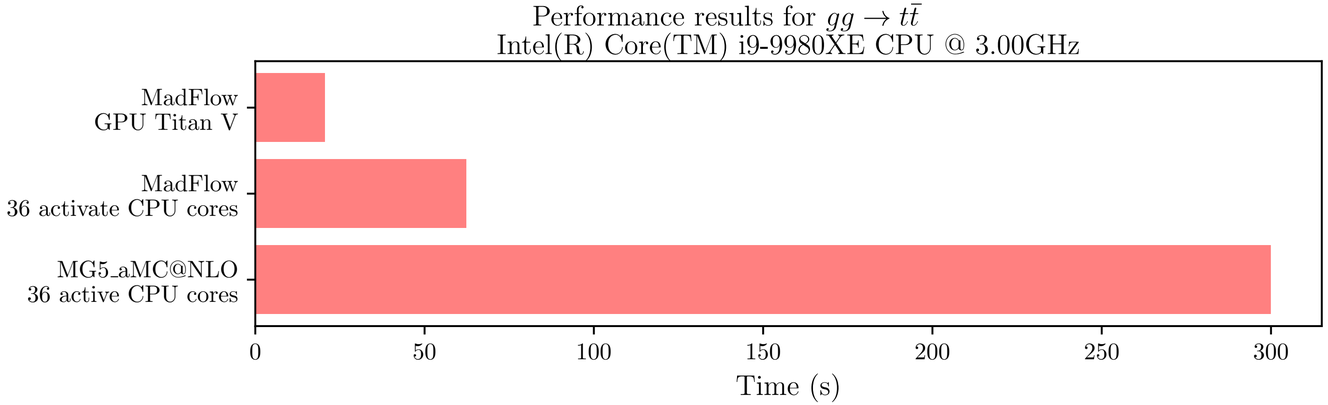
Beyond process-dependent code: MadFlow

[hep-ph] 2106.10279

github.com/N3PDF/madflow



- Exploit MadGraph interface to write the diagrams in python, extended to write them in a vectorized way and using tensorflow-friendly routines
- Write a phase space generator that's completely general (vectorized version of Rambo). We gave it the very original name of RamboFlow.
- We can then modify our previous example to use this Madgraph interface to *automagically* generate the matrix elements. Only at Leading Order.



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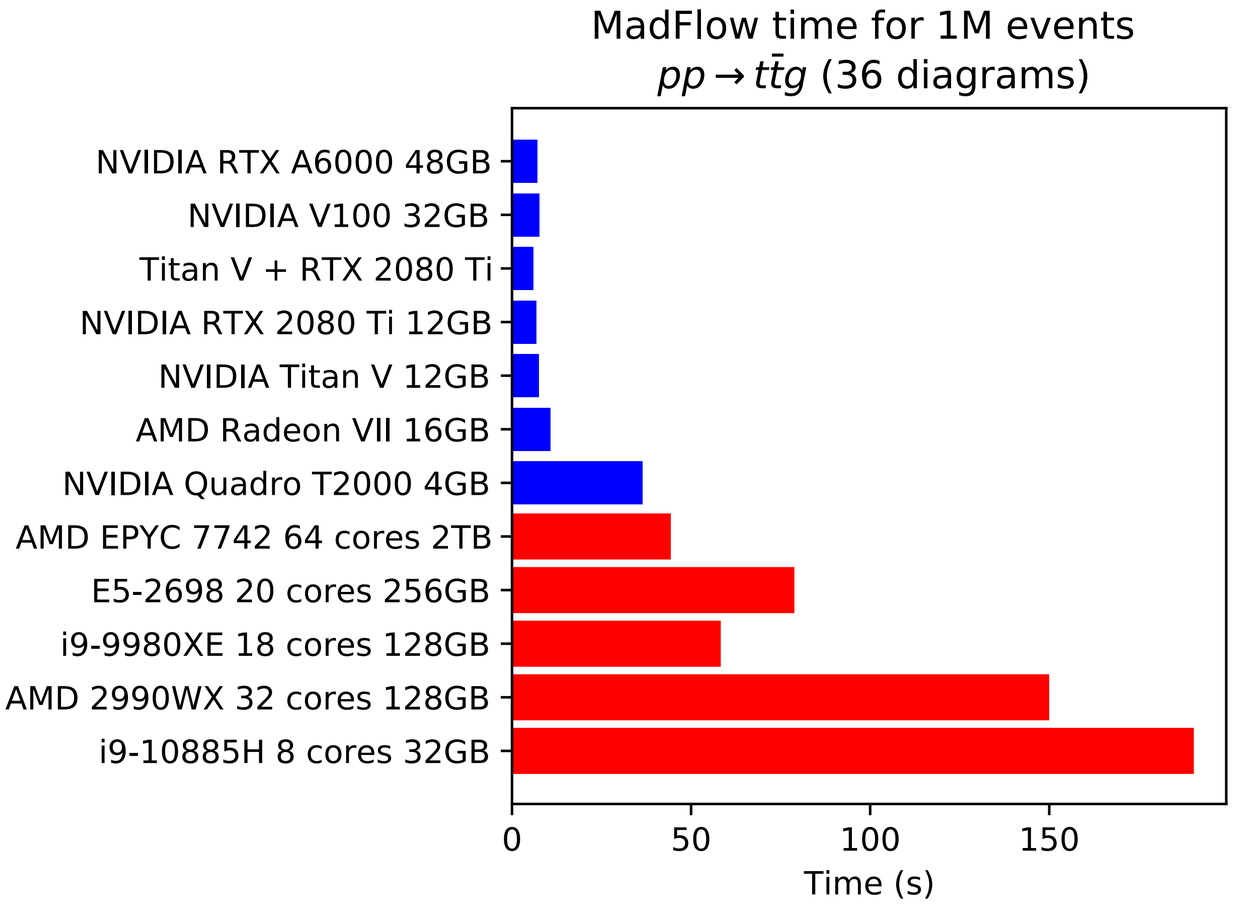


Beyond hardware agnostic code: overoptimization

Now we have to pay the debt that we bypassed at the beginning.

Until now we have been programming with tools that allowed us to use our existing codebase and that could run in any kind of hardware. As announced at the beginning, this introduced an overhead. This overhead is now explicitly visible.

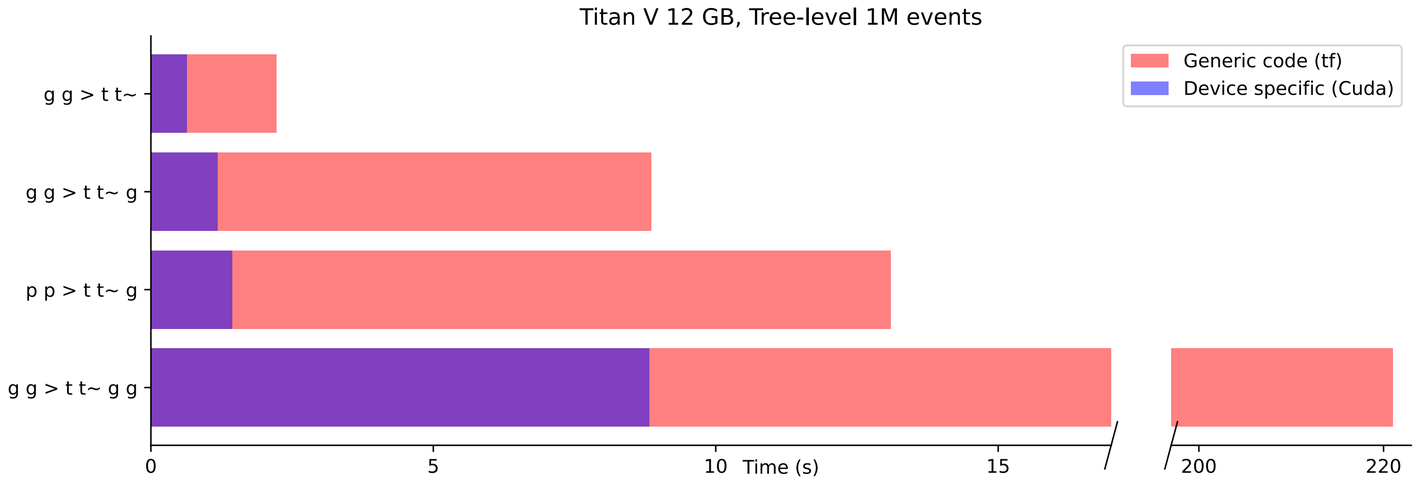
At the same time we can remember one of the advantages that we mentioned at the beginning

☑ Easily extensible and **interfaceable with other languages (C++, Cuda, Fortran, Rust)**

Let´s now use that power.

Since in this case the bottleneck is created by the sheer amount of diagrams, we can write a transpiler so that we can convert them in CUDA code that gets compiled before running the process.

The gains are mostly on memory, but that translates to a gain also in running time



Conclusions

- Full-fledged GPU Monte Carlo event generators required a great dedicated efforts
- Incremental improvements are not always appreciated…
- Having a small framework as a testing ground can be used to
  - Quickly test and benchmark possible ideas
  - Train students without paying a big “opportunity cost”
  - A computational version of a Toy Model