Vectorization of ROOT Mathematical Libraries

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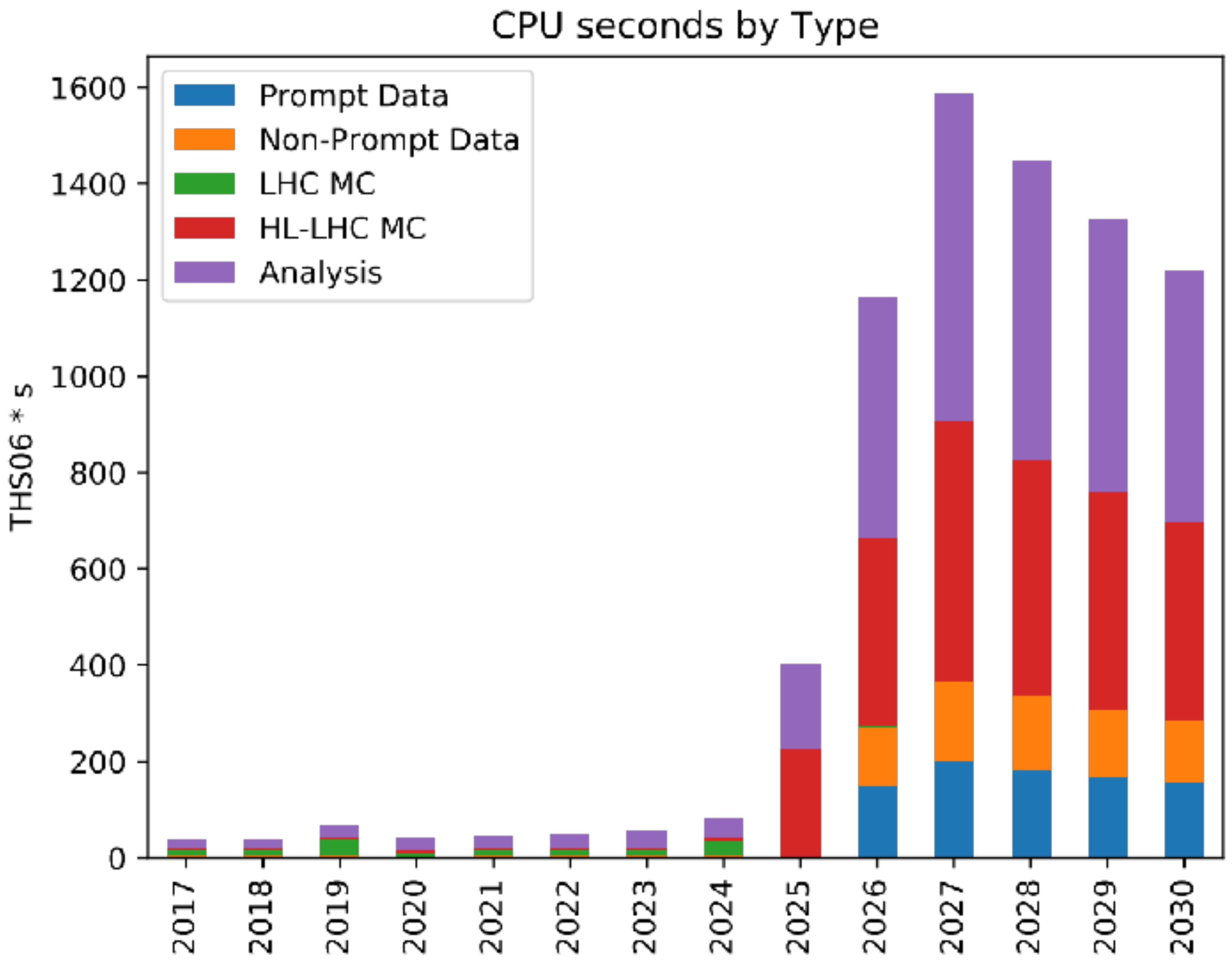
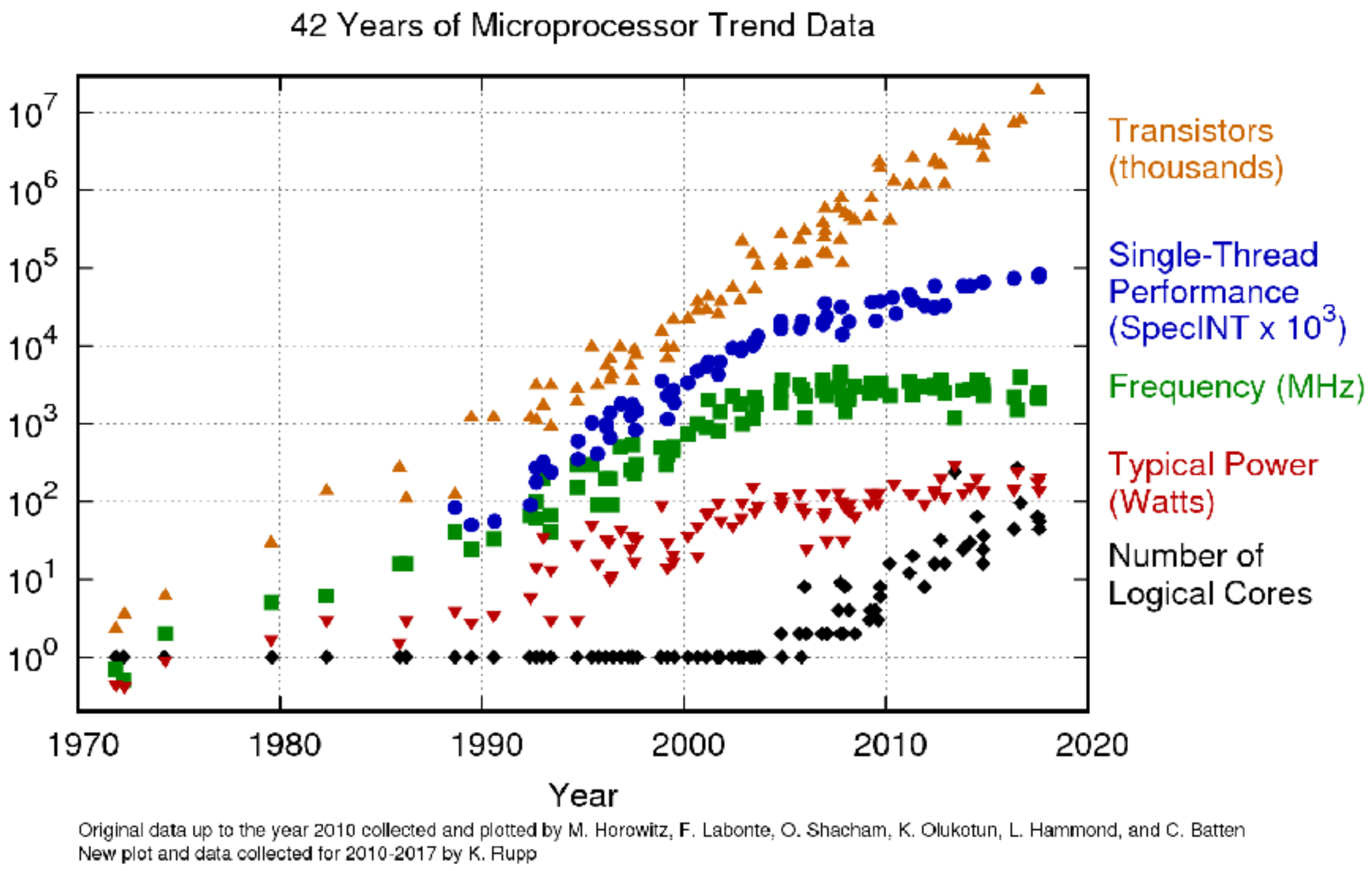
Outline

- Introduction
- VecCore library for vectorization
- VecCore performances
  - with different backends and compilers
- Integration of VecCore in ROOT
- Vectorization in fitting
  - vectorized TF1 and TFormula classes
- Vectorization in matrixes and vector classes
- Future plans
- Conclusions

Introduction

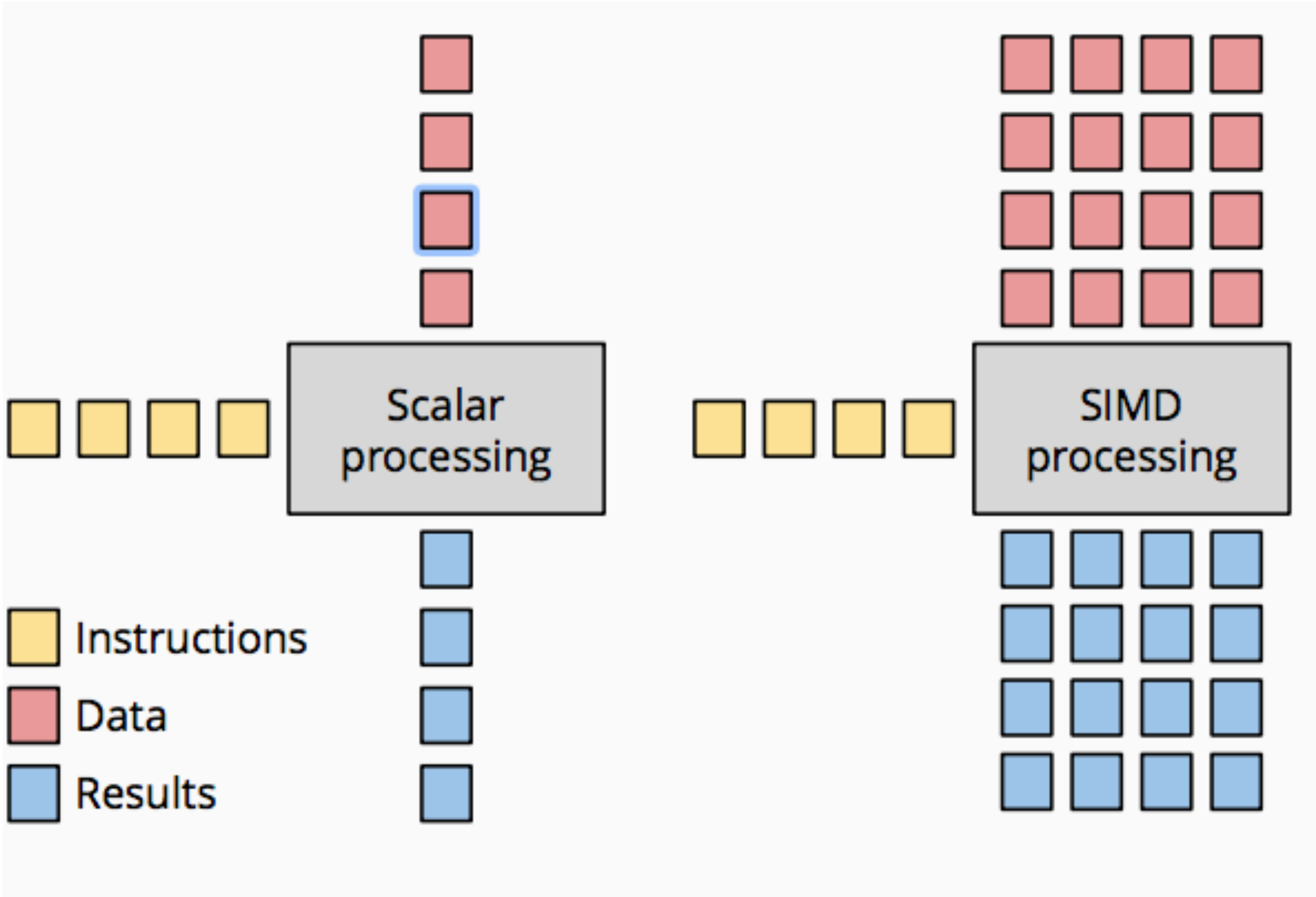
- HEP software needs to fully exploit SIMD vectorisation and parallelisation to achieve the desired performances in simulation, reconstruction and data analysis





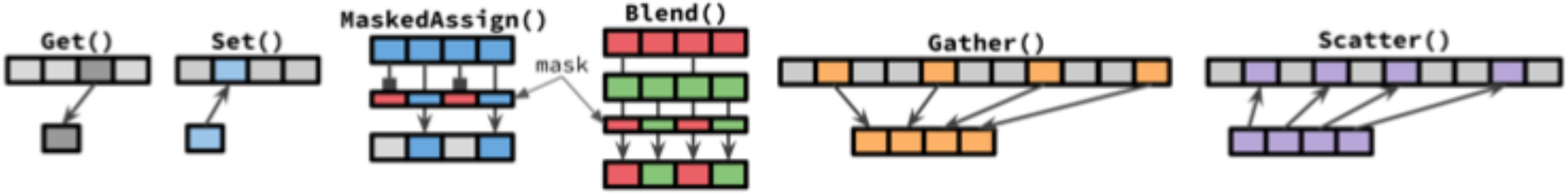
SIMD Vectorization

- Writing efficiently SIMD code is challenging
- Libraries exist that wrap SIMD intrinsic in a convenient interface
  - Vc
  - UME::SIMD
- They do not support all architectures or performances very dependent on specific platforms



VecCore Library

- Provide simple API to express SIMD algorithms
- Can support different back-end implementation
  - users can choose the optimal one depending on the running architecture
- API covering essential parts of SIMD instructions
  - it allows to implement majority of numerical algorithms
    - e.g. masking operations for dealing with branches



The VecCore API

```
namespace vecCore {

   template <typename T> struct TypeTraits;
   template <typename T> using Mask   = typename TypeTraits<T>::MaskType;
   template <typename T> using Index  = typename TypeTraits<T>::IndexType;
   template <typename T> using Scalar = typename TypeTraits<T>::ScalarType;

   // Vector Size
   template <typename T> constexpr size_t VectorSize();

   // Get/Set
   template <typename T> Scalar<T> Get(const T &v, size_t i);
   template <typename T> void Set(T &v, size_t i, Scalar<T> const val);

   // Load/Store
   template <typename T> void Load(T &v, Scalar<T> const *ptr);
   template <typename T> void Store(T const &v, Scalar<T> *ptr);

   // Gather/Scatter
   template <typename T, typename S = Scalar<T>>  T Gather(S const *ptr, Index<T> const &idx);

   template <typename T, typename S = Scalar<T>> void Scatter(T const &v, S *ptr, Index<T> const &idx);

   // Masking/Blending
   template <typename M> bool MaskFull(M const &mask);
   template <typename M> bool MaskEmpty(M const &mask);
   template <typename T> void MaskedAssign(T &dst, const Mask<T> &mask, const T &src);
   template <typename T> T Blend(const Mask<T> &mask, const T &src1, const T &src2);

}
```

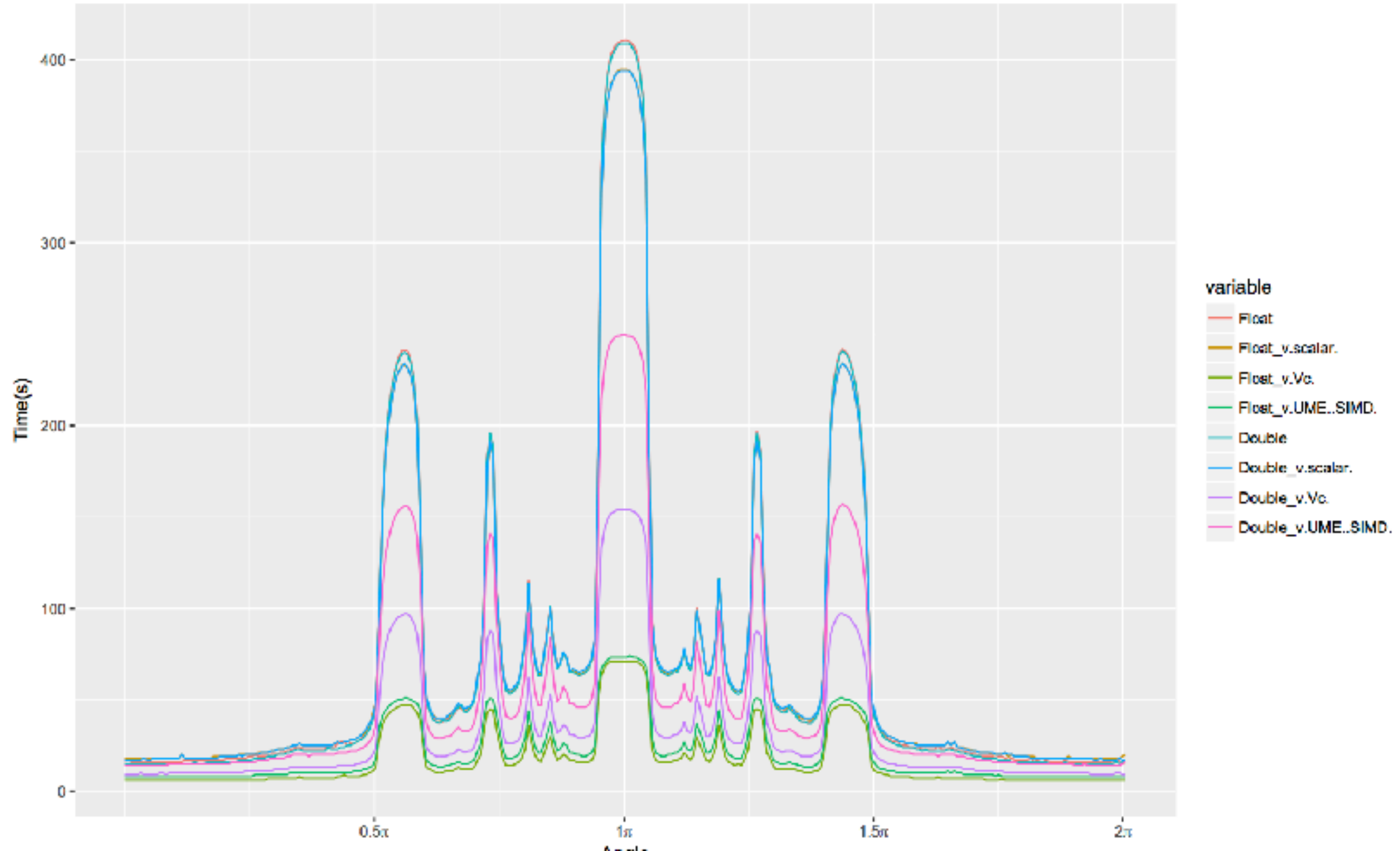
VecCore and ROOT

- VecCore is now integrated in ROOT together with the Vc back-end library)
  - e.g. configure ROOT with

    `cmake  -Dbuiltin_veccore=On -Dbuiltin_vc=On`
- When VecCore is enabled (`R__HAS_VECCORE` is defined), ROOT provides the VecCore SIMD vector types:
  - **`ROOT::Float_v`**
  - **`ROOT::Double_v`**
- The SIMD vector sizes (`ROOT::Double_v::size()`) will depend on the compiled architecture
  - `ROOT::Double_v::size()=2` when ROOT is compiled with SSE
  - `ROOT::Double_v::size()=4` for AVX (e.g. on Haswell)
  - `ROOT::Double_v::size()=8` for AVX-512 (e.g on KNL)

VecCore Performances

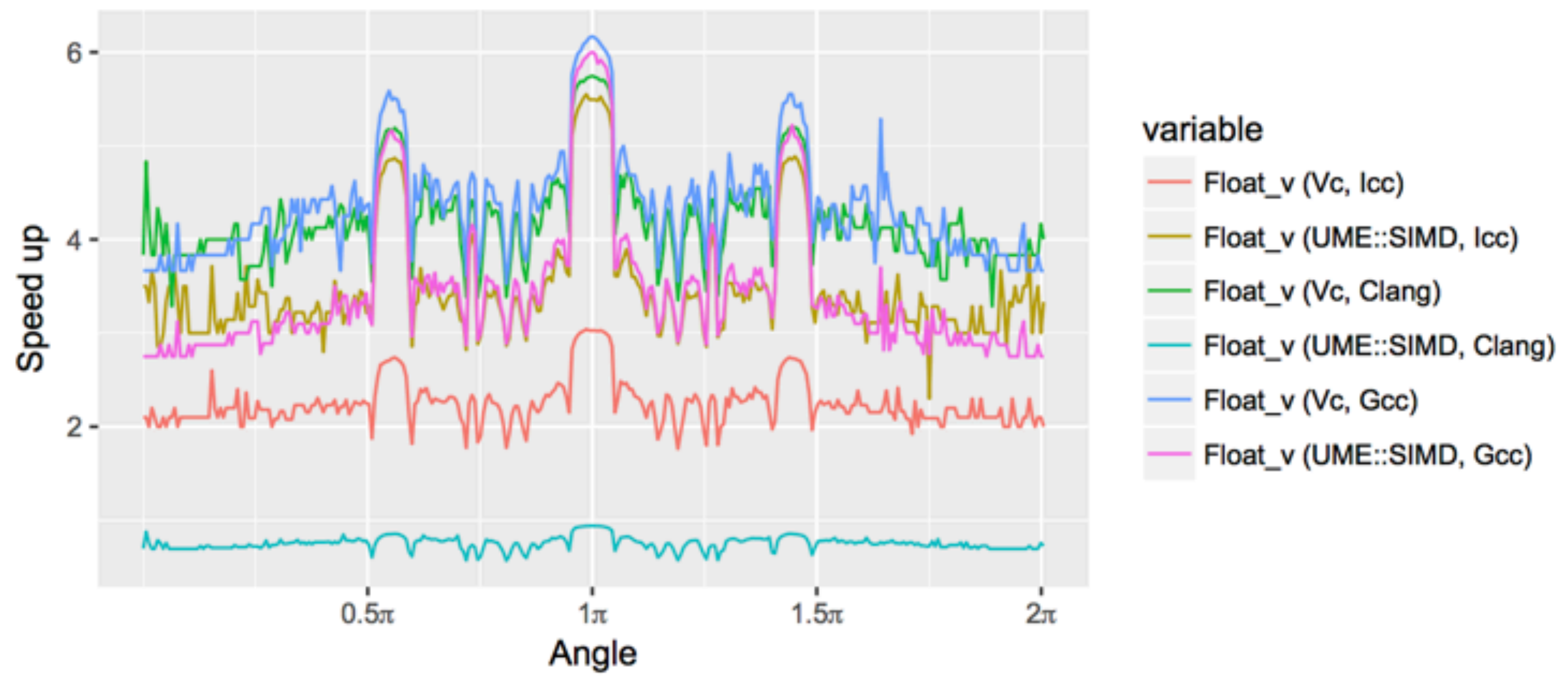
- Study vectorisation performances in a mathematical algorithm
  - Generation of Julia sets
  - Speed-up is less than ideal due to branching
    - different number of computations for each data points

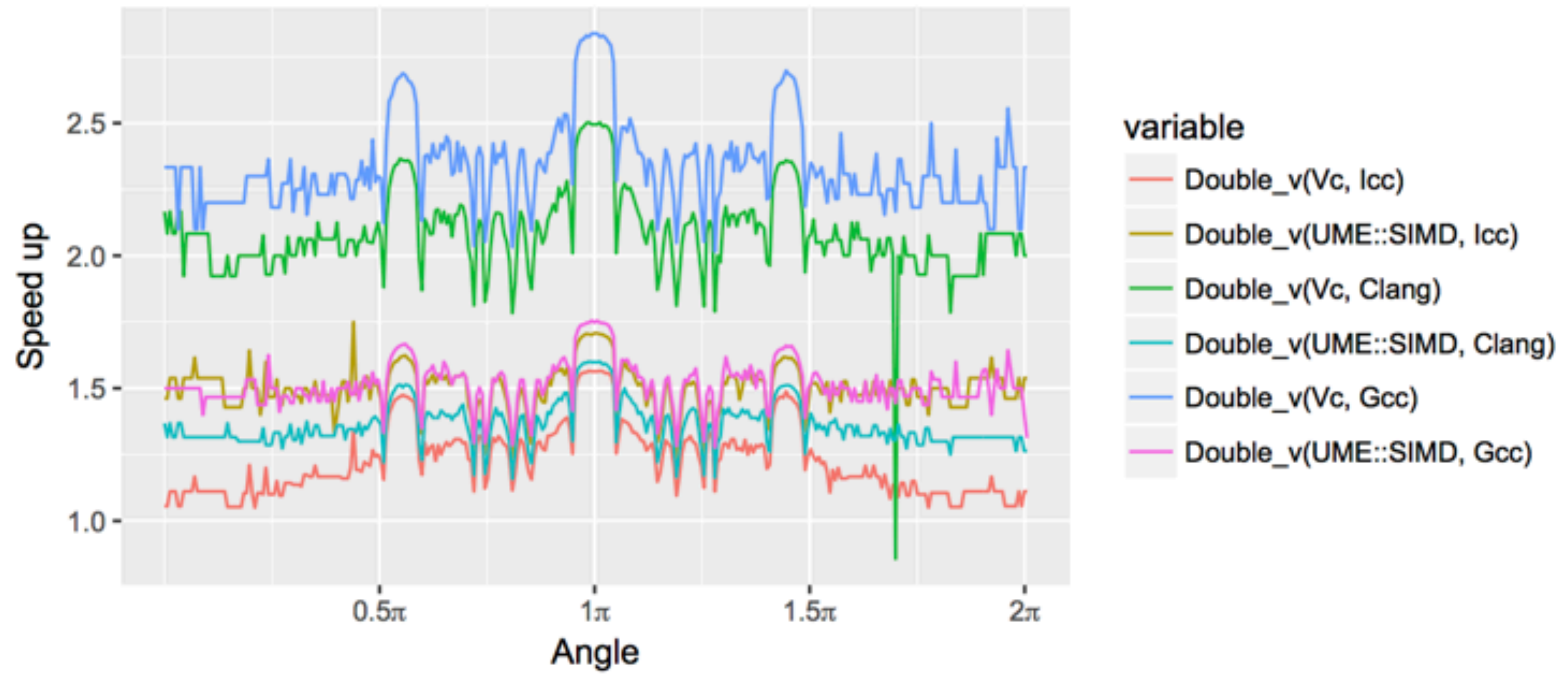


	Base type	float		double	
	Backend	UME::SIMD	Vc	UME::SIMD	Vc
Speed up	Reference	8	8	4	4
	Max.	6	6.17	1.75	2.84
	Min.	2.75	3.52	1.27	2.02
	Avg.	3.45	4.36	1.51	2.34

VecCore Performances

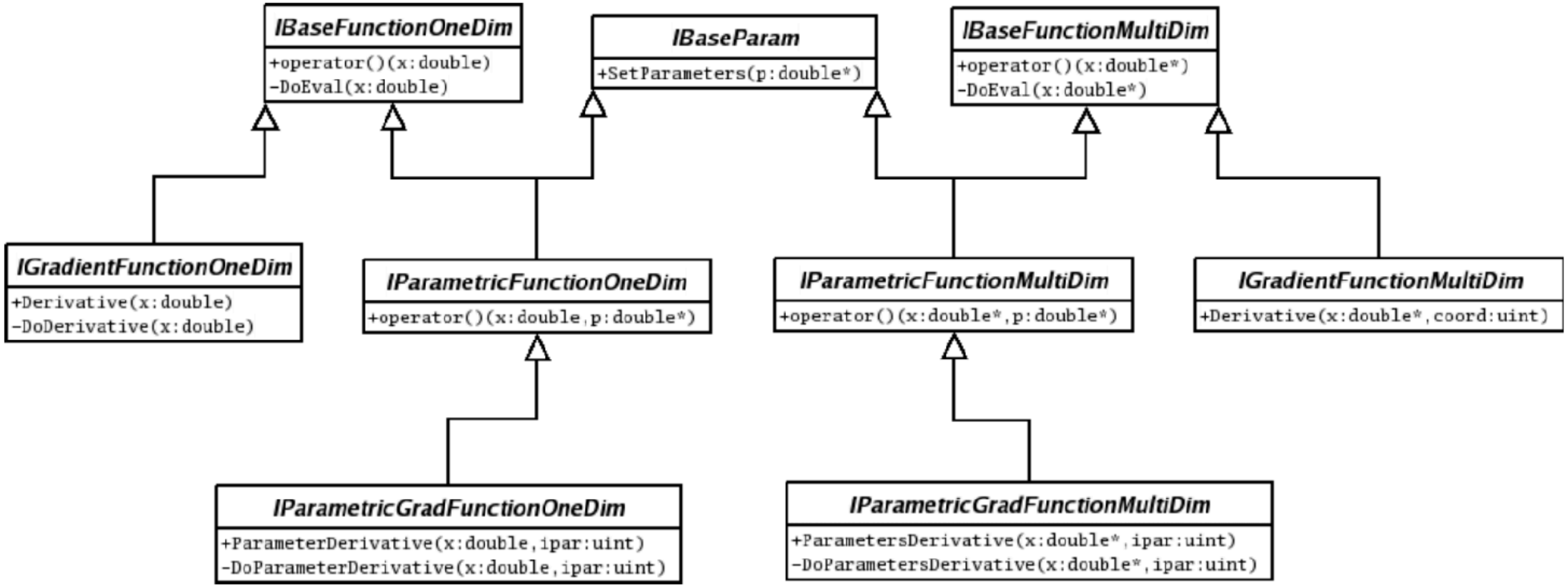
- Vc seems to outperform the UME::SIMD implementation
- Vc does not provide an implementation working for AVX-512
- gcc outperforms Clang and icc





VecCore and ROOT Math

Vectorization of ROOT Math interfaces for function evaluations



- Add generic interfaces for evaluation : operator()(T x) -> T where T can be instantiated as a ROOT::Double_v

New Generic Math Interfaces

- Interface for generic parametric function evaluation
  - used for example in fitting
  - vectorise on the data x which can be multi-dimensiona

```
template<class T>
class IParametricFunctionMultiDimTempl: virtual public IBaseFunctionMultiDimTempl<T>,
                                        virtual public IBaseParam {
 public:

    typedef T BackendType;

    …..

    // Evaluate the function at a point x[] and parameters p
    T operator()(const T *x, const double   *p) const { return DoEvalPar(x,p); }

  private:

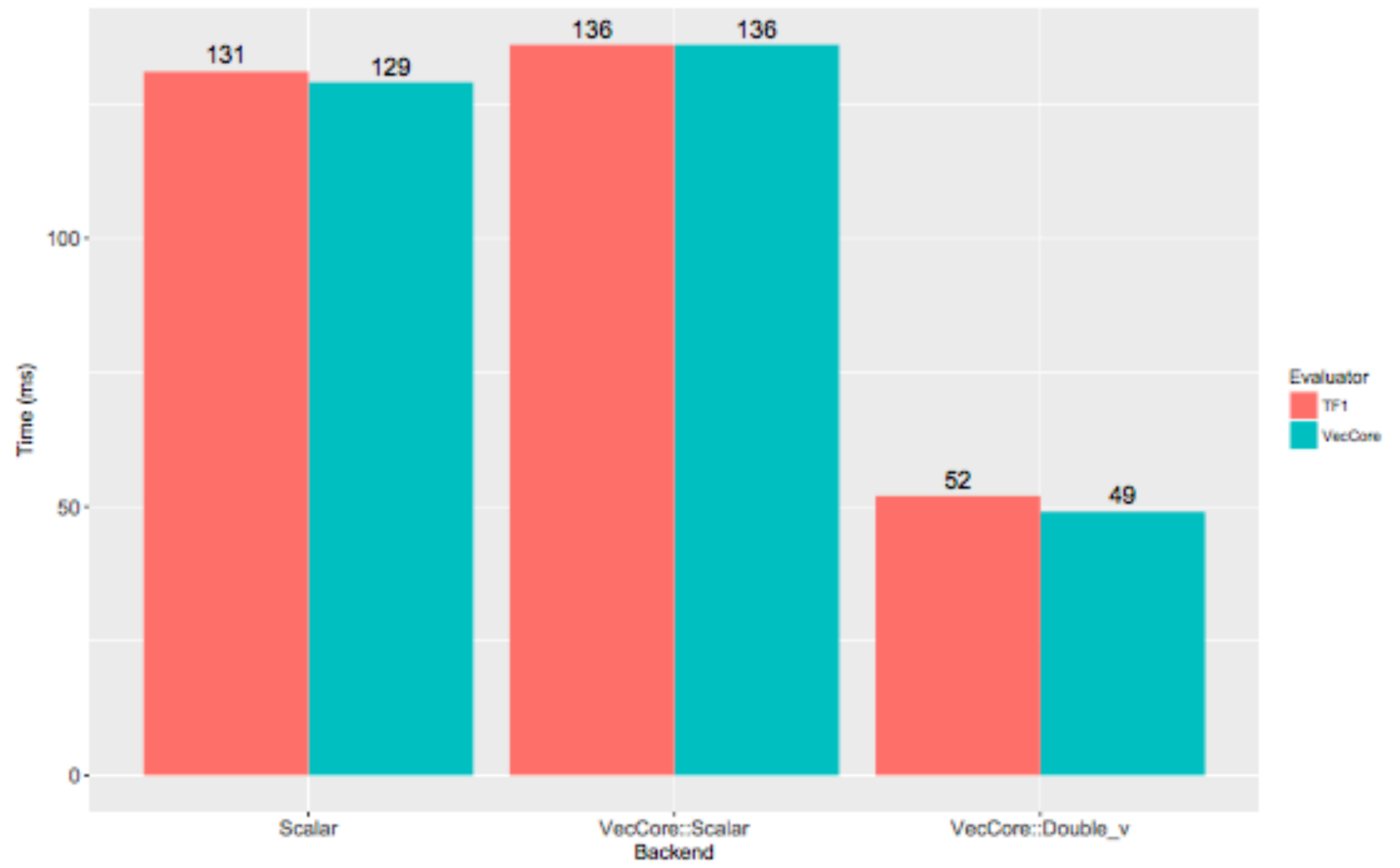
    virtual T DoEvalPar(const T *x, const double *p) const = 0;

    virtual T DoEval(const T *x) const;

};
```

TF1 Extensions

- TF1 class has been extended to support vectorised user functions
  - `TF1("fs",[](double *x, double *p){ return p[0]*sin(p[1]*x[0]); }, 0., 10., 2);`
  - `TF1("fv",[](ROOT::Double_v *x, double *p){ return p[0]*sin(p[1]*x[0]); }, 0., 10., 2);`
- Template evaluation accepting VecCore SIMD vector types
  - `template <class T> TF1::EvalPar(const T * x, double * p)  ->  T;`
- Vectorized TF1 function can then be used for fitting (e.g. in TH1::Fit)



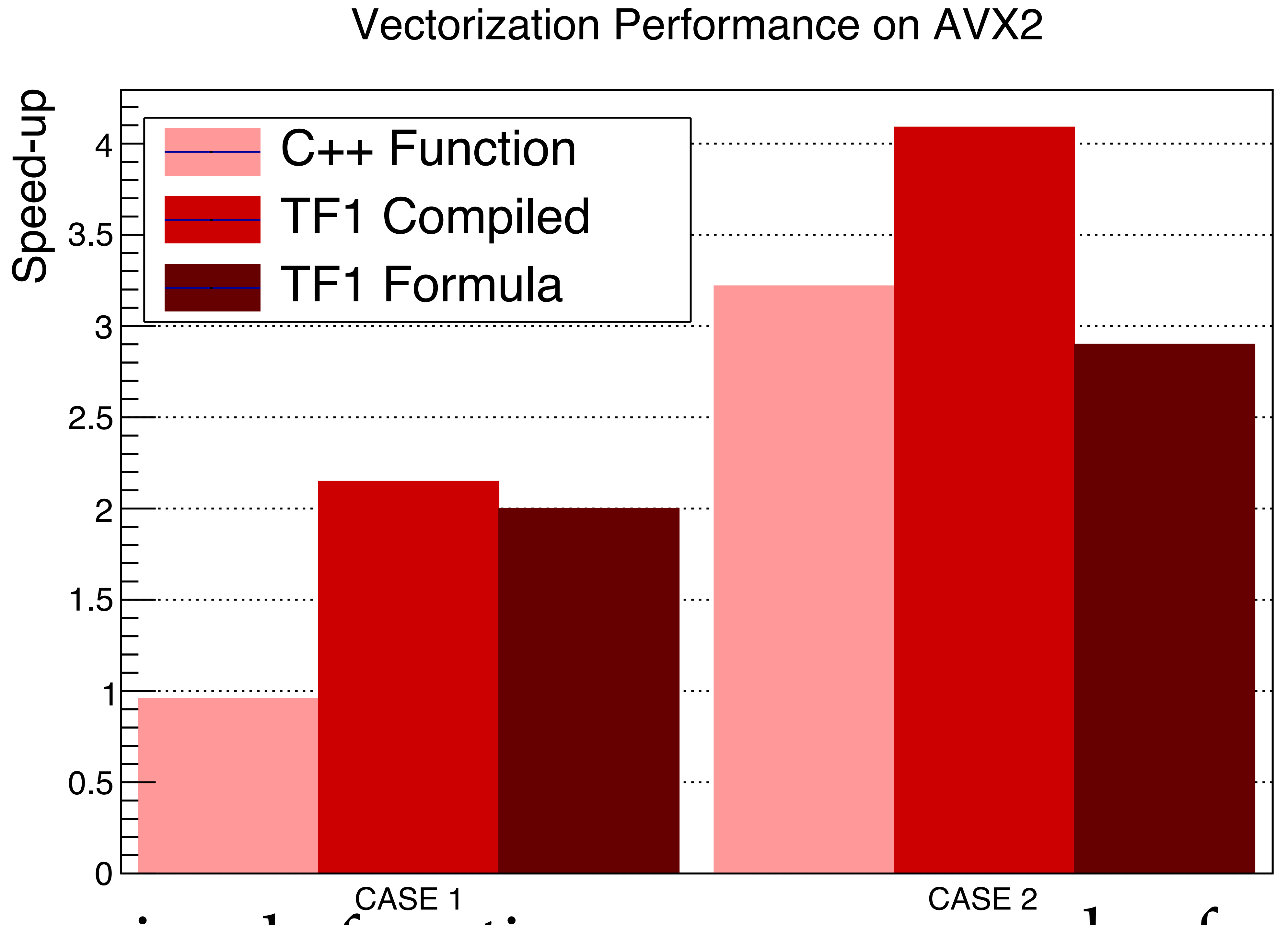
very small overhead when evaluating using a TF1 instead of a direct free function

Vectorization of TFormula

- ROOT TFormula class is used to build parametric functions which can be used for fitting and modeling directly from string expression
- e.g. `TFormula("f1","[a]*sin( [b]*x");`
  - expression is compiled using JIT provided by CLING
    - compiled signature is based on
      `f(double *x, double *p)->double`
  - Added capability to JIT compile with a vectorised signature:
    `f(ROOT::Double_v *x, double *p)->ROOT::Double_v`
- One can then easily have vectorised functions for fitting automatically

Vectorized TFormula Perfomances

- Performance results evaluating a math expression using a free C++ function with TF1 and TF1 based on Formula
- Study the speed-up by using vectorisation on AVX



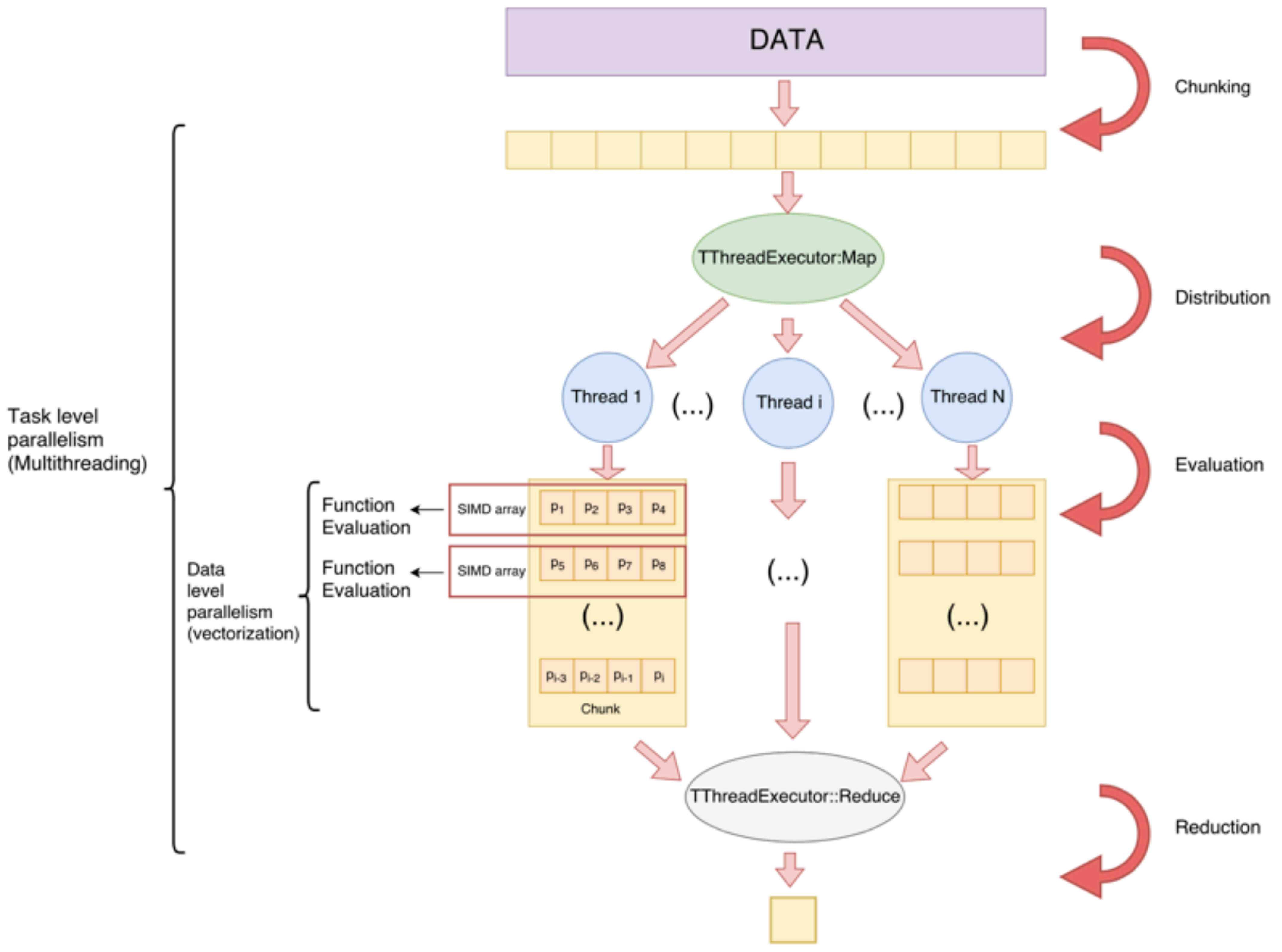
simple function more complex function

Fitting with Vectorized Functions

- Multi-dimensional input data x (coming from histograms or TTree's) is vectorised using `ROOT::Double_v`
  - organize data from AOS to SOA

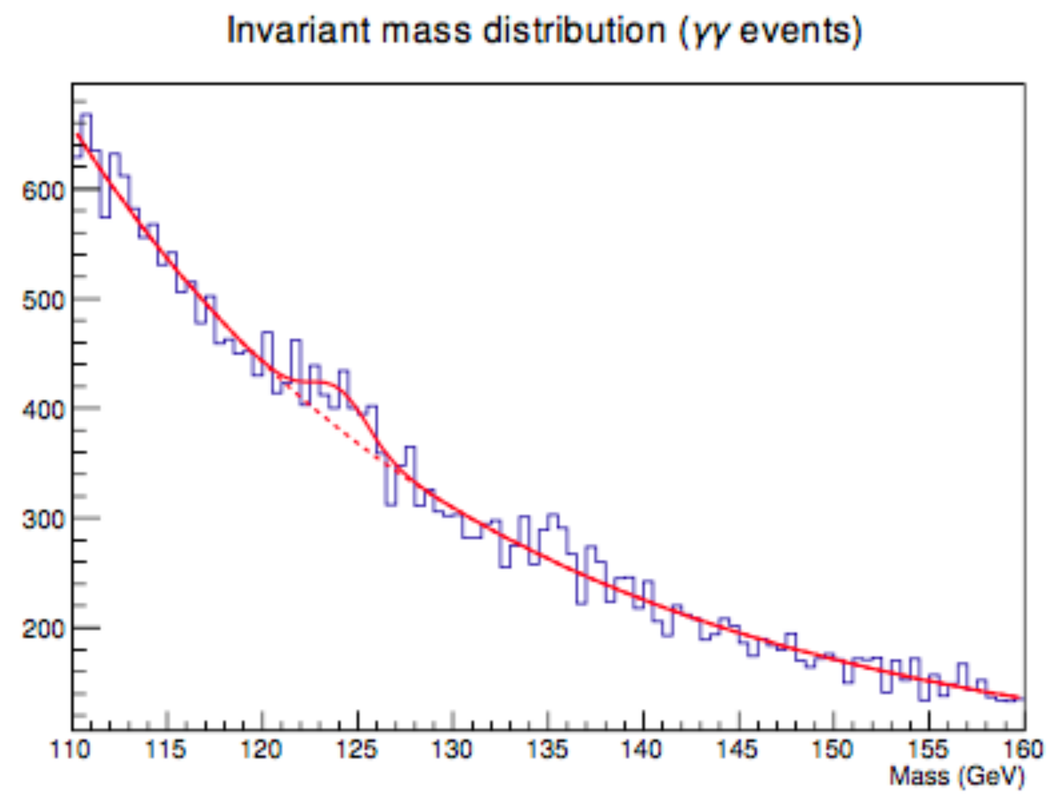
$$(x_0, y_0, z_0, \ldots, x_n, y_n, z_n) \rightarrow (x_0, \ldots, x_n, y_0, \ldots, y_n, z_0, \ldots, z_n)$$

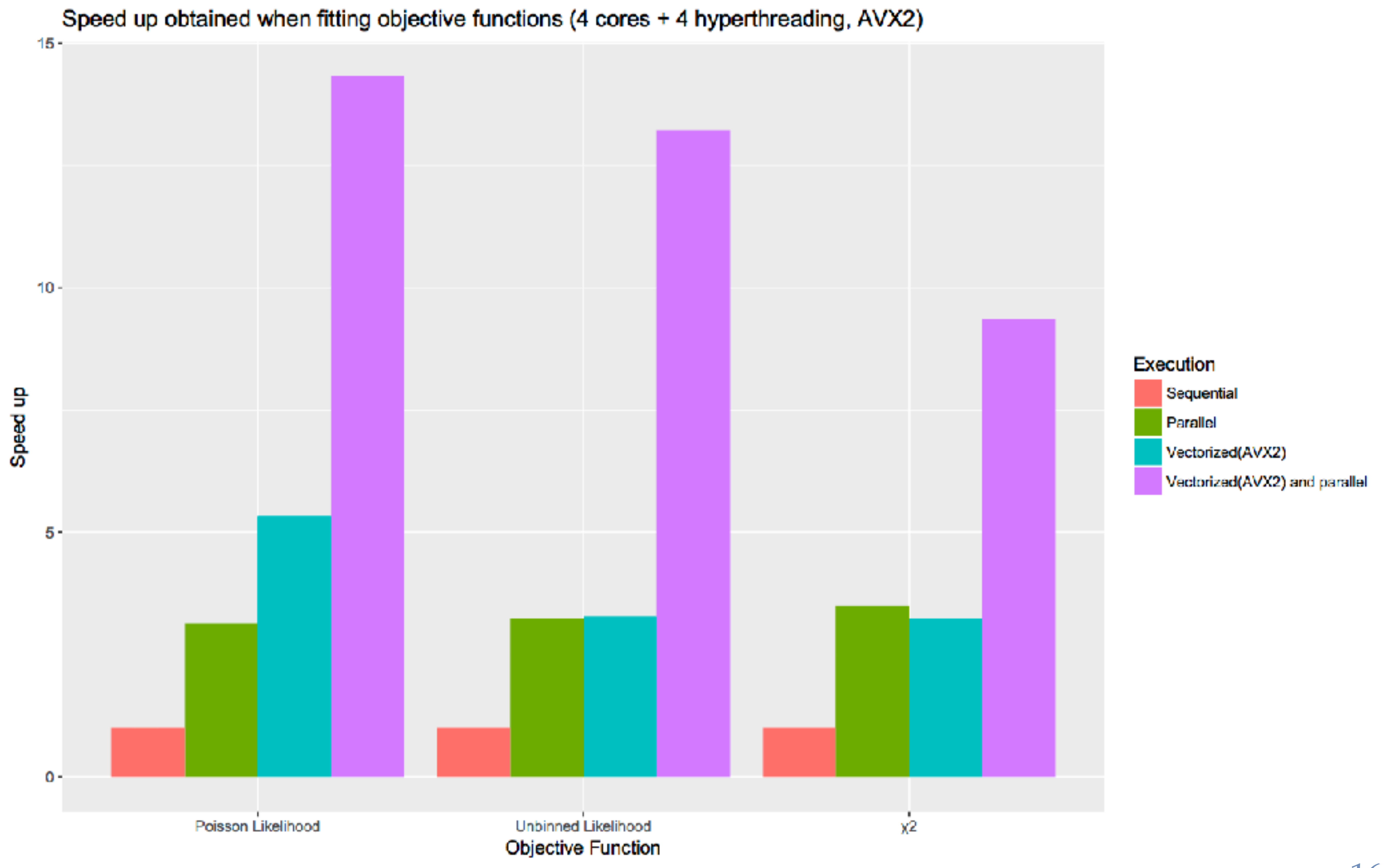
- Model function is evaluated in vectorised mode when computing the chi-square or likelihood function (objective function) for fitting
- Computation of objective function is also parallelized with multi-threads by chunking the data



Fitting Performances

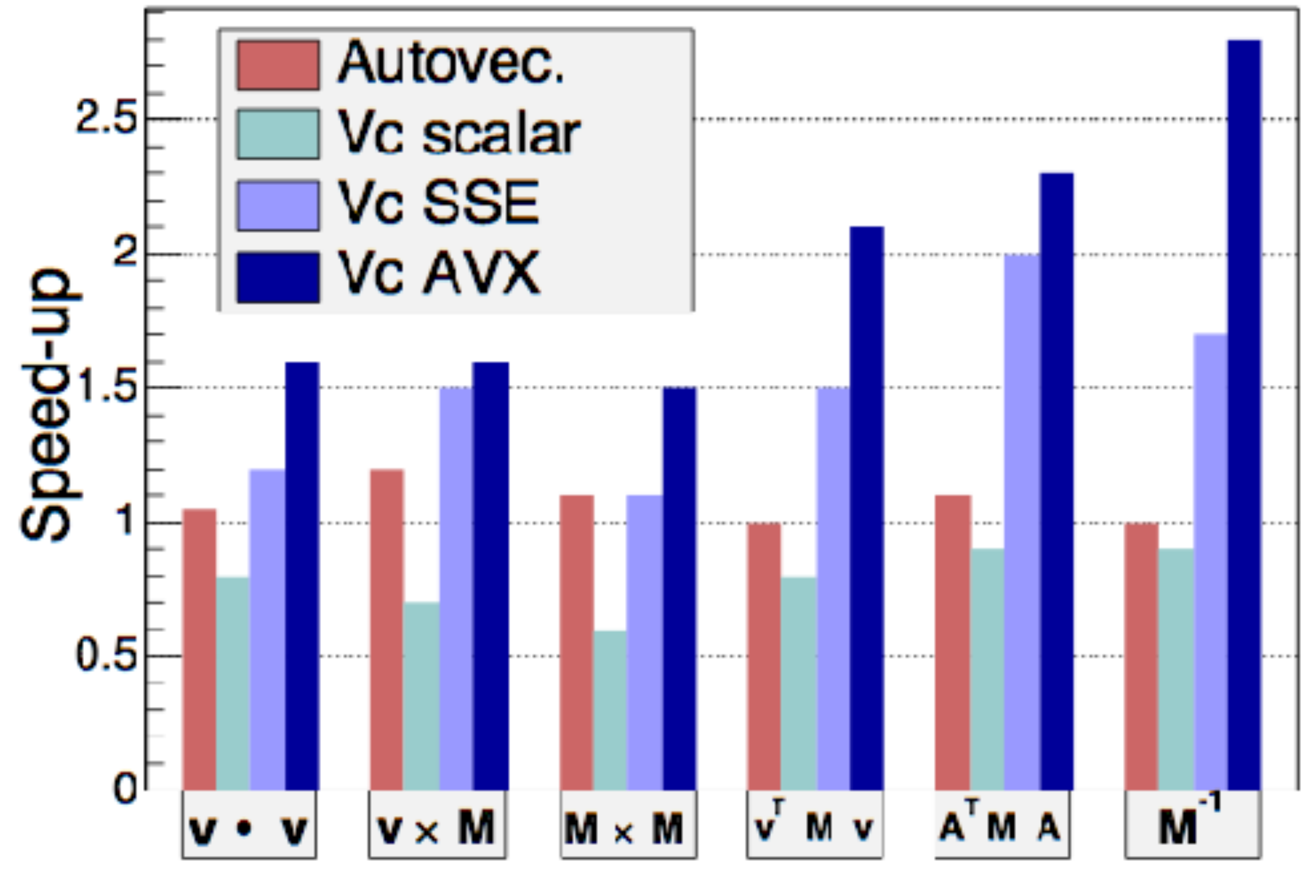
- Measure CPU performances in a typical HEP fitting
  - fit invariant mass spectrum to determine significance and location of the signal (e.g. H -> gg)

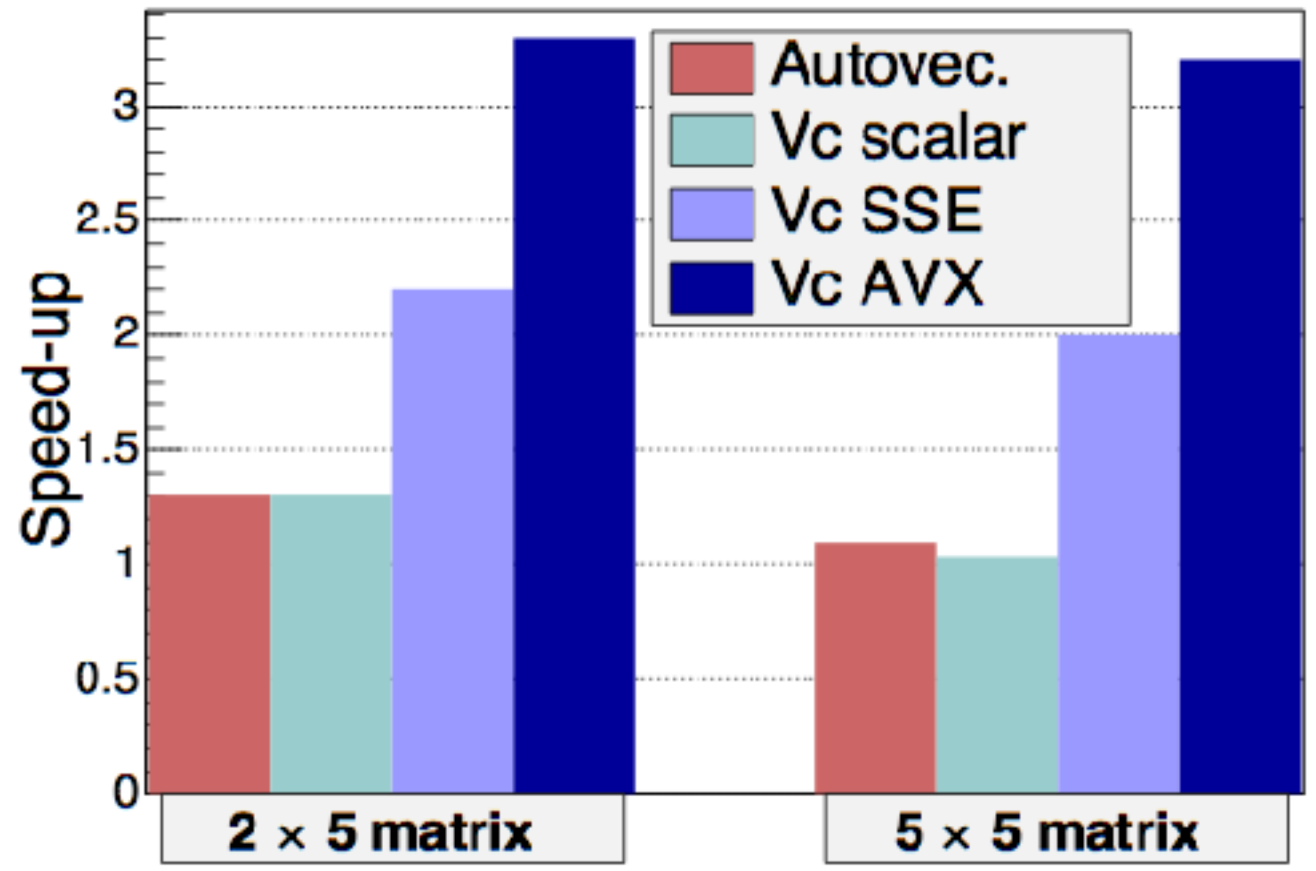




Vectorization in Matrix Operations

- ROOT provides a template vector and matrix classes (optimized for small sizes) which can be used in single and double precision
  - `SVector< double,N>`
  - `SMatrix< double,N,M>`
- Template classes for geometry and physics vectors with their transformations
  - `DisplacementVector3D< Cartesian3D<double>`
  - `LorentzVector<PxPyPzE4D<double> >`
- VecCore types (**`ROOT::Double_v`**) can be used as template parameters for vector and matrices classes and for the geometry vectors
  - vectorisation for operations on a list of vectors/matrices (vertical vectorisation)





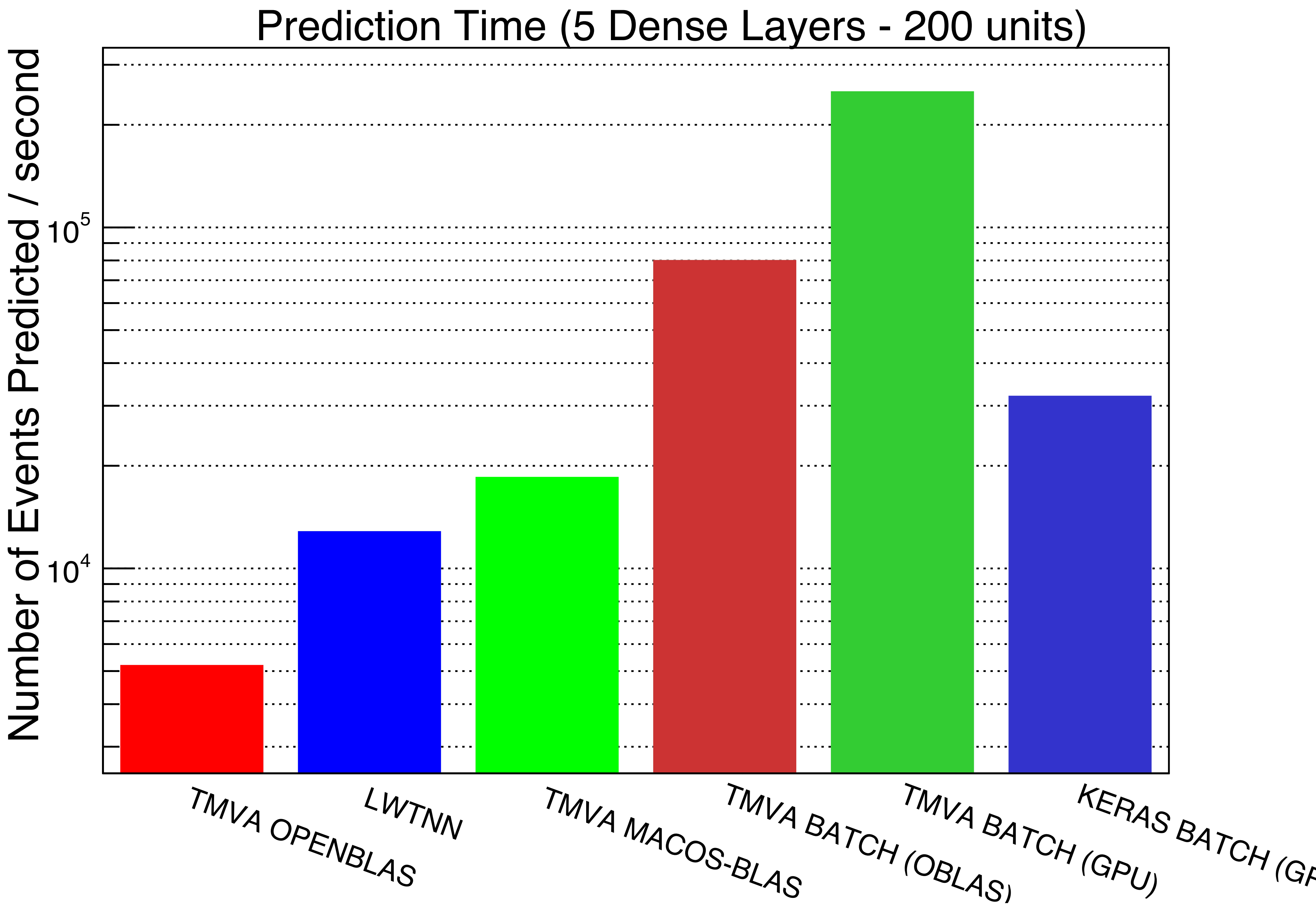
Future Plans: Math Functions

- Re-implement Mathematical functions in TMath and ROOT::Math (e.g. statistics functions) using VecCore
- Plans is to have a single template implementation, which can work for scalar and vector types
- Example:
  - ```
    template <class T>
    TMath::Gaus(const T & x, double mu, double sigma) -> T
    ```
- Basic Math functions (e.g. exp, sin, cos) are already provided by VecCore
    ```

Future Plans: Machine Learning

- Use VecCore for matrix operations in Neural Network
- Interested in optimise the single event evaluation.
- Vectorisation can be used for :
  - applying weight to input layer data (matrix multiplication)
    - compute activation function using vectorised implementations (e.g. tanh)

Performances for evaluating a deep neural network architecture



Conclusions

- Advantages by using VecCore library which provides a simpler programming model for SIMD
- Benchmark of VecCore and its backend shows that Vc outperforms UME::SIMD and gcc performs better than icc or clang
- ROOT uses internally VecCore by defining new vector types:
  - `ROOT::Float_v` and `ROOT::Double_v`
  - Extension of ROOT function classes and interfaces to support these new types
  - Integrate vectorisation also in TFormula class, thanks to ROOT JIT'ing
- Significant performances improvement in ROOT thanks to vectorisation
- Plan to deploy vectorisation even more: Math functions and Deep Learning

History of Intel SIMD

- Intel® Pentium Processor (1993)
  32bit
- Multimedia Extensions (MMX in 1997)
  64bit integer support only
- Streaming SIMD Extensions (SSE in 1999 to SSE4.2 in 2008)
  32bit/64bit integer and floating point, no masking
- Advanced Vector Extensions (AVX in 2011 and AVX2 in 2013)
  Fused multiply-add (FMA), HW gather support (AVX2)
- Many Integrated Core Architecture (Xeon Phi™ Knights Corner in 2013)
  HW gather/scatter, exponential
- AVX512 on Knights Landing, Skylake Xeon, and Core X-series (2016/2017)
  Conflict detection instructions

☐ = 32 bit word

Why Use SIMD ?

SIMD vectorization is already essential for high performance on modern Intel® processors, and its relative importance is expected to increase, especially on hardware geared towards HPC, such as Xeon Phi™ and Skylake Xeon™ processors.