CERN

ROOT
Data Analysis Framework

Vectorization of ROOT Mathematical Libraries

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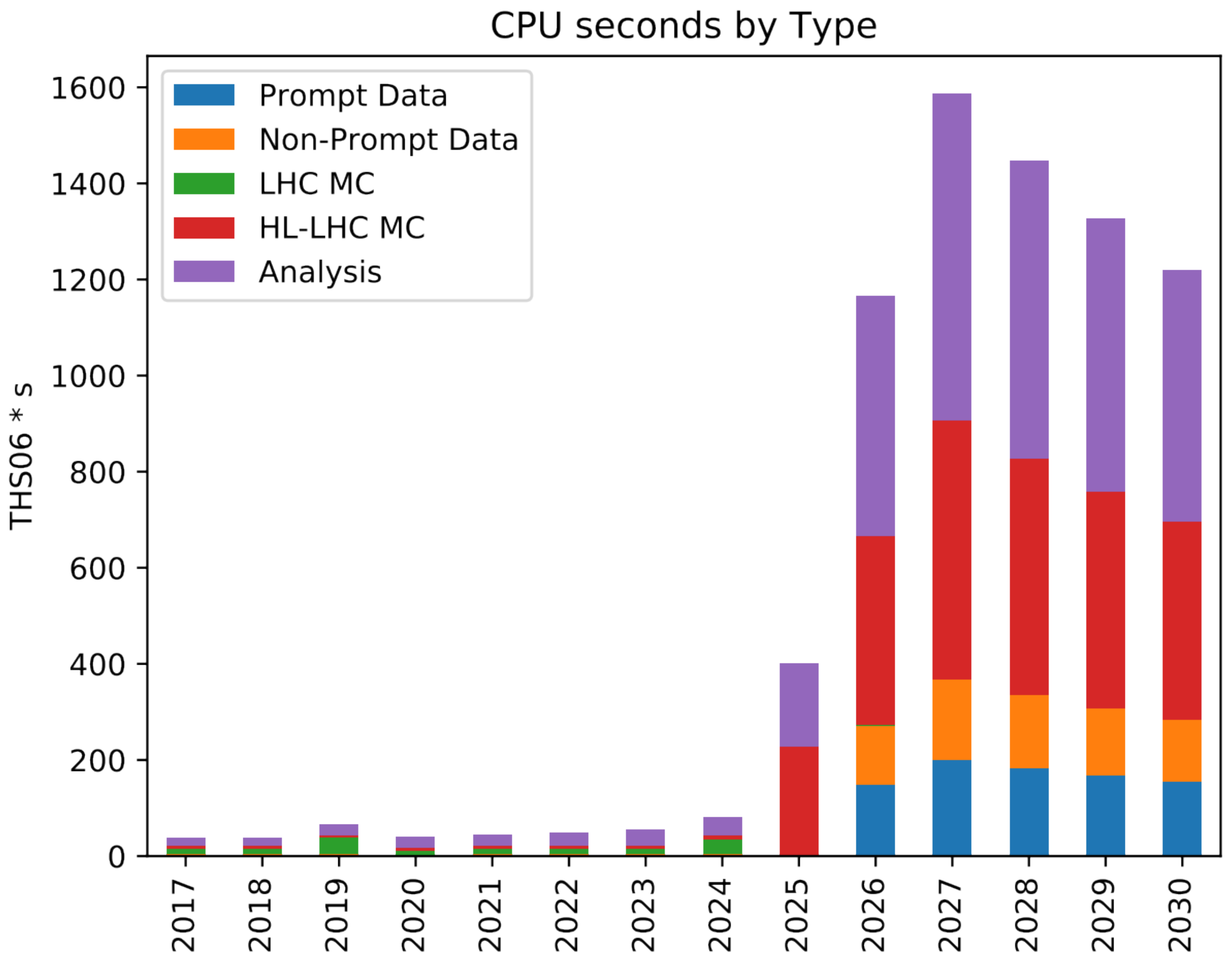
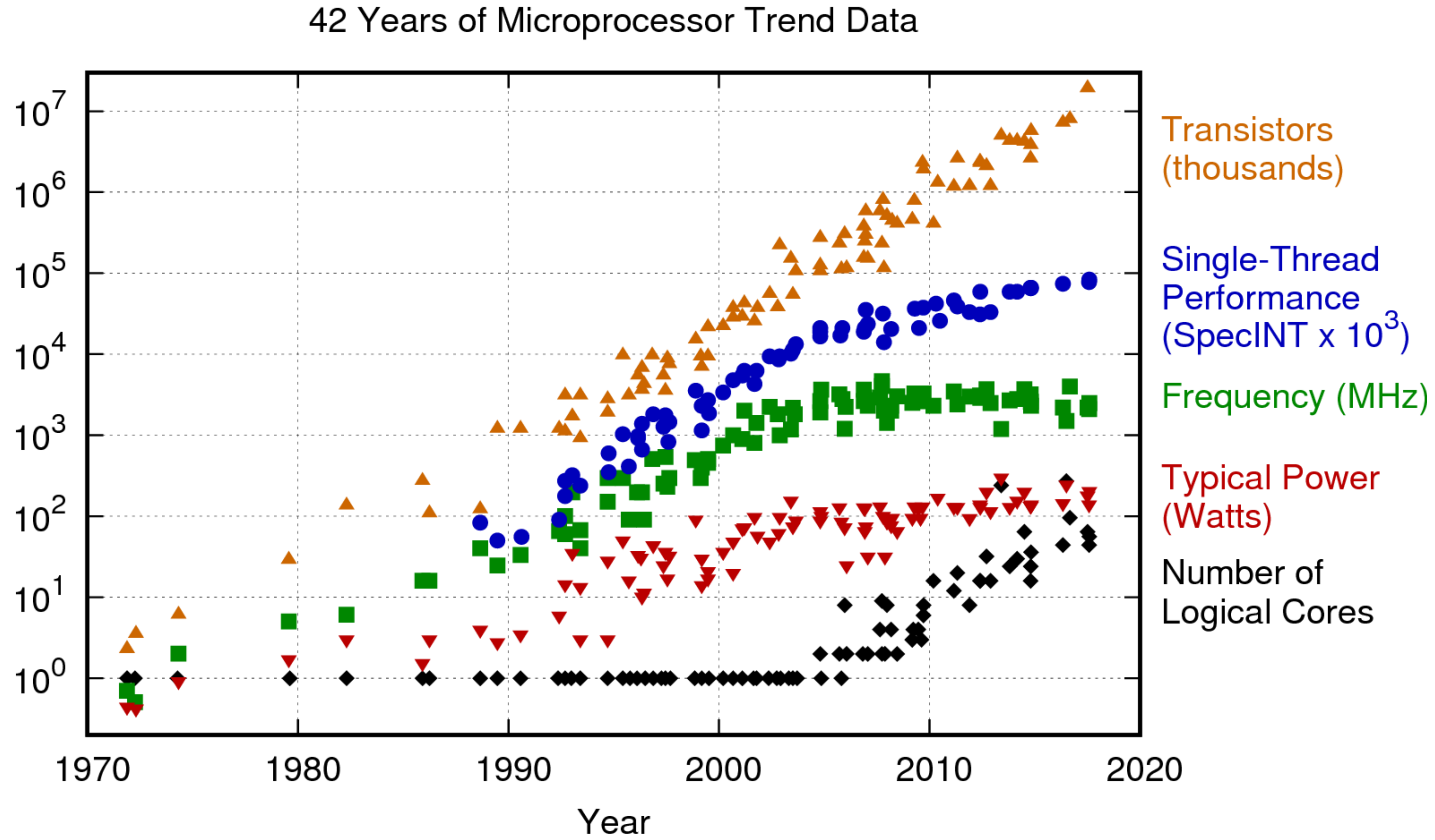
Outline

- Introduction
- **VecCore** library for vectorization
- Integration of VecCore in ROOT
- Vectorization in function evaluation (fitting), matrix 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

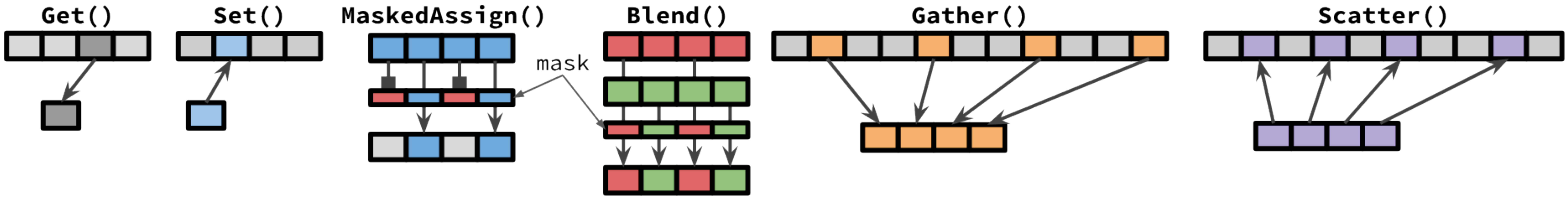




Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2017 by K. Rupp

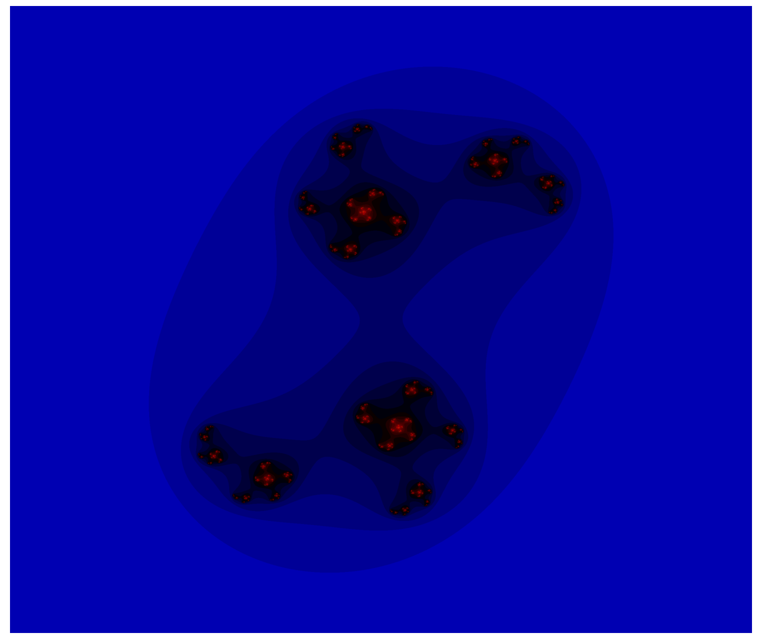
VecCore Library

- Provide simple API to express SIMD algorithms
  - write directly SIMD code is challenging
- Can support different back-end implementation
  - **Vc** and **UME::SIMD**
  - users can choose the optimal one depending on the running architecture
  - New **Vc** version will be part of the C++ standard. With VecCore easy migration
- API covering essential parts of SIMD instructions
  - it allows to implement majority of numerical algorithms
    - e.g. masking operations for dealing with branches

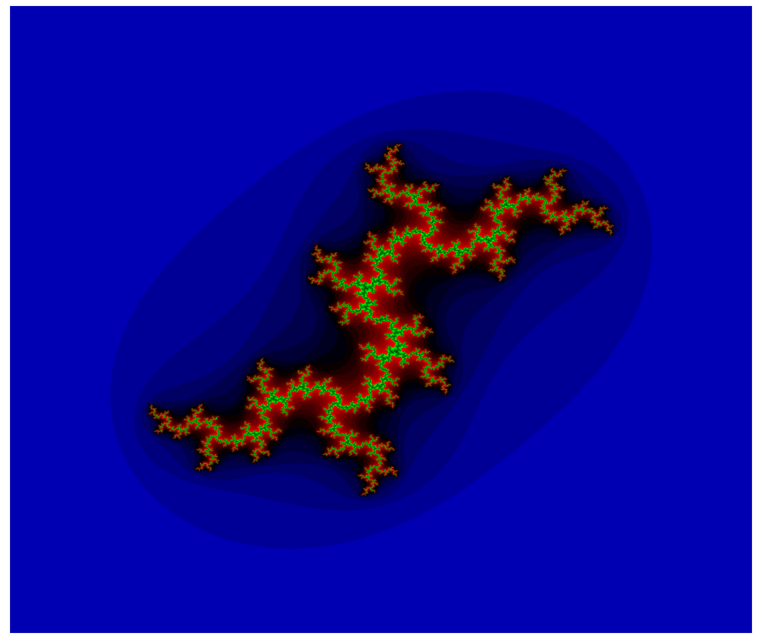


VecCore Performances

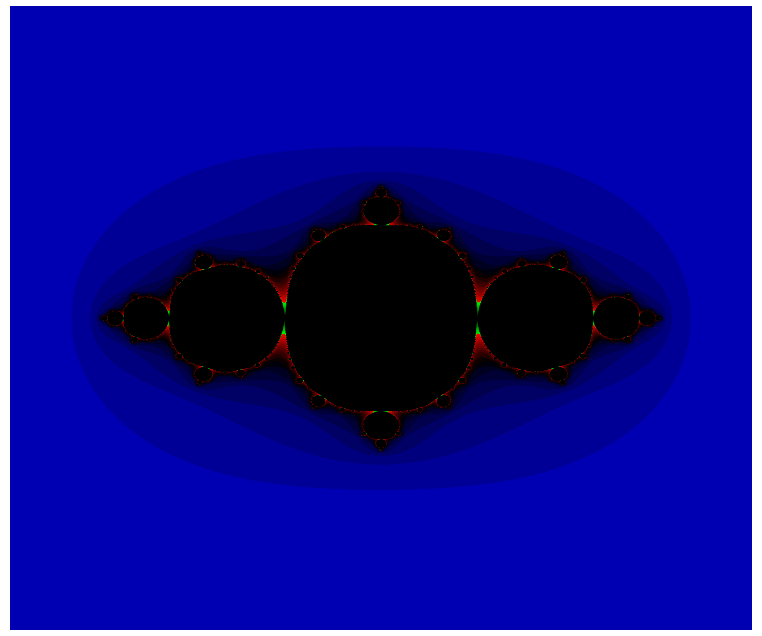
- Study vectorisation performances in a mathematical algorithm
  - Generation of Julia sets $z_{n+1} = {z_n}^2 + 0.7885e^{i\alpha}, \quad -2 \le z \le 2,\ \alpha \in [0, 2\pi), \quad n \le 100.$
  - Speed-up is less than ideal due to branching
  - different number of computations
    for each data points and varying as function of
    angle parameter



45^0

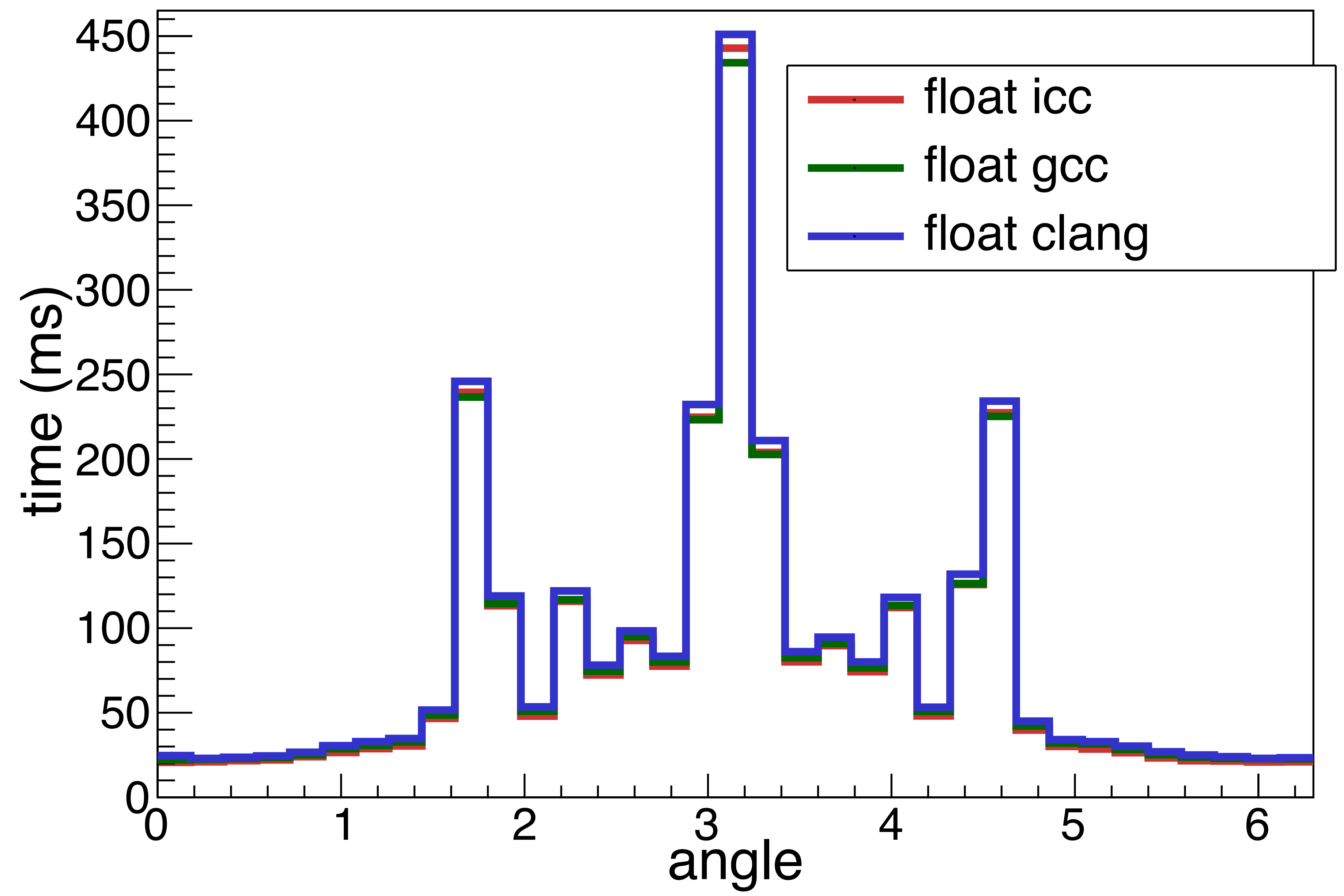


90^0



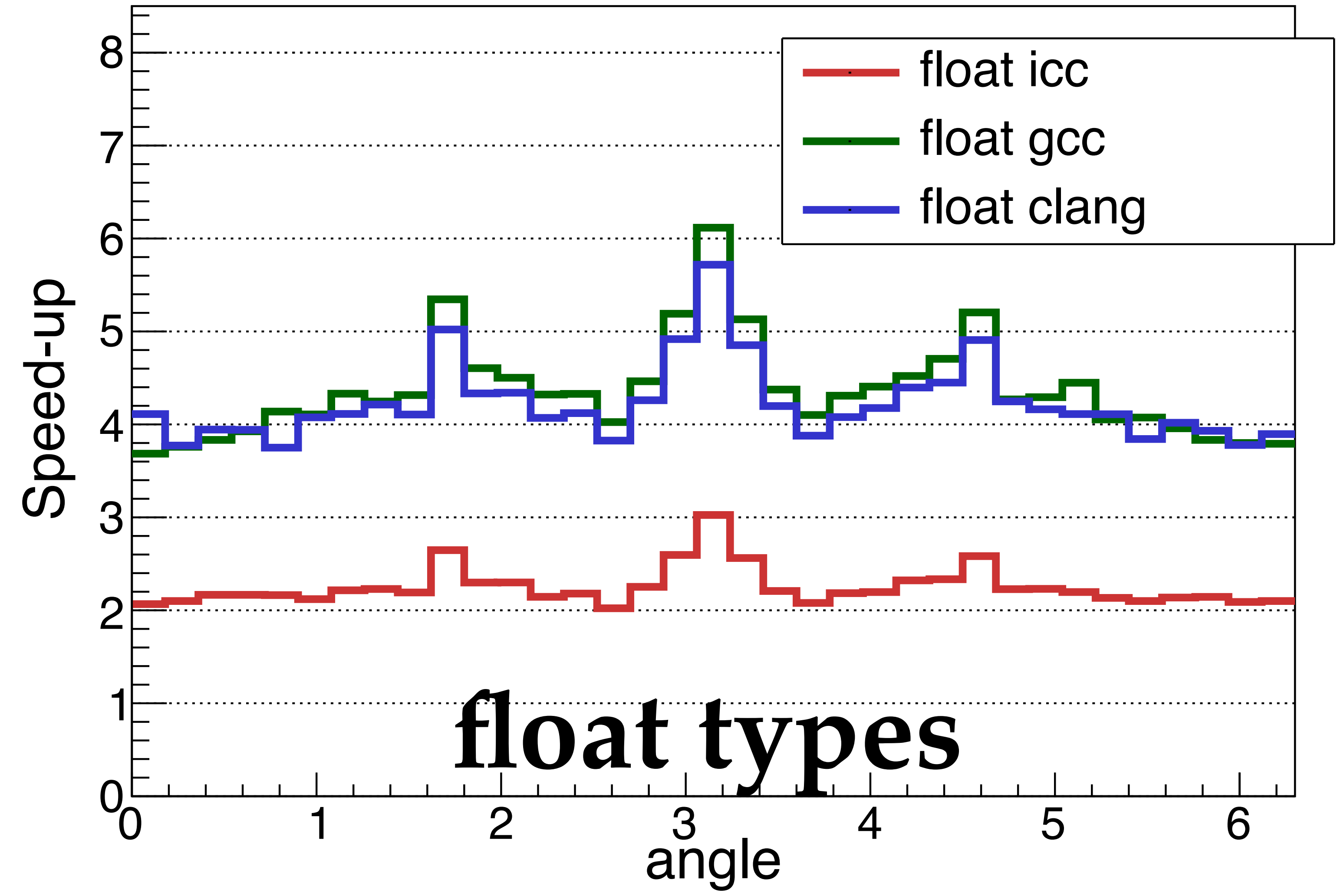
180^0

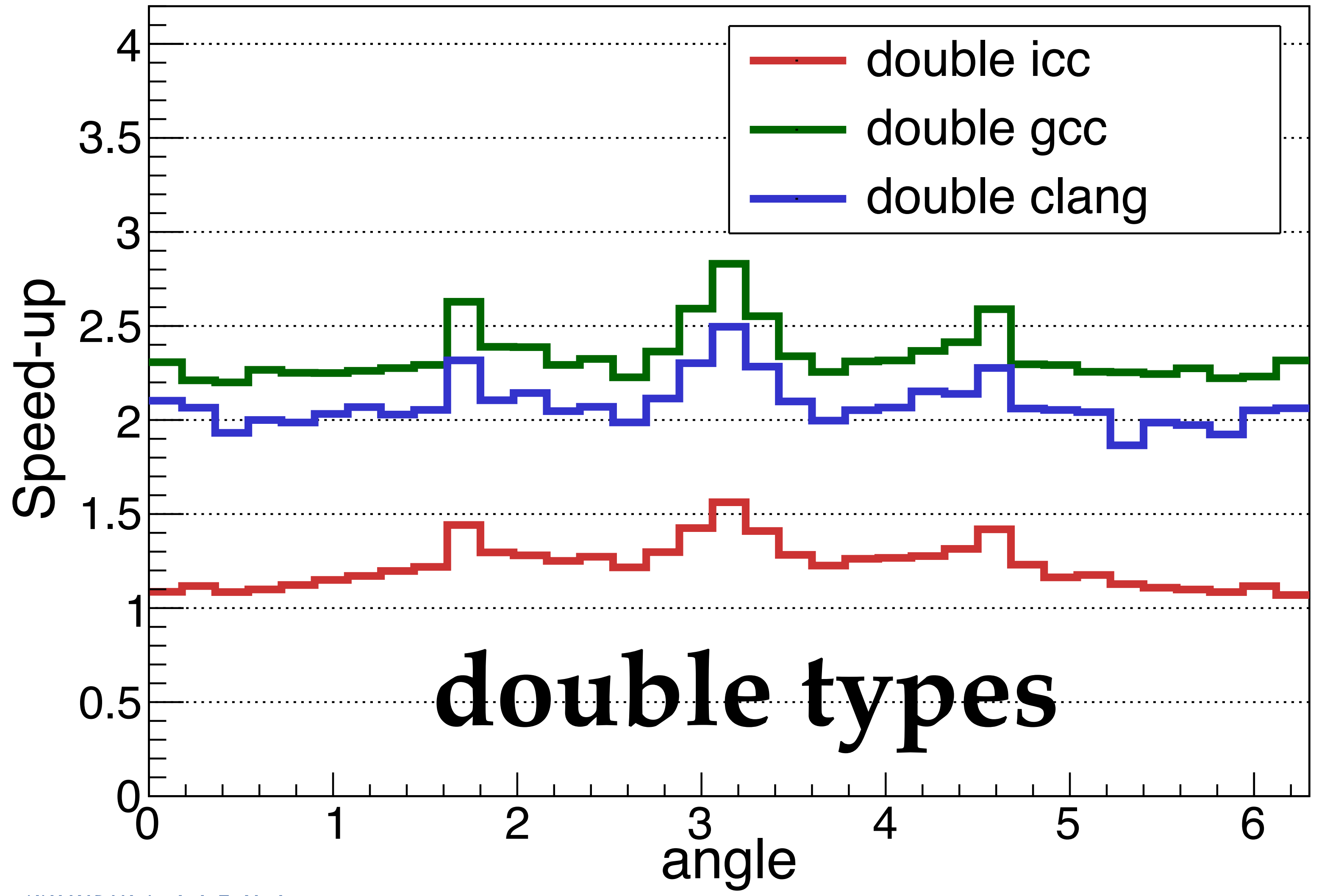
Generation time as function of angle when using scalar float types



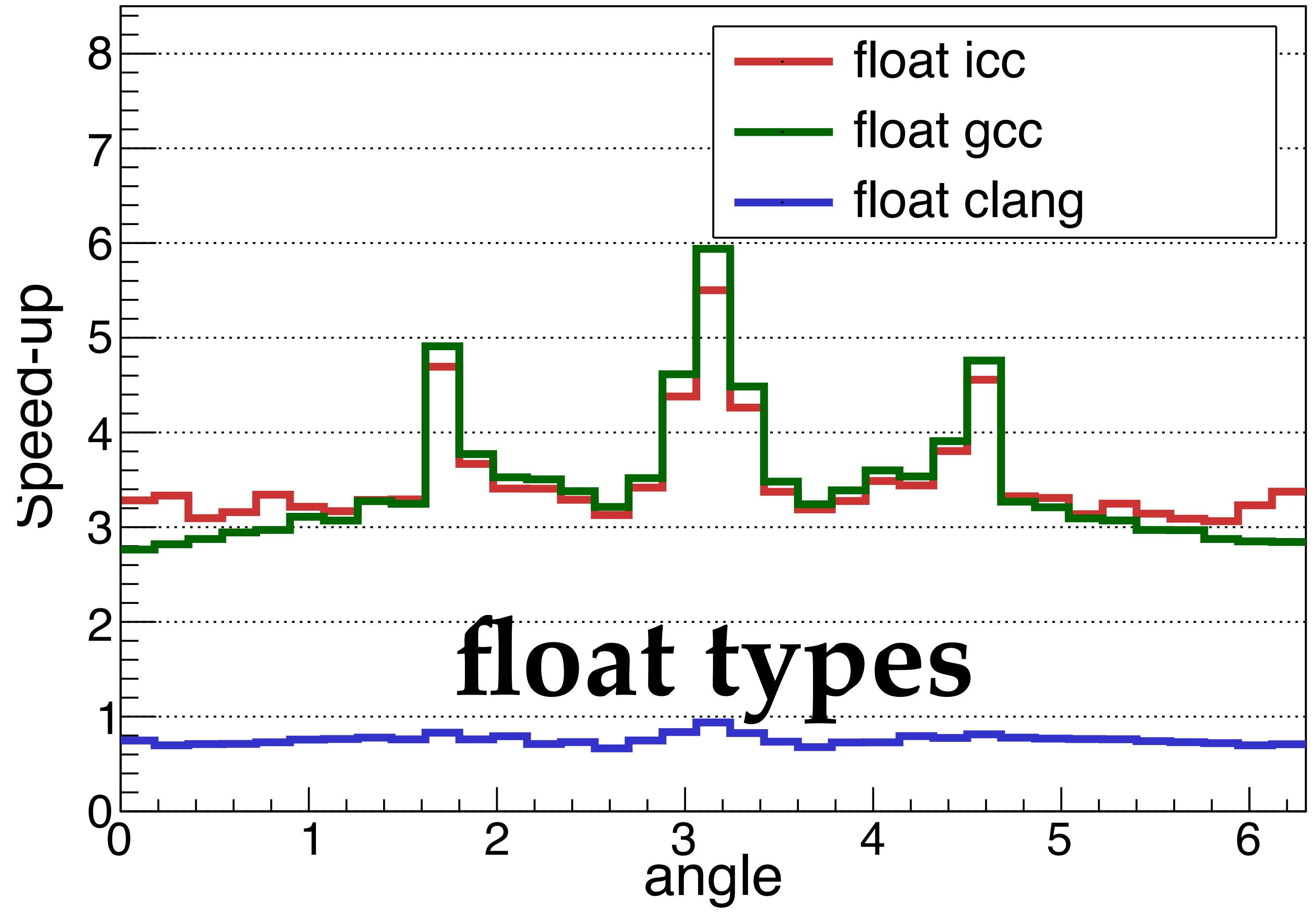
VecCore Performances

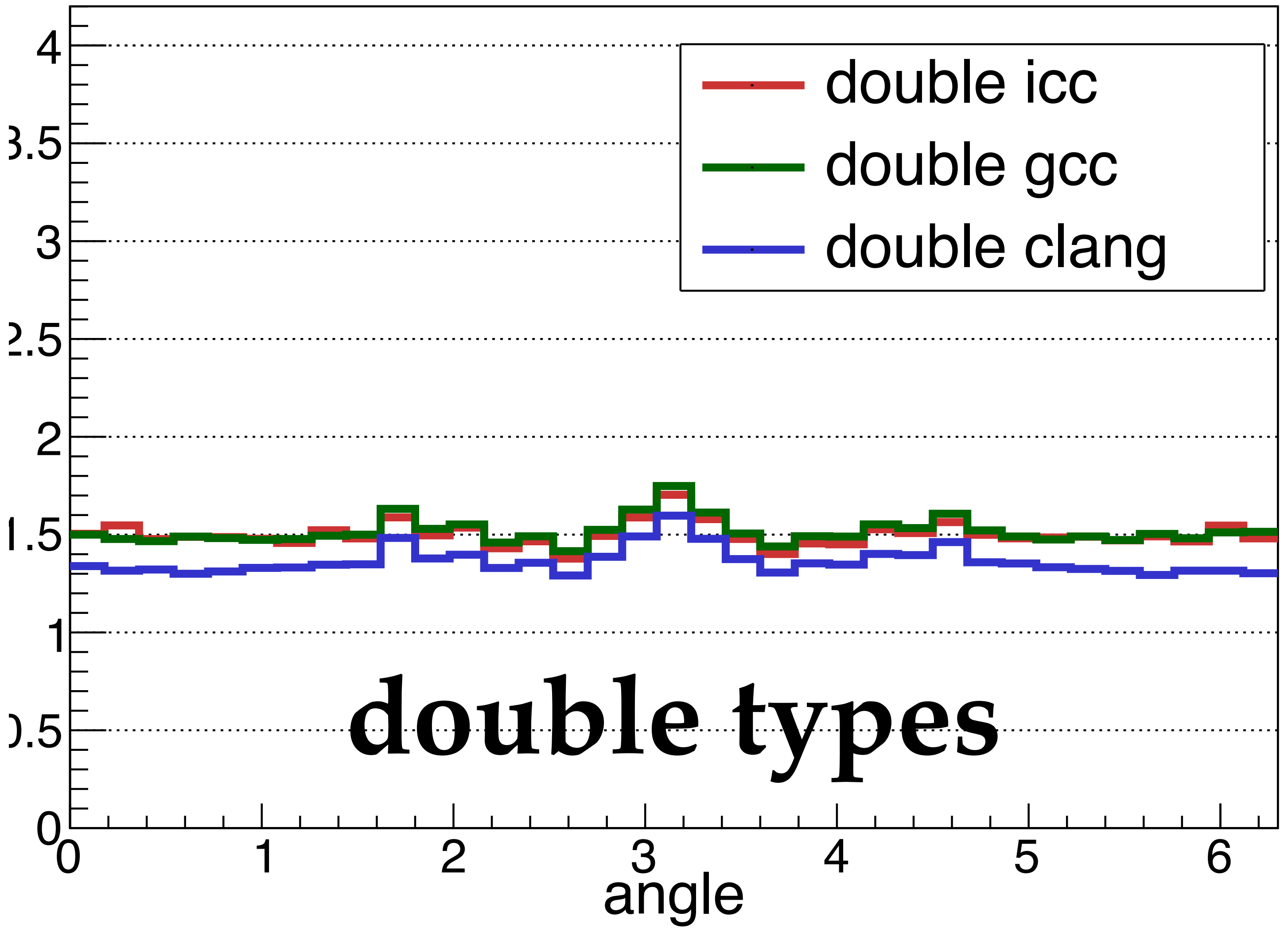
Vc





UME::SIMD





- **Vc** seems to outperform the **UME::SIMD** implementation
- *gcc* outperforms *clang* and *icc* (especially when using **Vc**
- **Vc** does not provide an implementation working for AVX-512

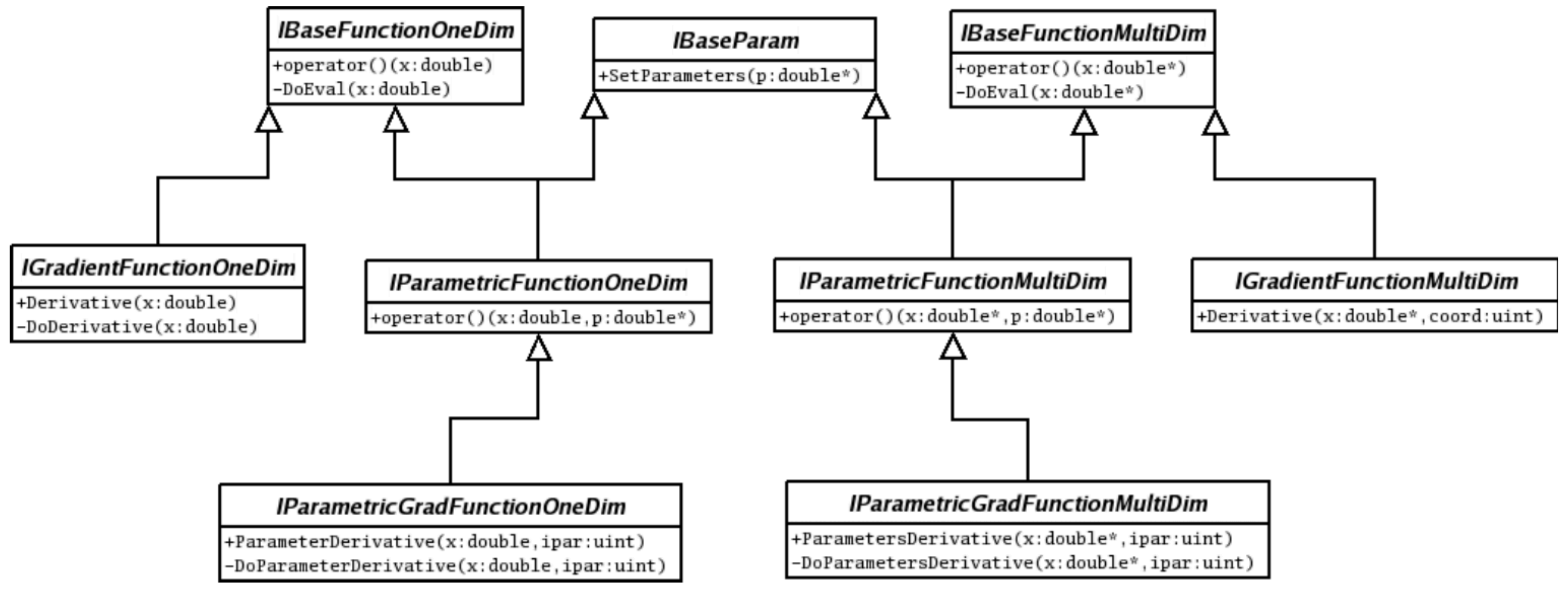
VecCore and ROOT

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

    `cmake  -Dbuiltin_veccore=On -Dbuiltin_vc=On`
- When VecCore is enabled (`R__HAS_VECCORE` is defined), ROOT provides these new VecCore SIMD vector types:
  - **`ROOT::Float_v`**
  - **`ROOT::Double_v`**
- The SIMD vector sizes (`ROOT::Double_v::size()`) will depend on the compiled instruction set
  - `ROOT::Double_v::size()=2` when code 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 and ROOT Math

- Vectorization of ROOT Math interfaces for function evaluations (used for fitting in ROOT)
  - vectorize on the data *x* which can be multi-dimensional




```
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;
};
```

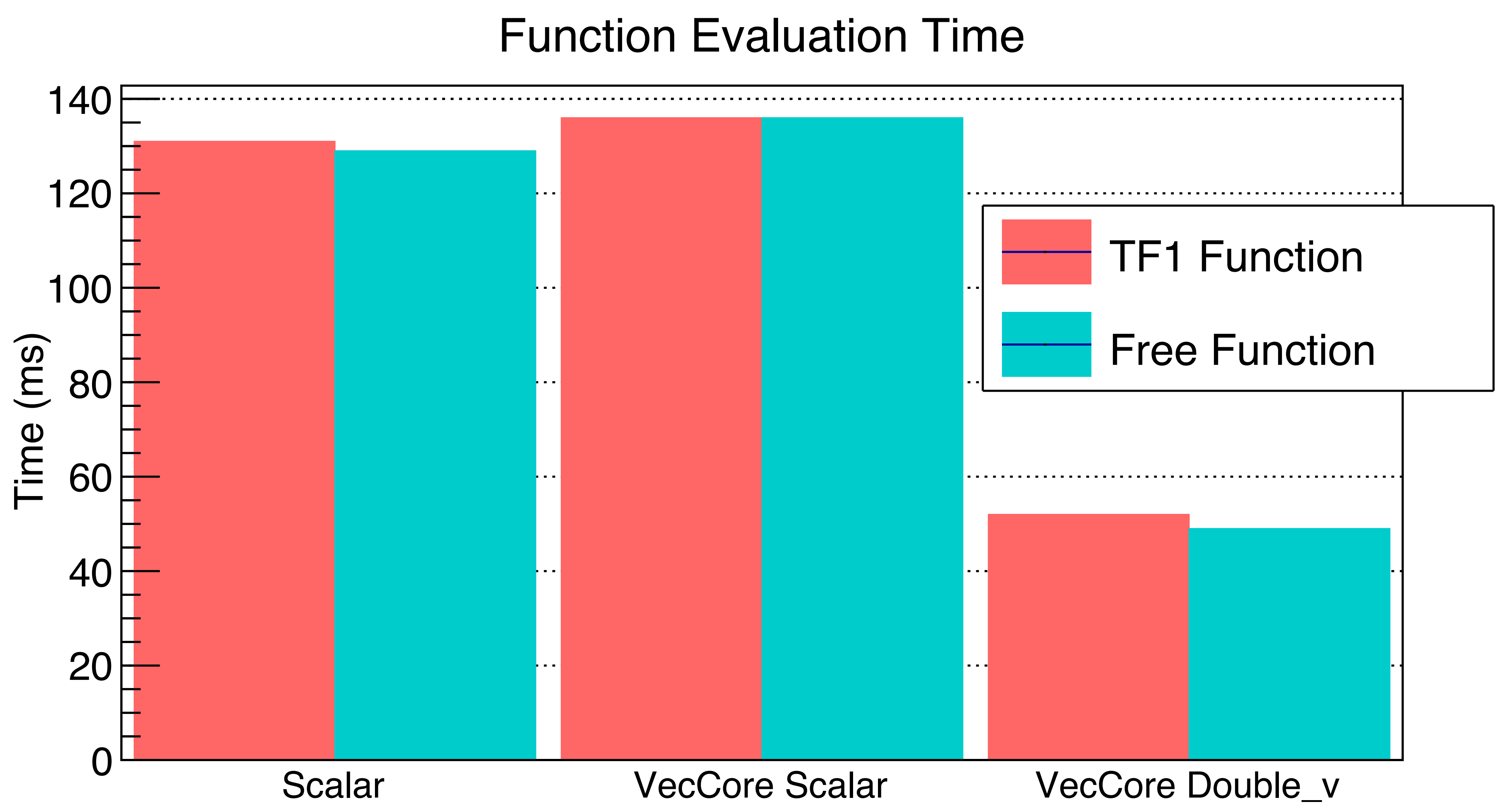
- Add generic interfaces for evaluation :

  `operator()(T  x) -> T`

  - where T can be instantiated as a `ROOT::Double_v` or just `double`
- Backward compatiblity is preserved !

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`)



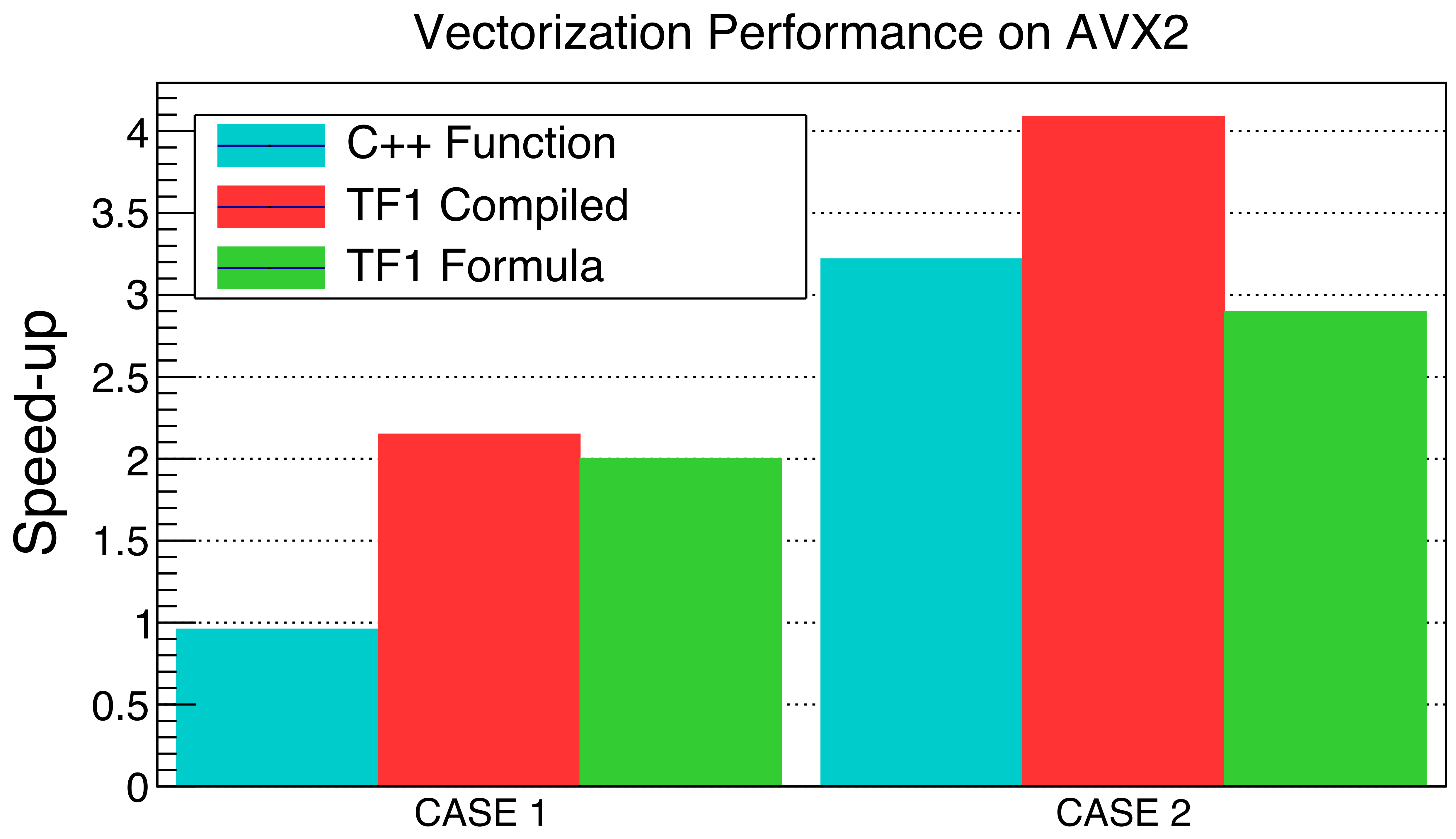
very small overhead when evaluating using a TF1 instead of a direct free function

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 `TFormula`
- Study the speed-up by using vectorisation on AVX



simple function complex function

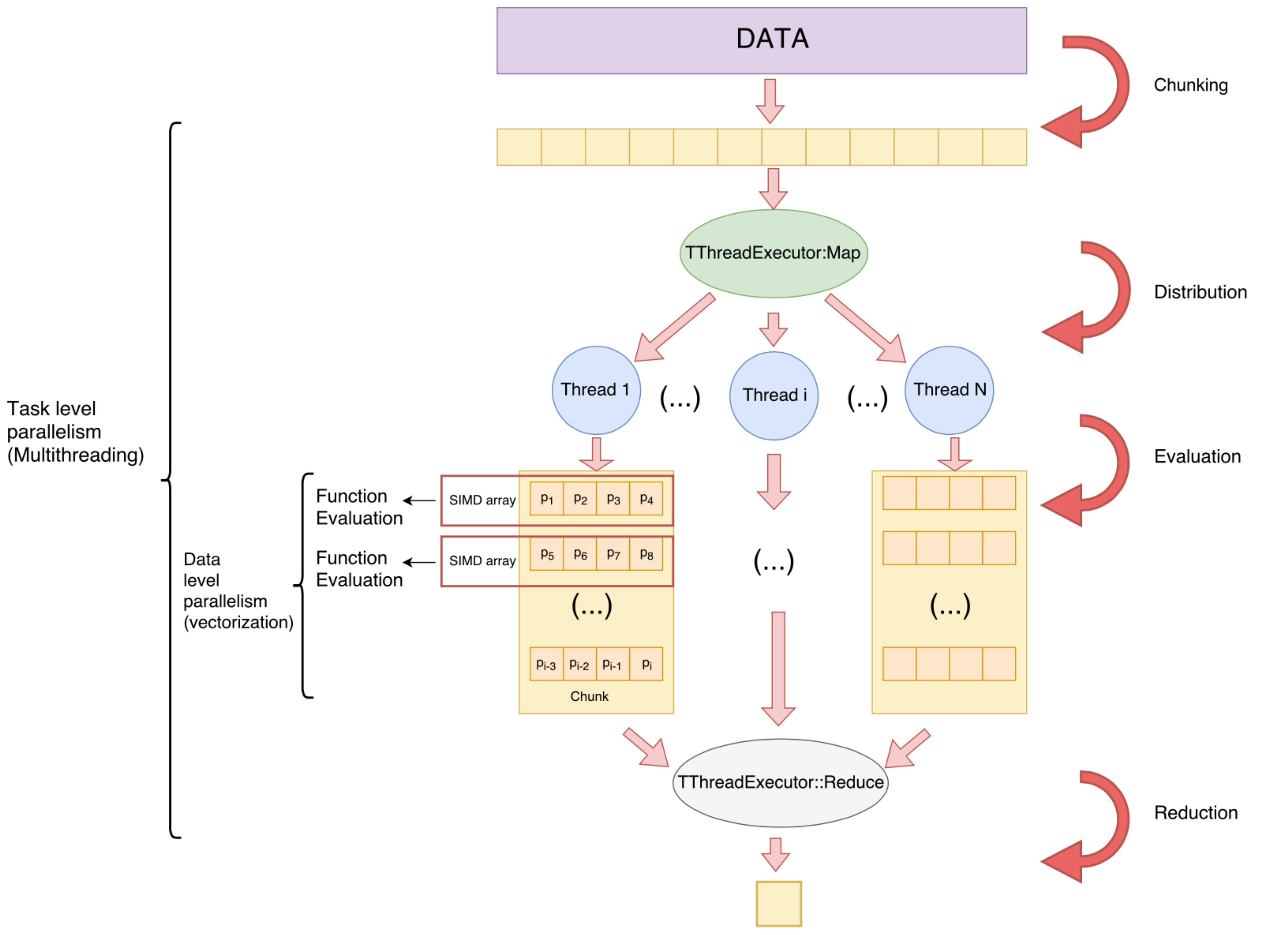
1. 2nd degree polynomial
2. exponential + gaussian

Fitting with Vectorized Functions

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

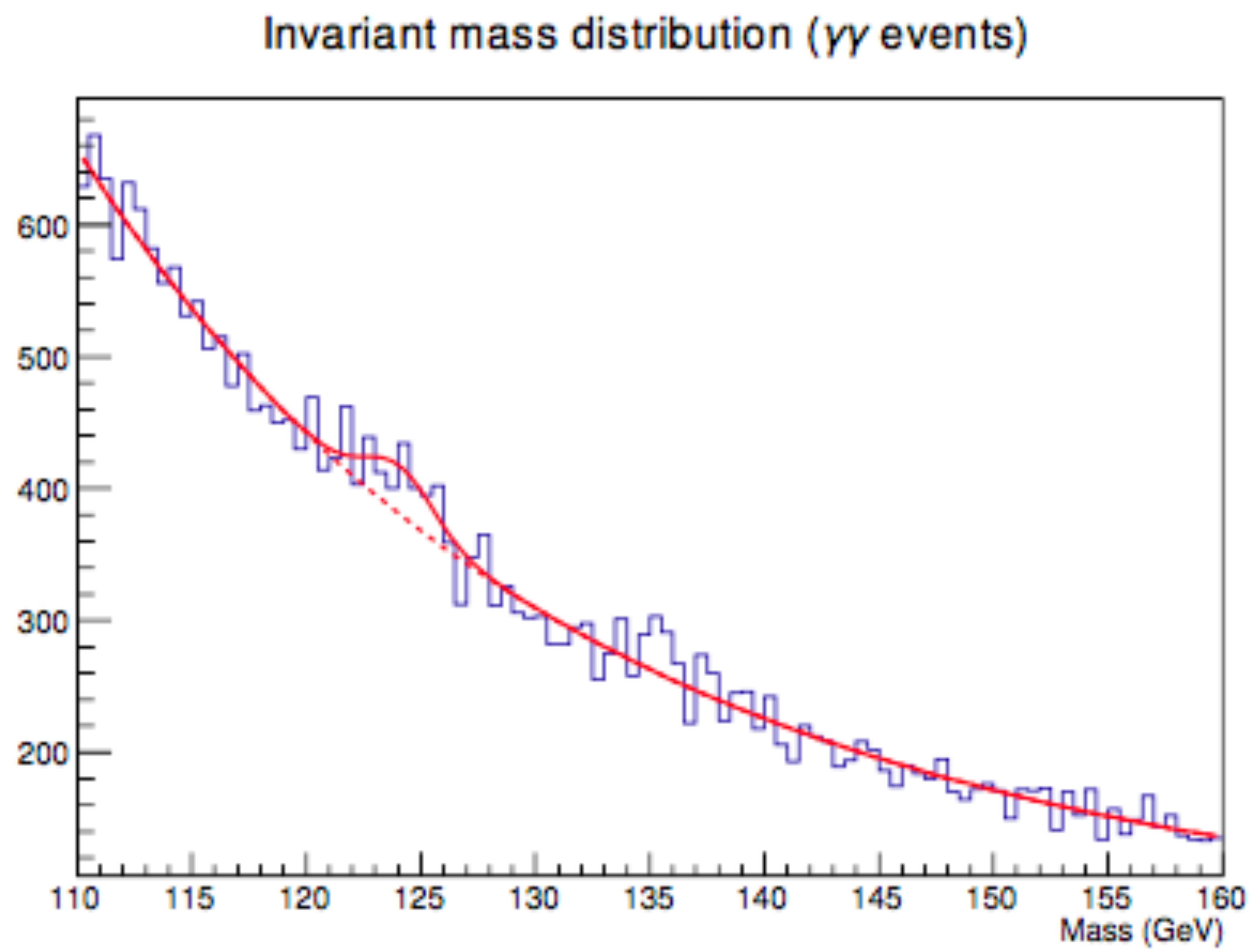
$$(x_0, y_0, z_0, ..., x_n, y_n, z_n) \longrightarrow (x_0, ..., x_n, y_0, ..., y_n, z_0, ..., z_n)$$

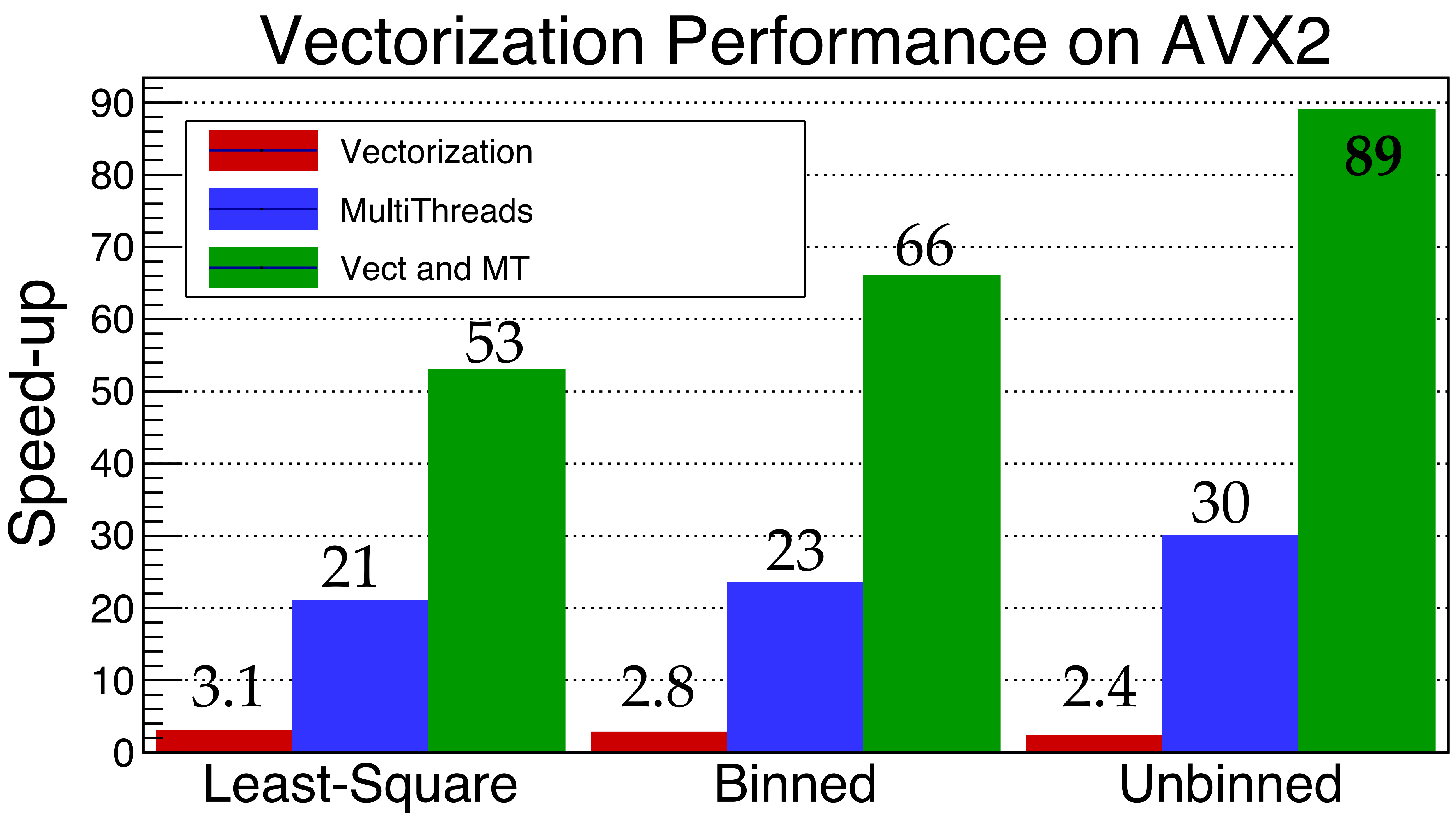
- Model function is evaluated in vectorized mode when computing the chi-square or likelihood function (objective function) for fitting
- Computation of objective function is also parallelized with multi-threads by chunking the data



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 -> $\gamma\gamma$)

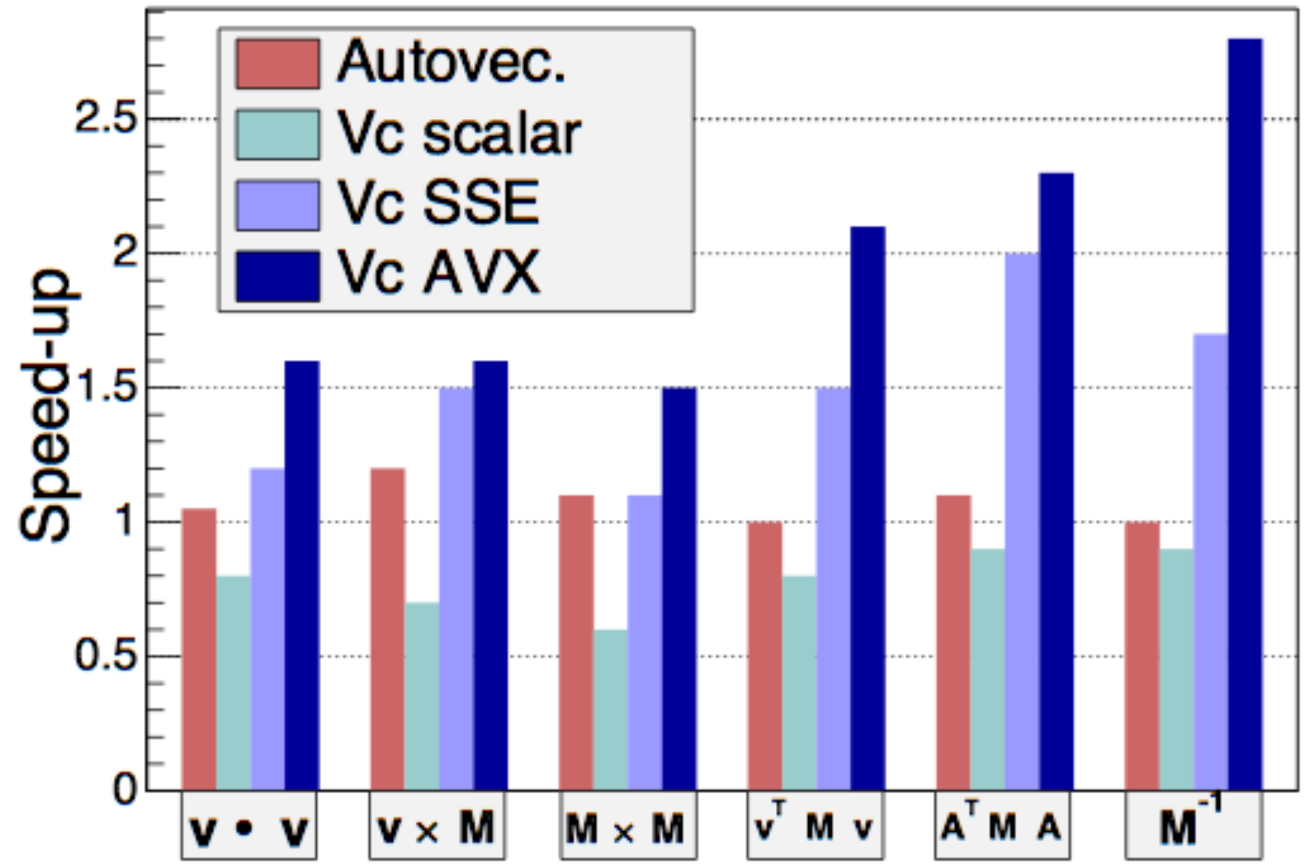


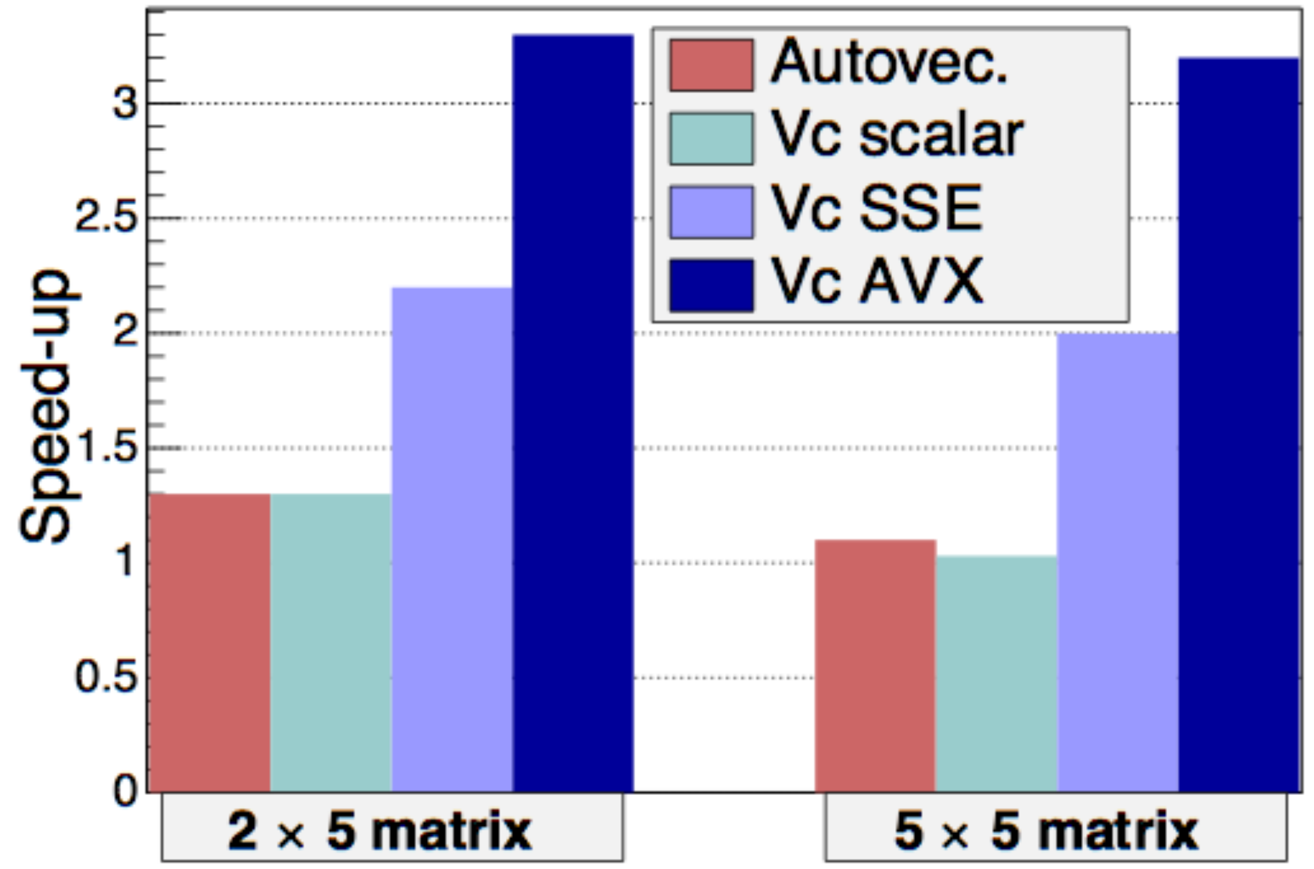


Intel Xeon CPU E5-2683 with 28 physical cores

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)





Transparent Data Parallelism: VecOps

Introduced `ROOT::RVec<T>`: vectorised operations made easy

- `std::vector` like interface, ergonomic support of analysis operations
- Can adopt memory or own it
- Vectorised arithmetic operations, math functions

```
RVec<double> mus_pt {15., 12., 10.6, 2.3, 4., 3.};
RVec<double> mus_eta {1.2, -0.2, 4.2, -5.3, 0.4, -2.};
RVec<double> good_mus_pt = mus_pt[mus_pt > 10 && abs(mus_eta) < 2.1];

RVec<float> vals = {2.f, 5.5f, -2.f};
RVec<float> sin_vals = sin(vals);
```

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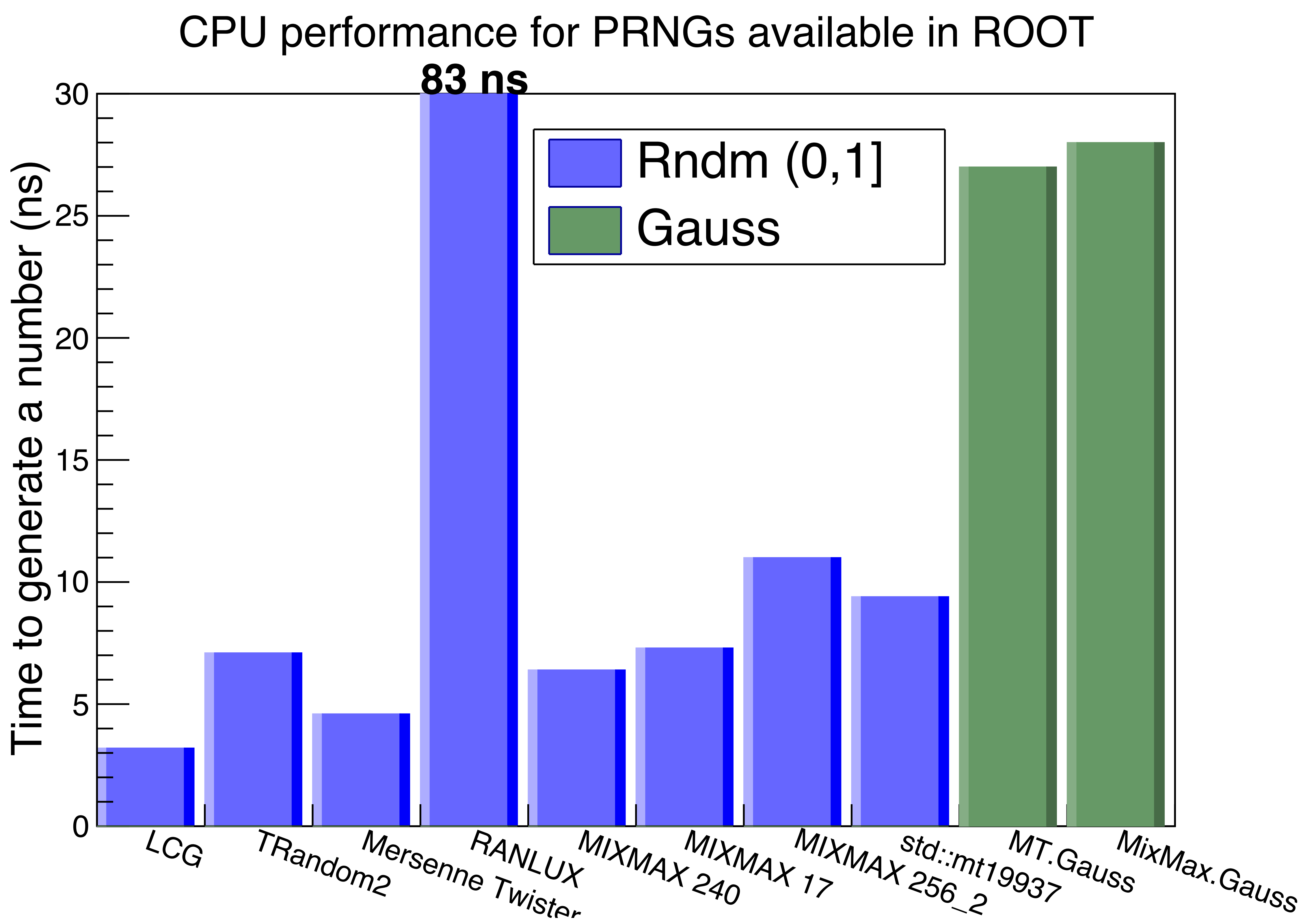
Future Plans: Math Functions

- 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, log, sin, cos`) are already provided by **VecCore**

Future Plans: Random Number

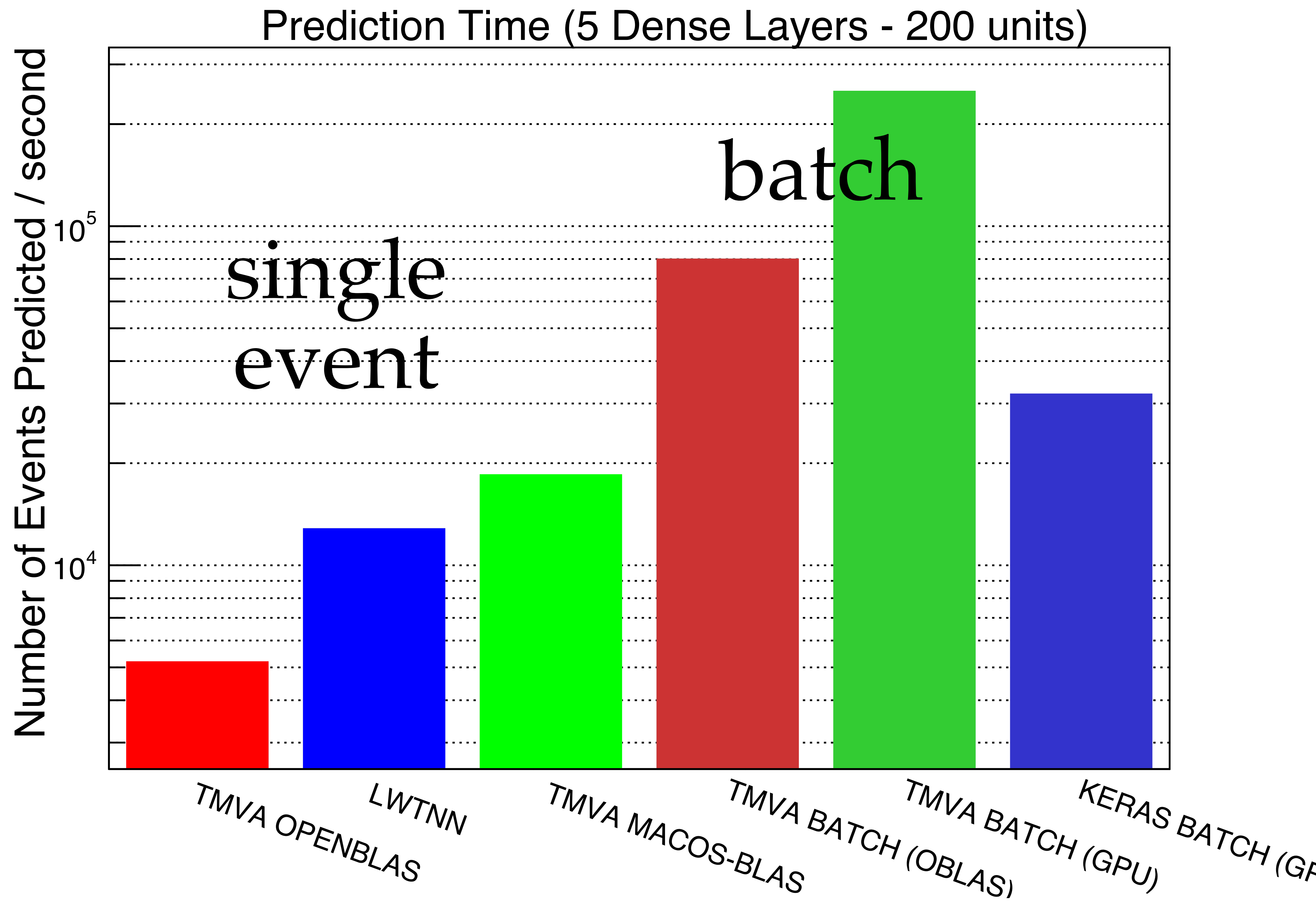
- Can use vectorization to speed-up pseudo-random number generations
- Horizontal (internal) or vertical vectorization can be used
  - By creating a vector state (based on VecCore) we can speed-up generators like Ranlux or MixMax
- on-going effort in collaboration with GeantV project and MIXMAX network (https://indico.cern.ch/event/731433/)



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 vectorization
- Plan to deploy vectorization even more:
  - math functions, random numbers and deep learning

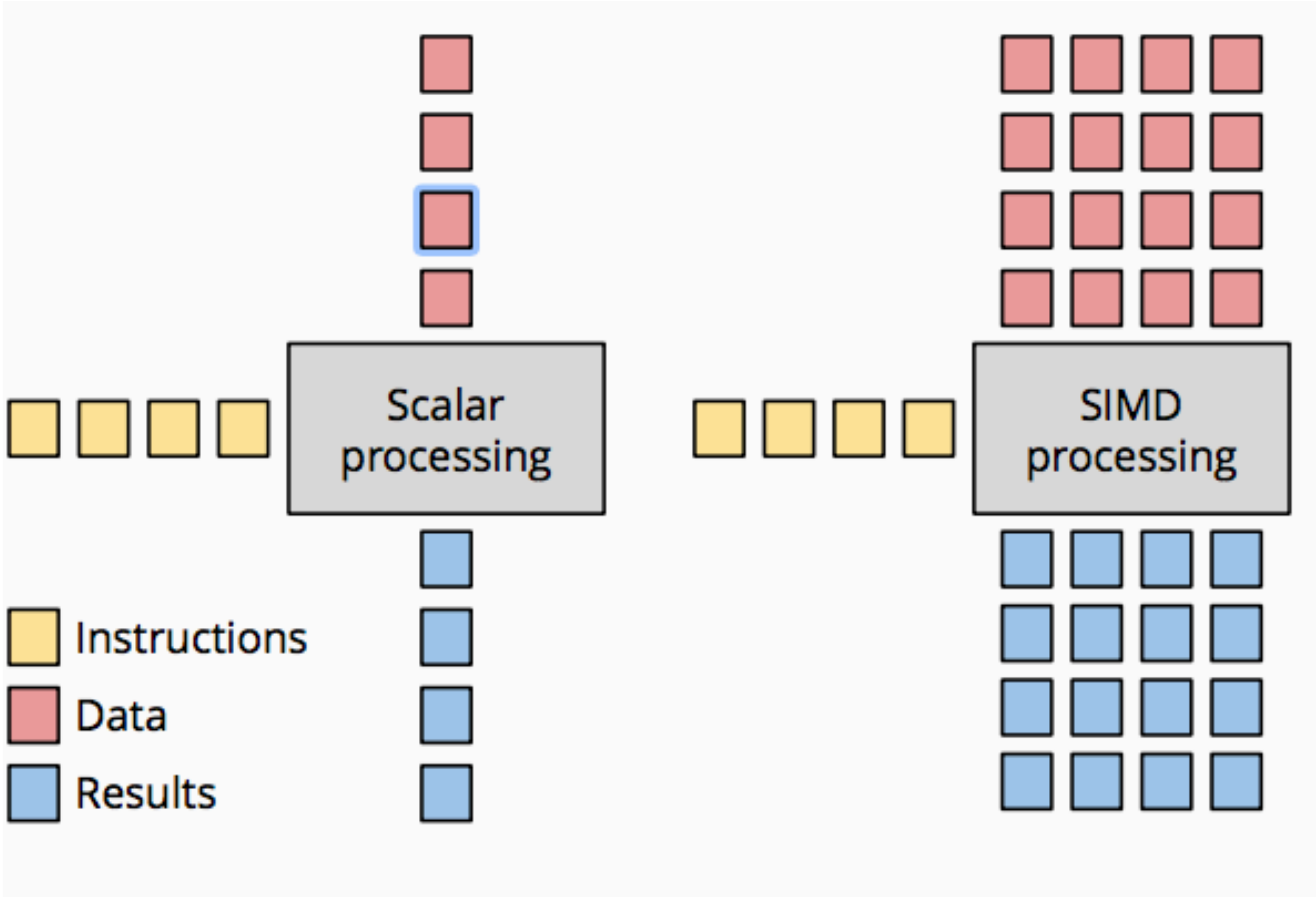
Thank you !

References:

- ROOT: https://root.cern.ch
- VecCore : https://github.com/root-project/veccore
- Vc : https://github.com/VcDevel/Vc
- UME::SIMD: https://github.com/edanor/umesimd
- SIMD C++ standardization:
  - http://www.open-std.org/JTC1/SC22/WG21/docs/papers/2013/n3759.html

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



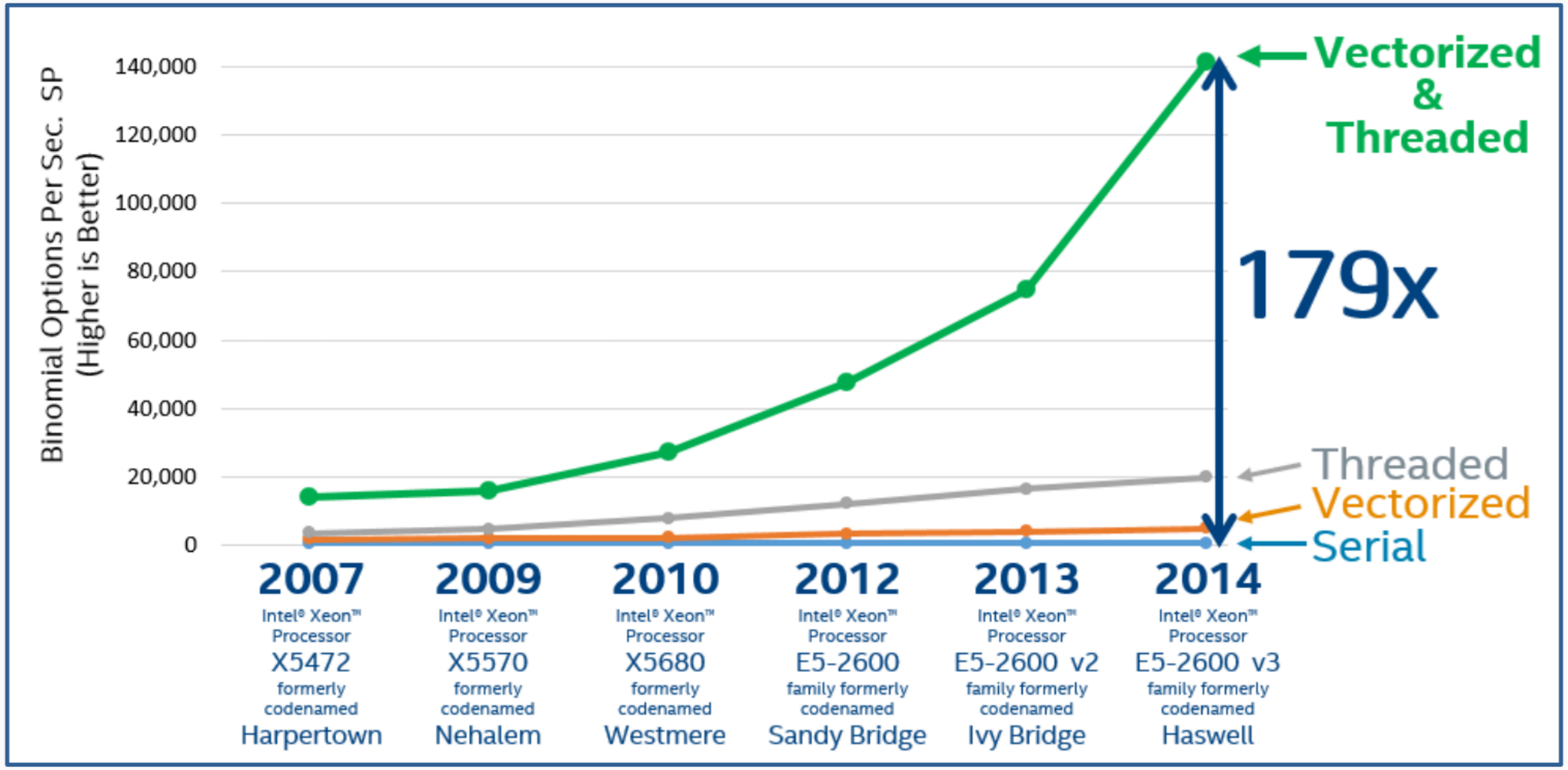
History of Intel SIMD

- 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.



The VecCore API

```cpp
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);

}
```