# Towards full electromagnetic physics vectorisation in the GeantV transport framework

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on behalf of the GeantV development team

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# INTRODUCTION


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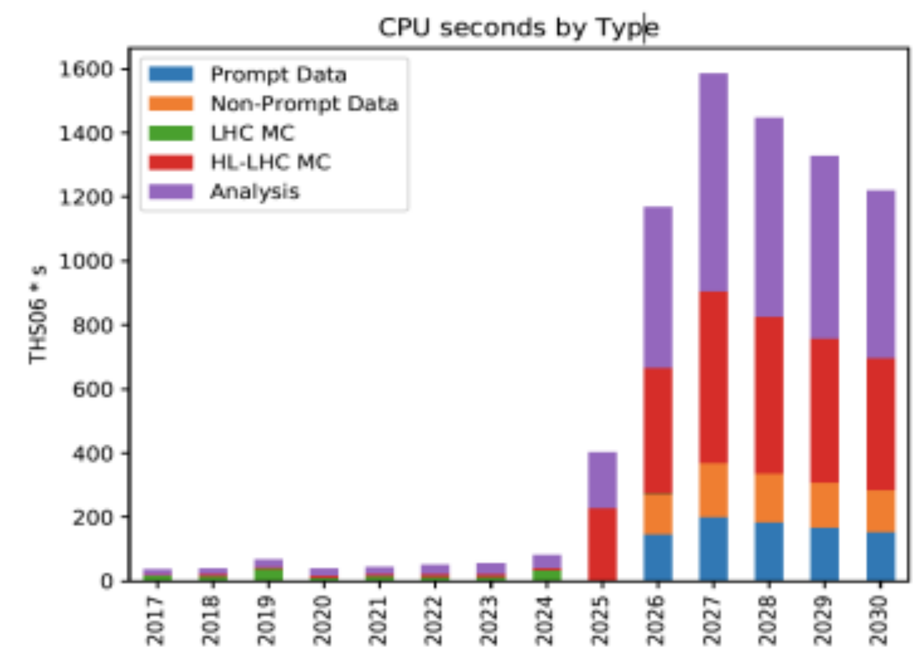
# INTRODUCTION

- Event simulation is one of the **most time consuming** parts of the workflow, in the HEP sw ecosystem
  - For high-luminosity LHC phase (HL-LHC), the upgraded experiments expect to collect **150 times more data** than in Run 1
- The **GeantV R&D project** was launched in 2013, aiming at exploring emerging computer technologies in order to significantly increase run-time performance of detector simulation




**CMS and Atlas estimated CPU needs for HL-LHC (source: CWP)**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# INTRODUCTION

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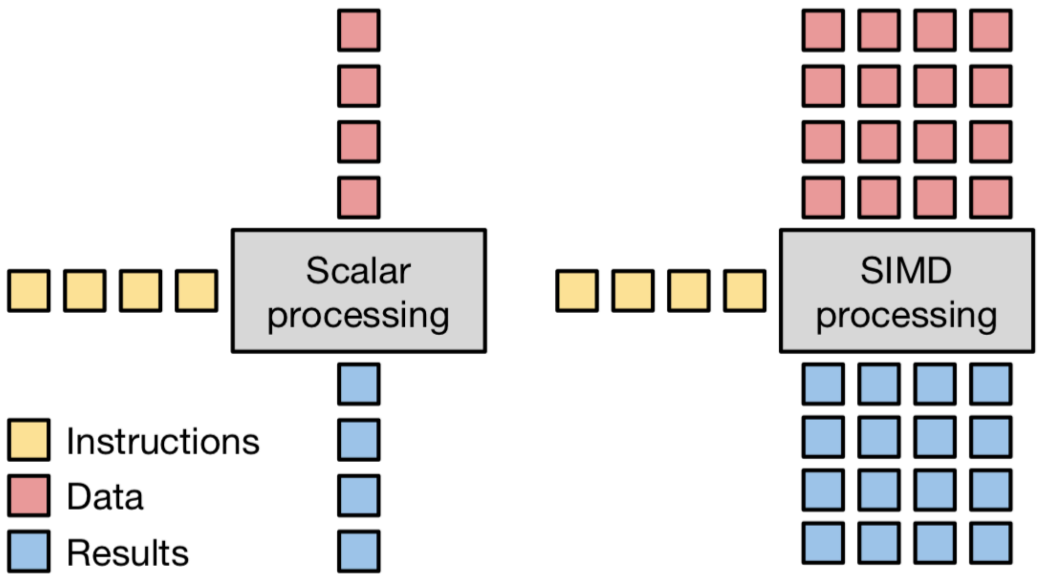
  - For high-luminosity LHC phase (HL-LHC), the upgraded experiments expect to collect **150 times more data** than in Run 1
- The **GeantV R&D project** was launched in 2013, aiming at exploring emerging computer technologies in order to significantly increase run-time performance of detector simulation
- The project studies performance gains when changing the classic particle transport approach, propagating **multiple tracks from multiple events in parallel**
  - improving code and data locality in the process
  - enabling SIMD/SIMT execution models: Vectorization+Multithreading
- **Vectorization of physics library** is important as key part of the algorithmic chain





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# WHEN CAN WE PROFIT FROM VECTORIZATION

- Functions with many **math computations**
  - Such as +, *, /, sqrt, sin, cos, exp, log (ordered according to approximate computation complexity)
- Functions with **minimal branching**
  - Branching **may** require to evaluate both branches for vectorized code

**Scalar code**

```
if (cond > rndArray[0]) {
  eps  = Math::Exp(-al1 * rndArray[1]);
  eps2 = eps * eps;
} else {
  eps2 = eps02 + (1. - eps02) * rndArray[1];
  eps  = std::sqrt(eps2);
}
```

**Vector code**

```
MaskD_v cond1 = cond > rnd1;
if (!MaskEmpty(cond1)) {
  vecCore::MaskedAssign(eps, cond1, Math::Exp(-al1 * rnd2));
  vecCore::MaskedAssign(eps2, cond1, eps * eps);
}
if (!MaskEmpty(!cond1)) {
  vecCore::MaskedAssign(eps2, !cond1, eps02 + (1.0 - eps02) * rnd2);
  vecCore::MaskedAssign(eps, !cond1, Math::Sqrt(eps2));
}
```

- Functions not bounded by **memory access**
  - Load 4 doubles into SIMD register is one instruction but it is not faster than loading values one by one


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# GEANTV EM PHYSICS LIBRARY

**Current State**

| particle | processes | model(s) GeantV | model(s) Geant4 |
|---|---|---|---|
| $e^-$ | ionisation | Møller [100eV-100TeV] | Møller [100eV-100TeV] |
| | bremsstrahlung | Seltzer-Berger [1keV-1GeV] | Seltzer-Berger [1keV-1GeV] |
| | | Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV] | Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV] |
| | Coulomb sc. | GS MSC model [100eV-100TeV] | Urban MSC model [100eV-100MeV] |
| | | | Mixed model [100MeV-100TeV] |
| $e^+$ | ionisation | Bhabha [100eV-100TeV] | Bhabha [100eV-100TeV] |
| | bremsstrahlung | Seltzer-Berger [1keV-1GeV] | Seltzer-Berger [1keV-1GeV] |
| | | Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV] | Tsai (Bethe-Heitler) w. LPM. [1GeV-100TeV] |
| | Coulomb sc. | GS MSC model [100eV-100TeV] | Urban MSC model [100eV-100MeV] |
| | | | Mixed model [100MeV-100TeV] |
| | annihilation | Heitler ($2\gamma$) [0-100TeV] | Heitler ($2\gamma$) [0-100TeV] |
| $\gamma$ | photoelectric | Sauter-Gavrila + EPICS2014 [1eV-100TeV] | Sauter-Gavrila + EPICS2014 [1eV-100TeV] |
| | incoherent sc. | Klein-Nishina$^+$ [100eV-100TeV] | Klein-Nishina$^+$ [100eV-100TeV] |
| | $e^-e^+$pair production | Bethe-Heitler$^+$ [100eV-80GeV] | Bethe-Heitler$^+$ [100eV-80GeV] |
| | | Bethe-Heitler$^+$ w. LPM [80GeV-100TeV] | Bethe-Heitler$^+$ w. LPM [80GeV-100TeV] |
| | coherent sc. | - | Livermore |
| + | energy loss fluct. | - | Urban |

- Every model is **tested and verified against the corresponding Geant4** model (cross section per atom, cross section per volume, and kinematic of primary and secondary particles)
- **EM showers** in GeantV can be **fully simulated** in real applications (i.e. FullCMS, TestEM3, TestEM5, FullLHCb) and the results are verified against the corresponding Geant4 simulation


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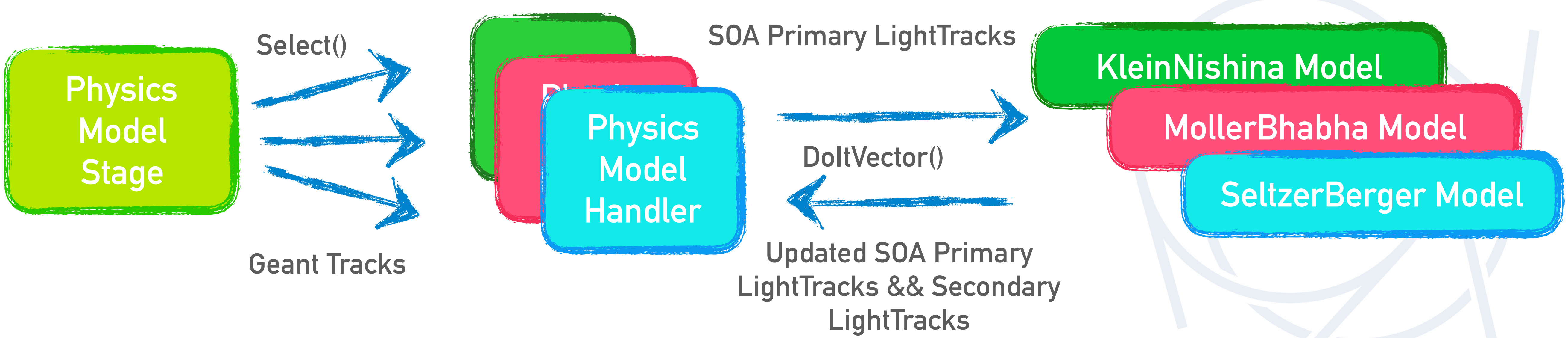
# ELECTROMAGNETIC PHYSICS – FINAL STATE GENERATION

- Once the particle undergoes a physics process, the **final state generation stage** occurs:
  - Differential cross sections are used to update the **kinematic properties** of the primary particle and to **produce secondary particles** (if necessary)
  - Sampling with rejection / Sampling with Alias tables + approximations
- The final state generation involves **two main** parts in GeantV:
  - **Framework** part: filtering of tracks (according to particles type, physics process), gathering relevant track information into SOA form (LightTracks), call the physics model
  - **Model** part: Specific code for the selected physics model: update primaries, create secondaries..





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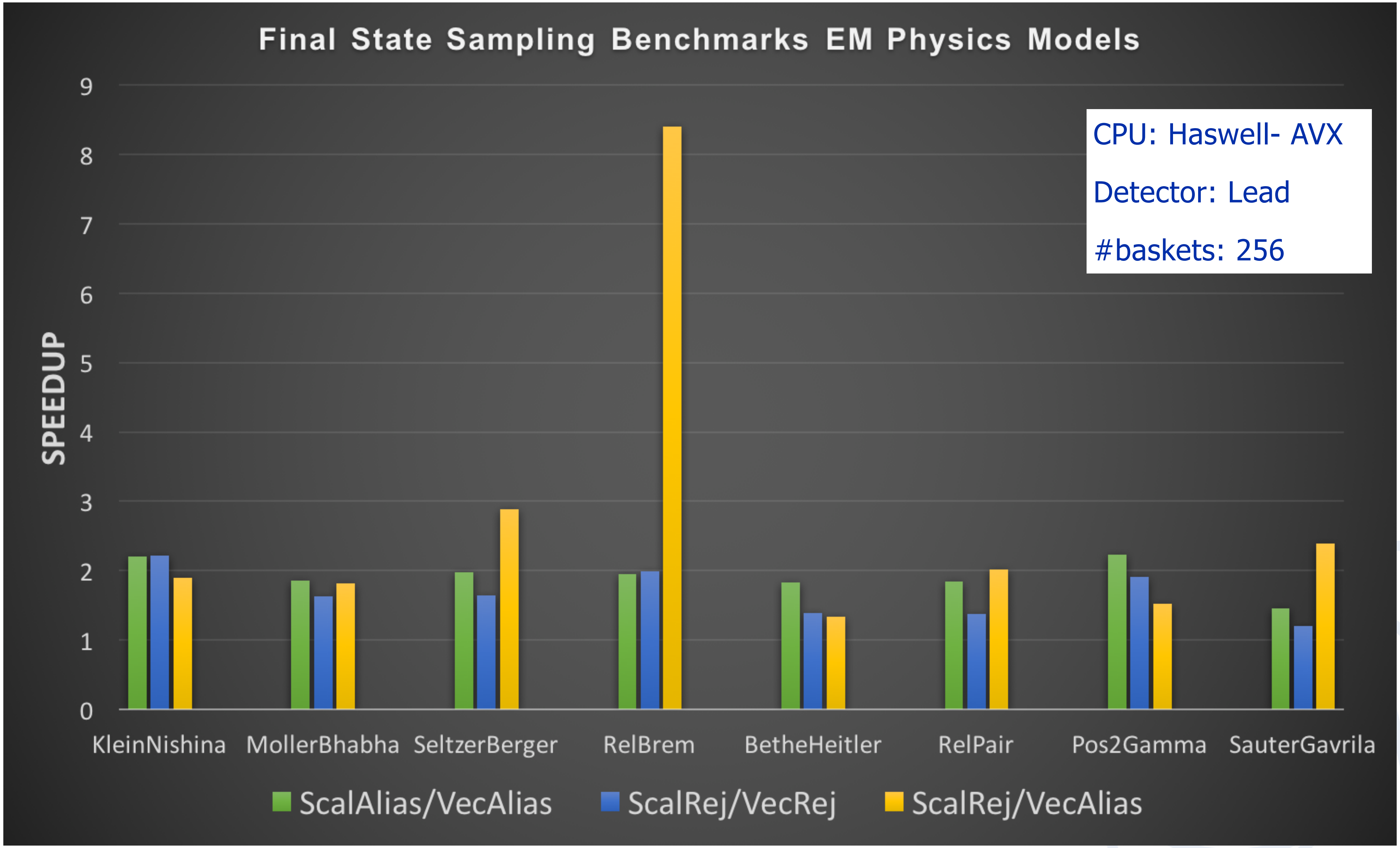
# MODEL LEVEL TEST BENCHMARKS




See next talk, from A. Gheata for benchmarks on the full simulation chain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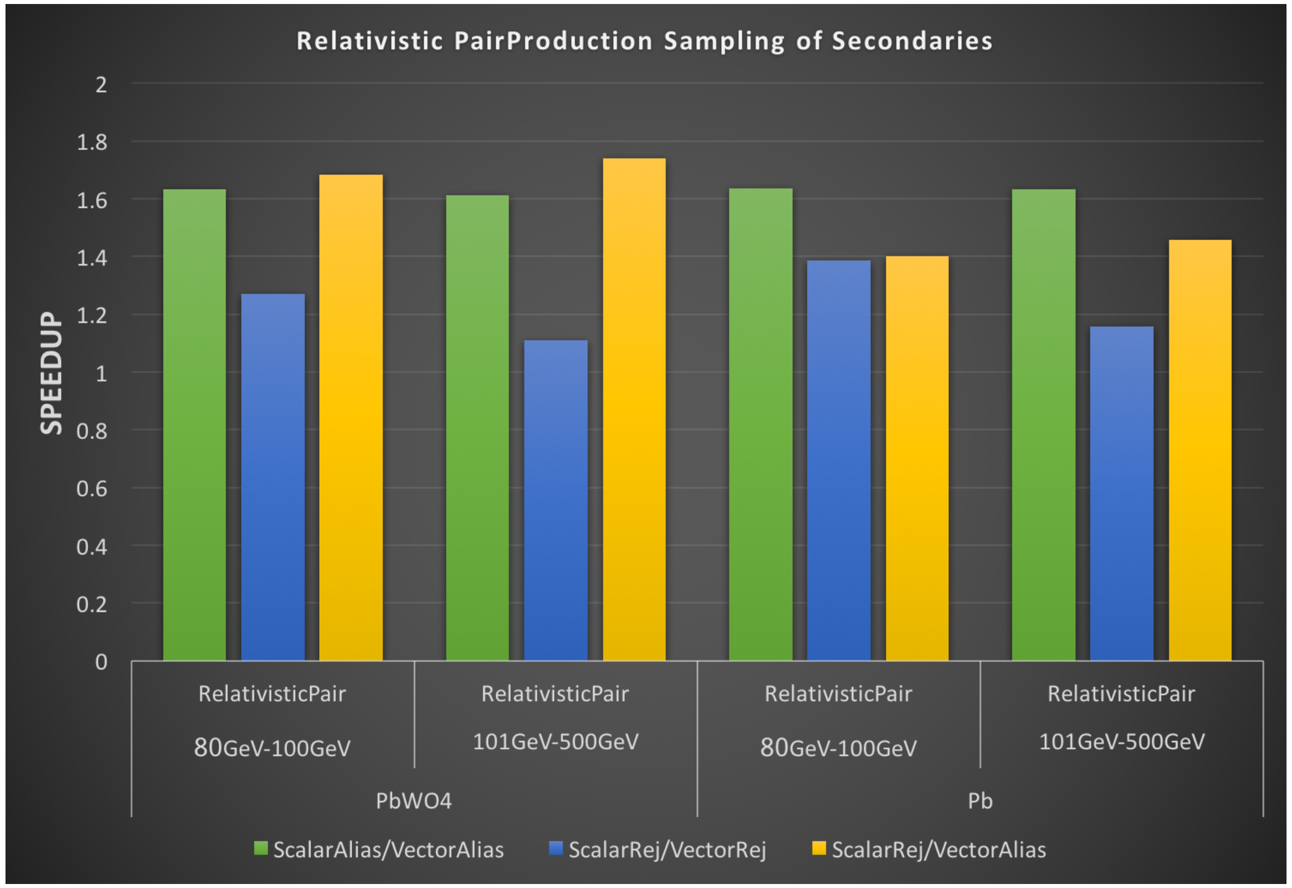
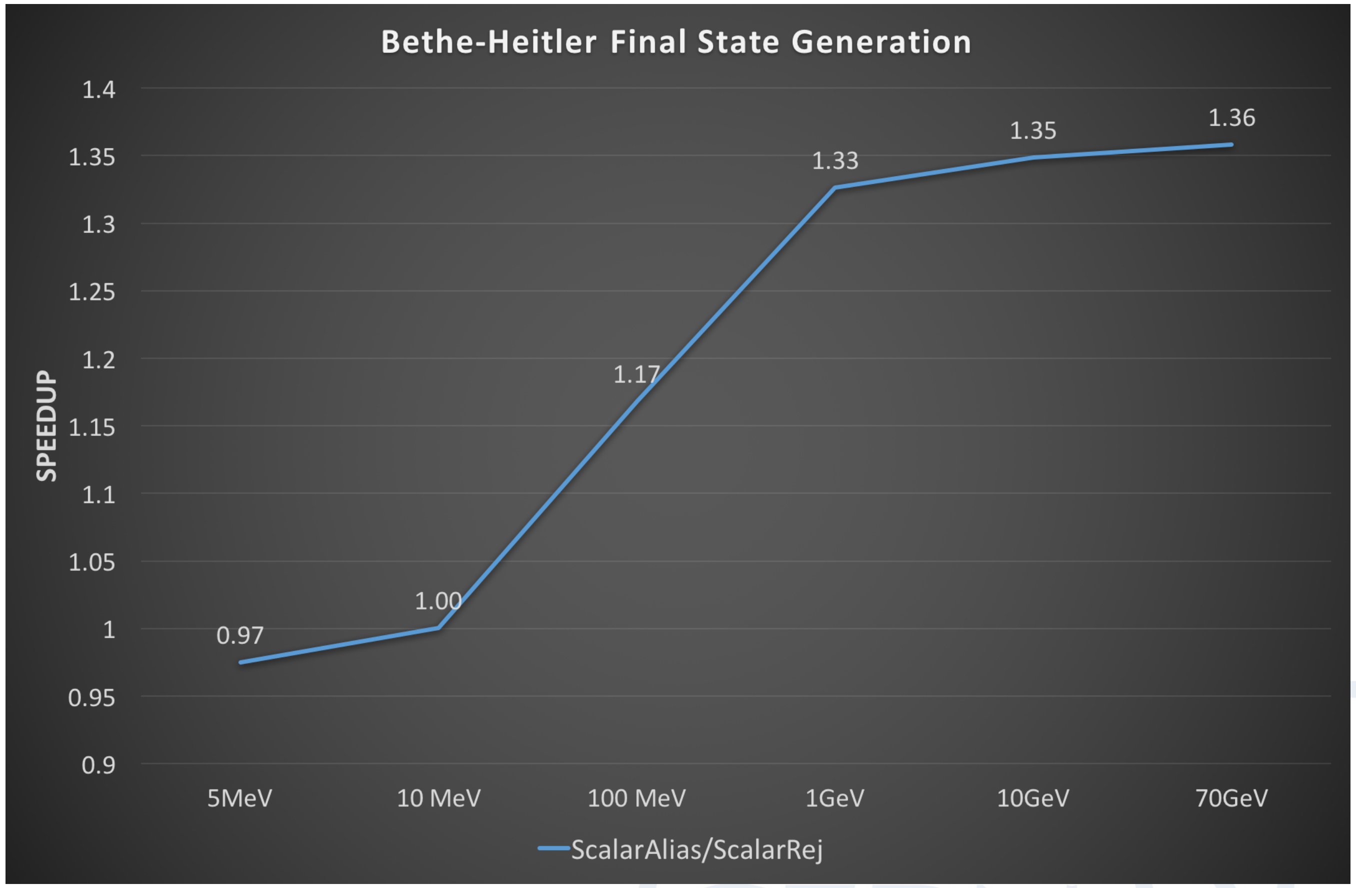
# TUNING THE SIMULATION THROUGH MODELS




CPU: Haswell - AVX
Detector: Pb/PbWO4
Model for Energy Range [80GeV-100TeV]
#baskets: 256

CPU: Haswell - AVX
Detector: Pb
Model for Energy Range [2 $e^-{}_m c^2$-80GeV]
Scalar execution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# SUMMARY

- Physics model integrated in the GeantV framework and validated against corresponding Geant4 simulation
- Most of the **EM physics library** models are now **vectorized**
  - Work in progress on Multiple scattering
  - Optimization of the current vectorized implementations
- SpeedUp
  - At the level of final-state EM Model: between 1.5-3 on Haswell, 2-4 on Skylake with AVX2
  - See A. Gheata talk for the impact on realistic EM showers in calorimeters and fullCMS applications

# WORK IN PROGRESS

- Work on **other parts** of the physics framework
  - ComputeIntLenght(), generation and insertion of secondary particles, etc..
- VecMath library and Vectorized pRNG (handling reproducibility issues)
- Study the possibility to substitute double precision computations with single one, in some parts of the physics library (i.e. transport in magnetic field)
- Add **AVX512** support (UME::SIMD)
  - currently there is no way to test consistently AVX512

**GeantV project is hosted at: https://gitlab.cern.ch/GeantV/geant**
**GeantV website: http://geant.cern.ch**


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# THANKS FOR THE ATTENTION!

# QUESTIONS?

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# BACKUP

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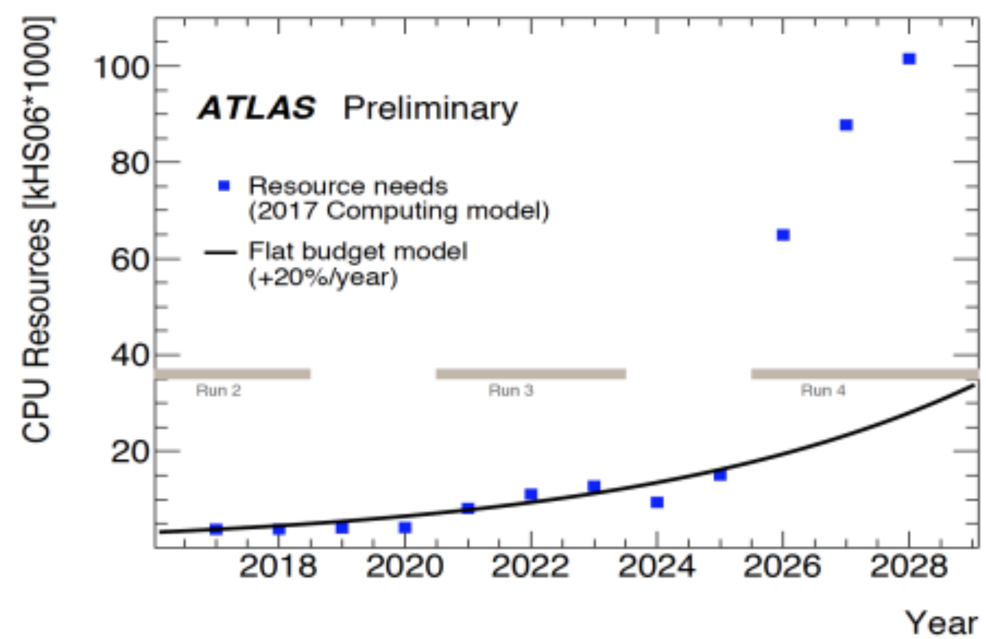
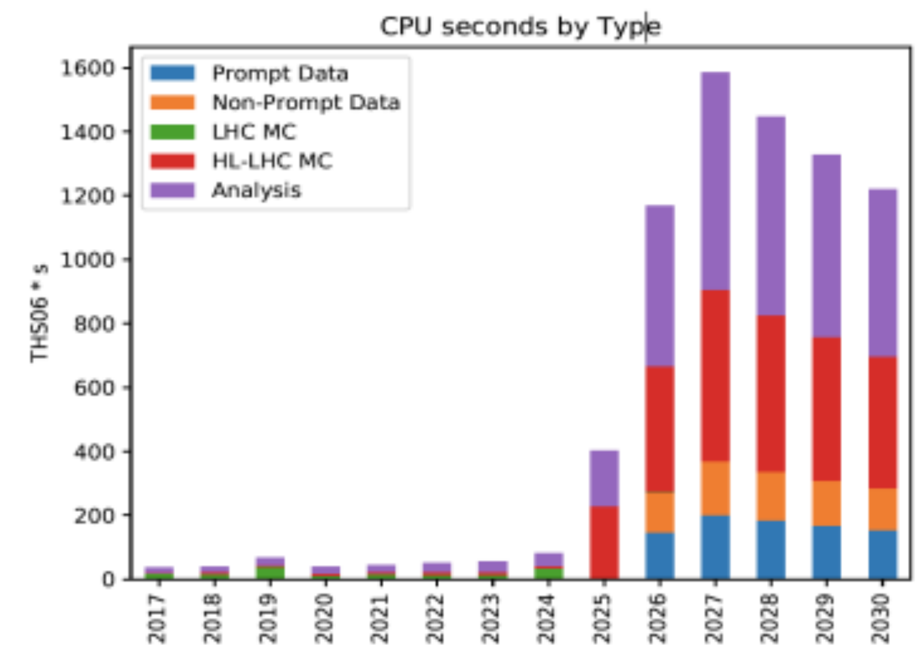
# NEED FOR FASTER SIMULATION CODE FOR HEP COMMUNITY

- During the first two runs, the LHC experiments produced, reconstructed, stored, transferred, and analysed **tens of billions** of simulated events
- As part of the high-luminosity LHC physics program (HL-LHC), the upgraded experiments expect to collect **150 times more data** than in Run 1
- More than **50%** of WLCG power used for simulations
- **GeantV**: path towards a faster toolkit **2-5 x Geant4**

Estimated ~10x CPU needs for the HL-LHC era

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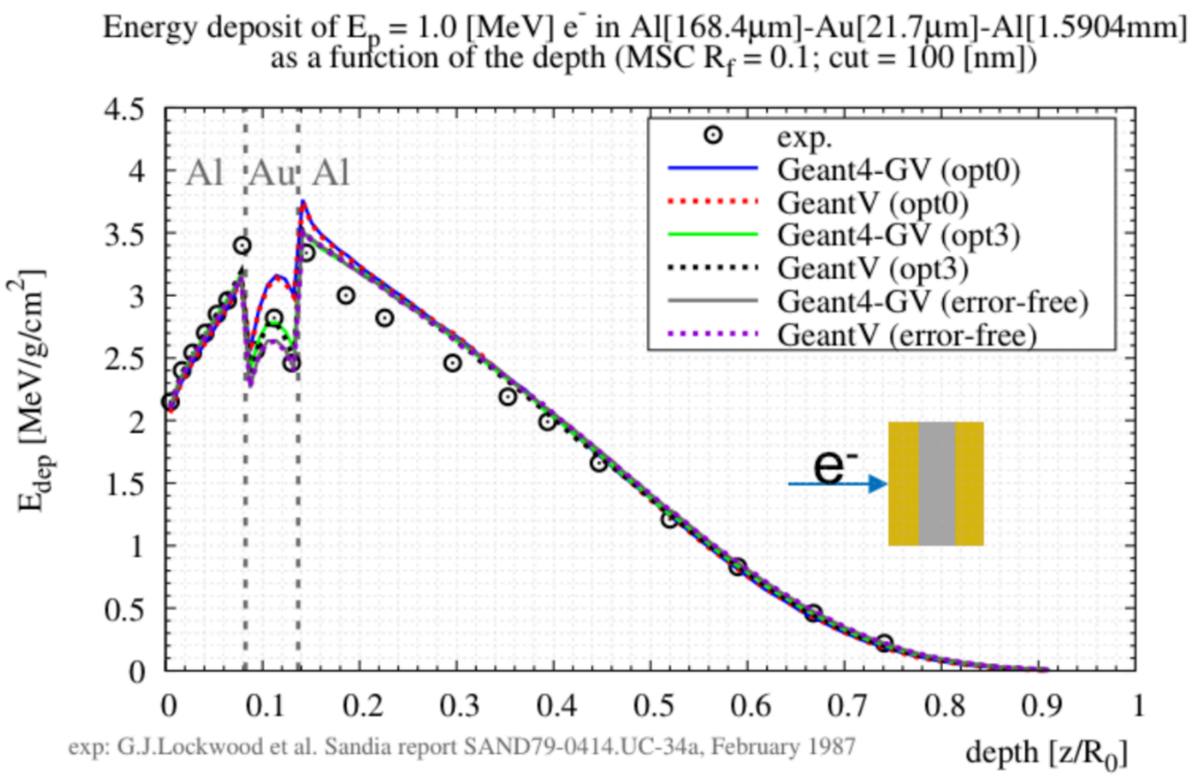
# EM PHYSICS MODELS VALIDATION

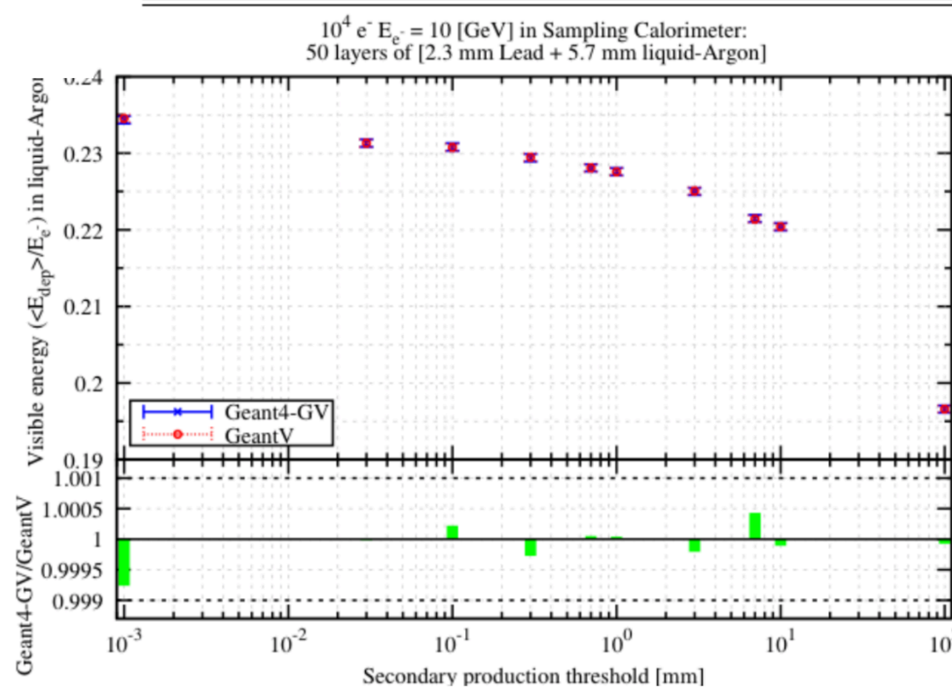



Multi-layered target

Scalar EM models revisited in a vectorization friendly way (e.g. vectorizable sampling) and validated against Geant4 version.

$10^5$ 1 [GeV] e- in ATLAS bar. simpl. cal. : 50 layers of [2.3 mm Pb + 5.7 mm lAr]; p.cut = 0.7 [mm]

| | $e^-/e^+$: ionisation, bremsstrahlung, msc; $\gamma$: Compton, conversion | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | GeantV | | | | Geant4 | | | |
| material | $E_d$[GeV] | rms [MeV ] | tr.l. [m] | rms [cm] | $E_d$[GeV] | rms [MeV ] | tr.l. [m] | rms [cm] |
| Pb | 0.69450 | 15.198 | 51.015 | 1.189 | 0.69448 | 15.234 | 51.016 | 1.192 |
| lAr | 0.22792 | 14.675 | 106.11 | 7.592 | 0.22796 | 14.656 | 106.13 | 7.582 |




Mean number of :

| | | |
|---|---|---|
| gamma | 405.87 | 406.15 |
| electron | 9411.49 | 9419.44 |
| positron | 53.77 | 53.71 |
| charged steps | 11470 | 11476 |
| neutral steps | 49177 | 49222 |

*credit: M. Novak*

Work in progress on vectorization of all the EM physics - expected to be included in the beta release!

ATLAS simplified sampling calorimeter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# MAXIMUM SPEEDUP ACHIEVABLE

- Depends on the **vector width** but..
- Generally **is less than the vector register width**
  - some operations are **slower** for vector registers

Reciprocal Throughput* for Division DP (SandyBridge)

| | |
|---|---|
| Scalar | 10-20 cycles |
| Vector | 20-44 cycles |

    - Maximum speedup for division will be ~ 2 for this CPU
  - **Overhead** payed to gather data into SIMD vectors
- Another important factor is the **number of execution units** for particular instructions = number of instructions that can be executed simultaneously.

*The average number of core clock cycles per instruction for a series of independent instructions of the same kind in the same thread.

**


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# RESULTS: MODEL LEVEL TEST BENCHMARKS

| Model | Haswell (avx) | |
|---|---|---|
| | Scalar Time [ms] | SpeedUp |
| Klein-Nishina alias | 56.4 | 2.2 |
| Klein-Nishina rej | 48.37 | 2.21 |
| Moller-Bhabba alias | 51.32 | 1.85 |
| Moller-Bhabba rej | 50.21 | 1.62 |
| Seltzer-Berger brems alias | 73.19 | 1.98 |
| Seltzer-Berger brems rej | 106.63 | 1.64 |
| Relativistic brems alias | 76.96 | 2 |
| Relativistic brems rej | 330.57 | 2 |
| Bethe-Heitler pair alias | 86.53 | 1.82 |
| Bethe-Heitler pair rej | 62.98 | 1.39 |
| Relativistic pair alias | 91.66 | 1.37 |
| Relativistic pair rej | 83.42 | 1.83 |
| Positron2Gamma alias | 60.78 | 2.23 |
| Positron2Gamma rej | 41.34 | 1.91 |
| Sauter-Gavrila alias | 66.4 | 1.45 |
| Sauter-Gavrila rej | 108.89 | 1.2 |

Test with Lead, #baskets: 256


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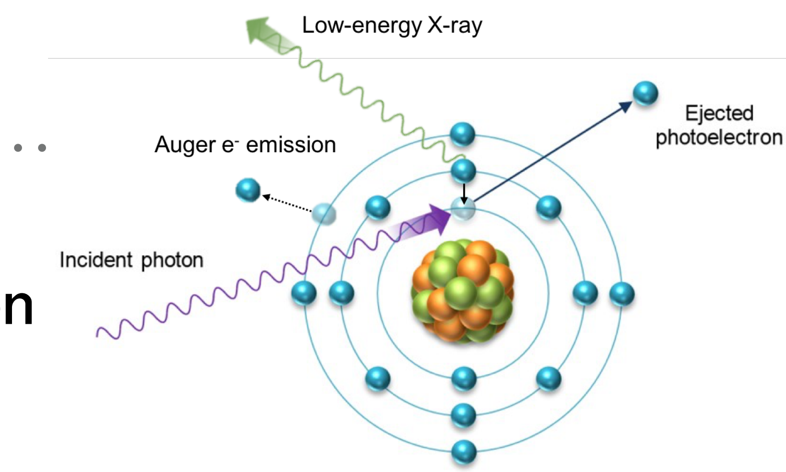
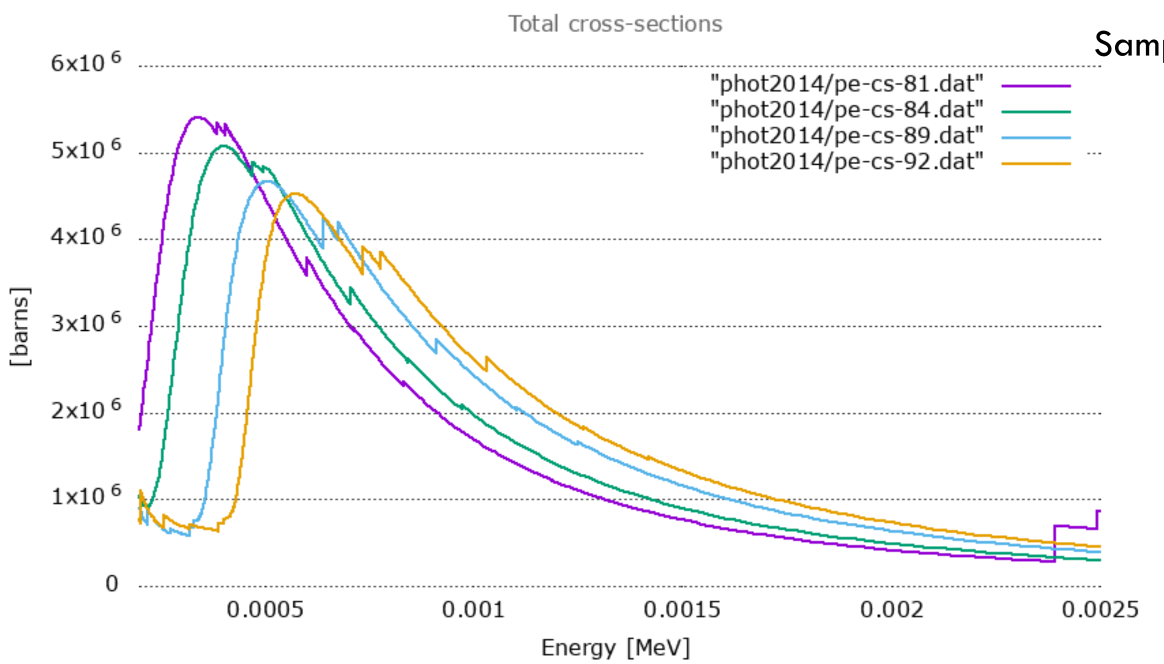
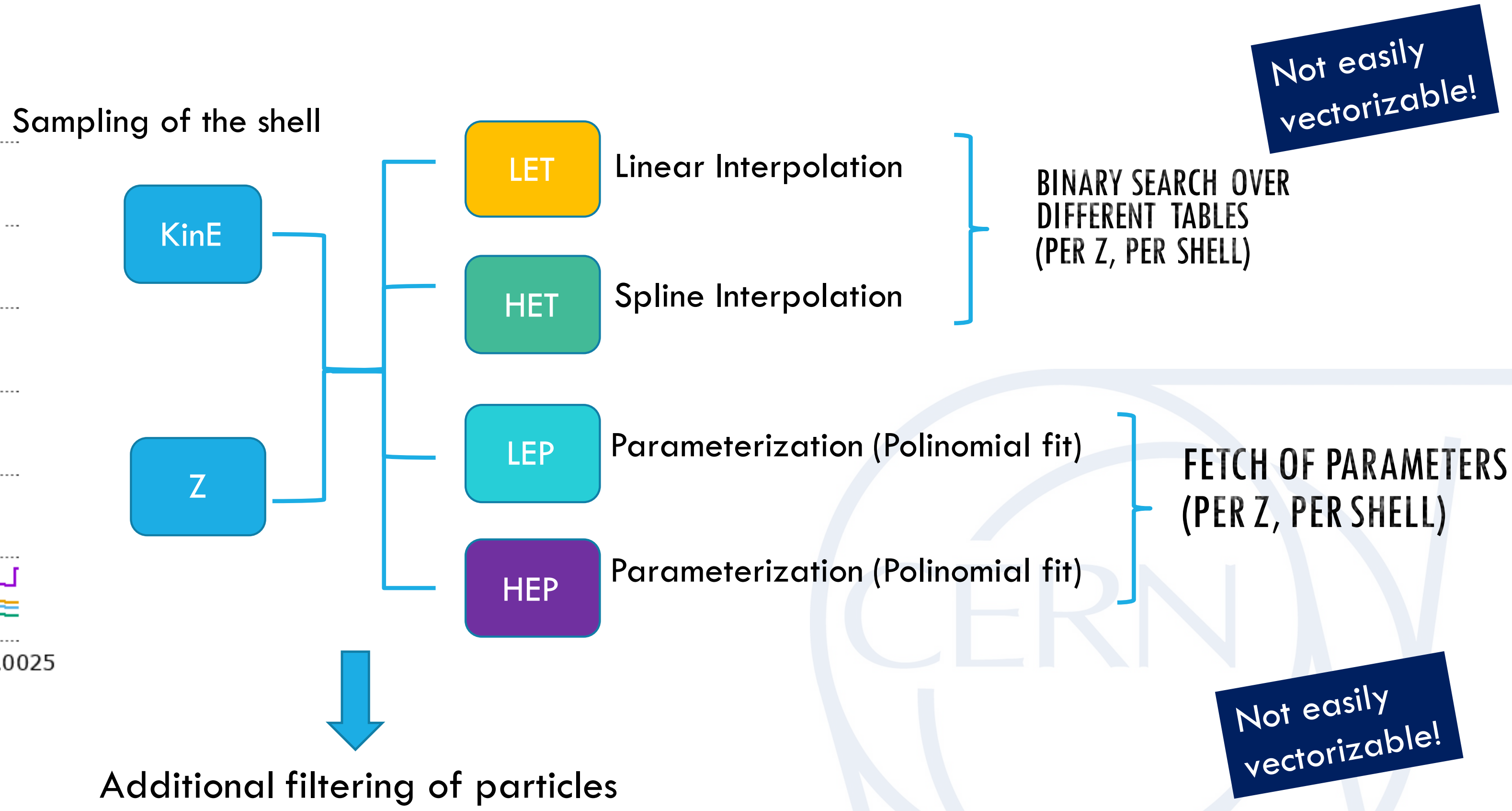
# EXAMPLE: PE EFFECT




## - Photoelectric effect total cross-section is not an easy function

- Fit in two different energy ranges, but not below k-shell binding energy
  - Tabulated cross-sections left for low energies
- For the final state sampling one need to sample
  - the angle: described by the SauterGavrila differential cross-section
  - the subshell: This is going through a binary search algorithm (not vectorizable) + linear or spline interpolation





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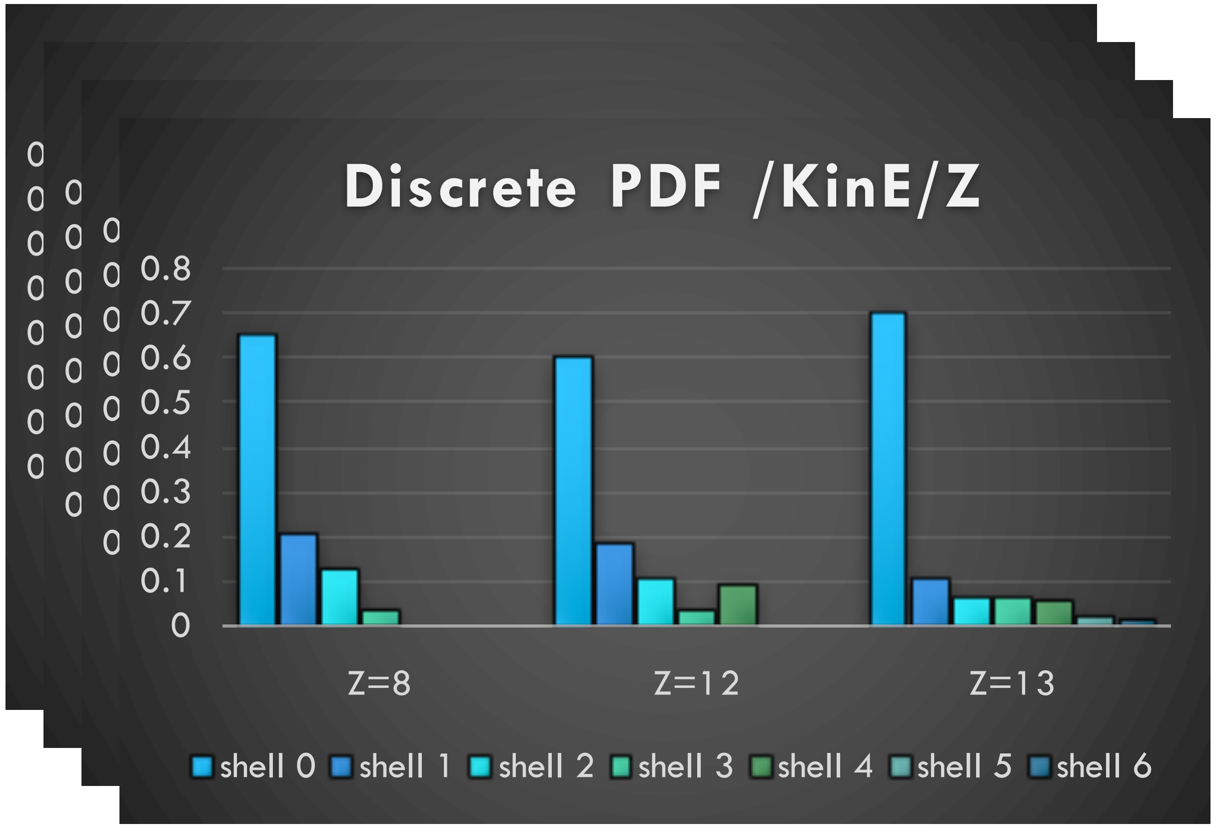
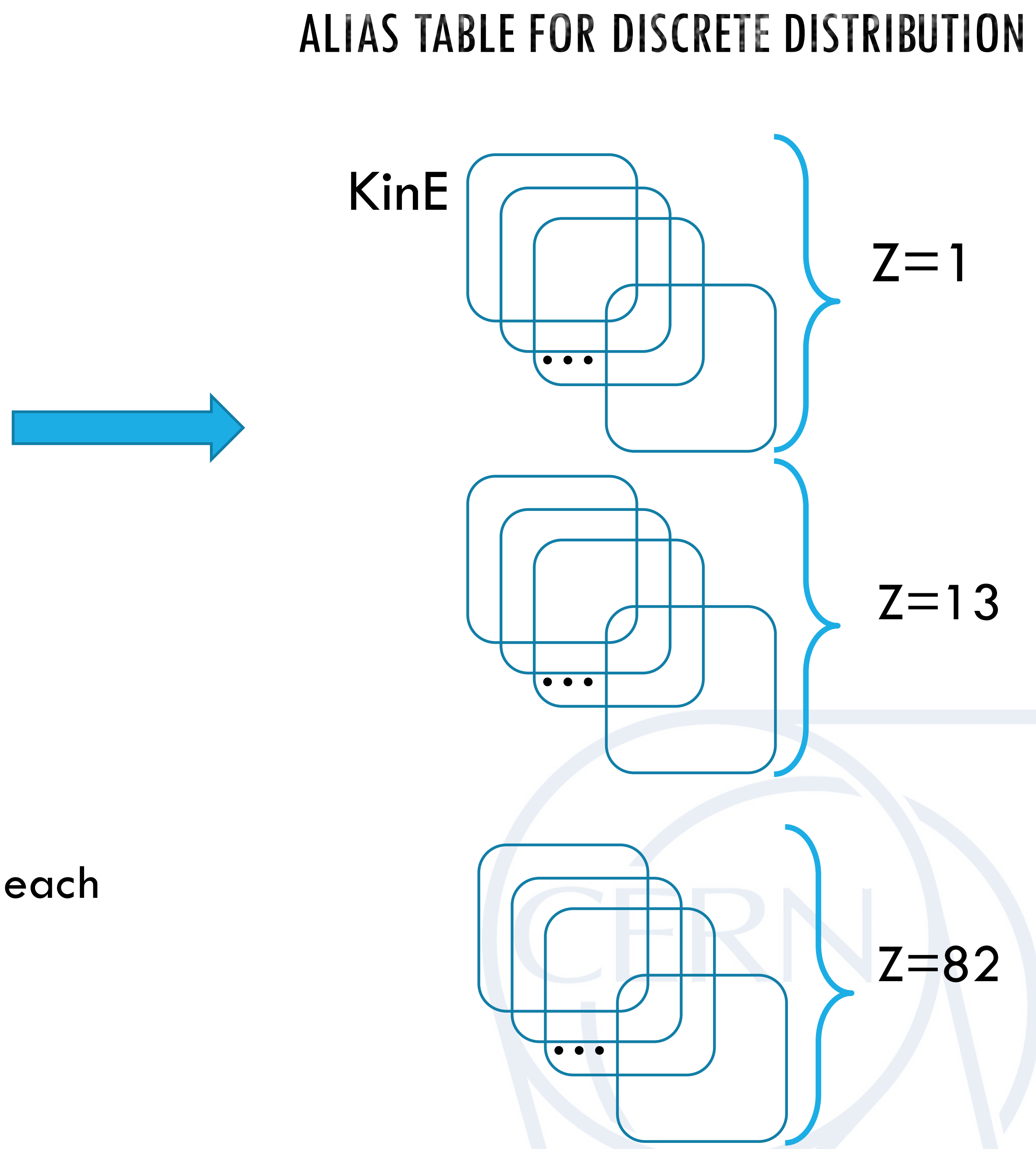
# VECTORIZATION WITH DISCRETE ALIAS TABLES




- We generated a denser ss-cs dataset
  - to build equally spaced (in energy) discrete PDFs for each element (linearly interpolated)
  - From them we can build Alias Table
    - PRO: sampling of shells with only one case
    - CONS: Gathering operations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# VECTORIZATION OF REJECTION SAMPLING


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1 Prepare values that are needed for sampling, in form of arrays


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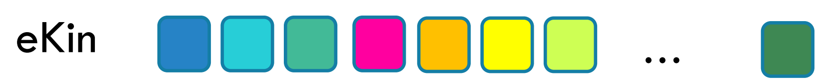




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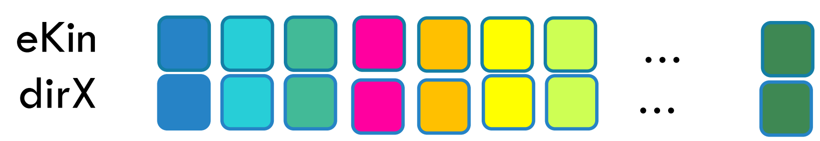



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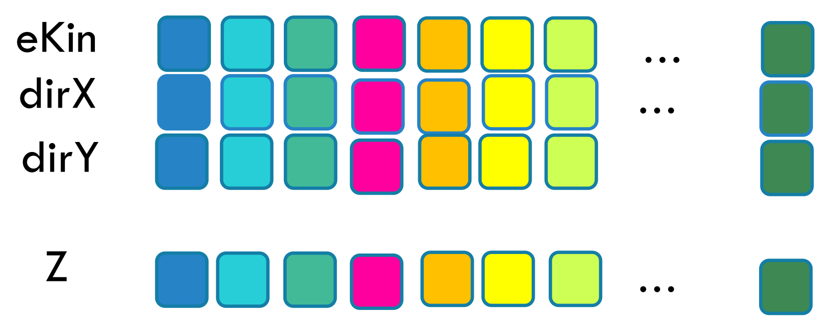



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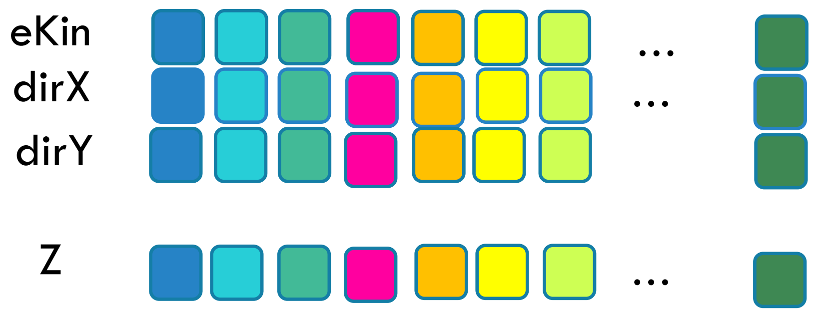


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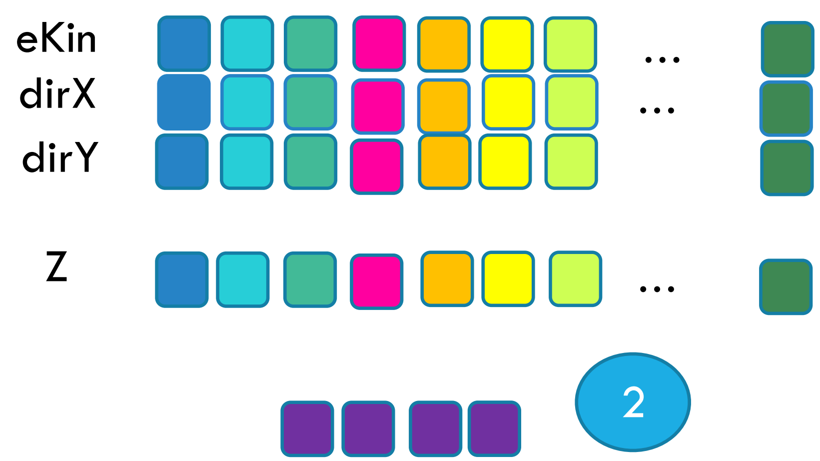


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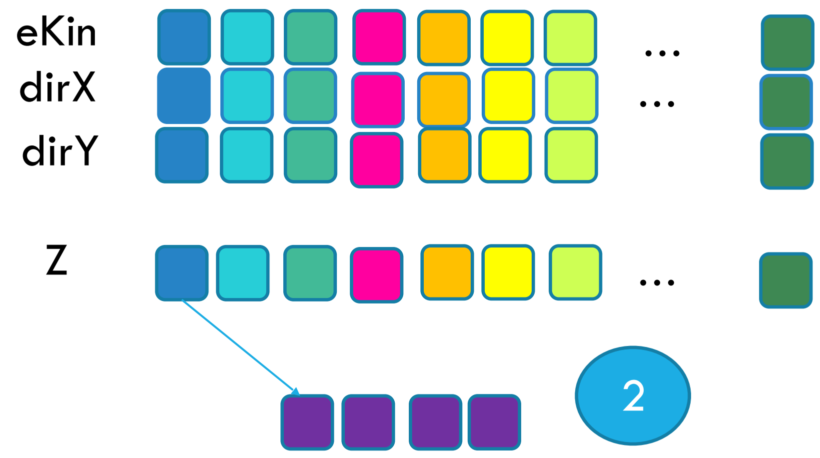


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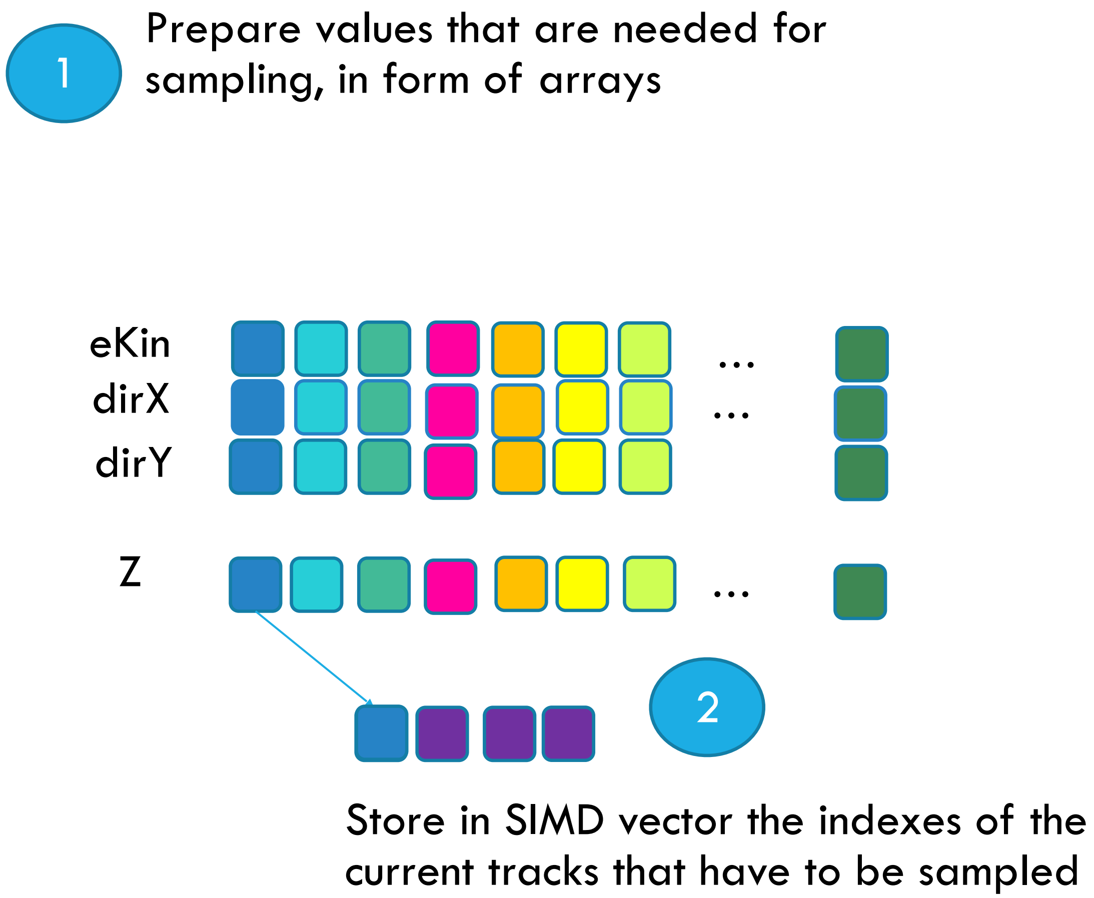



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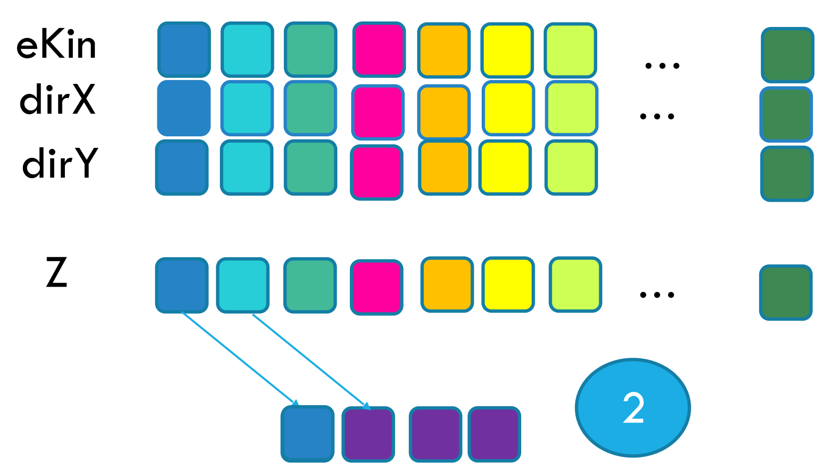


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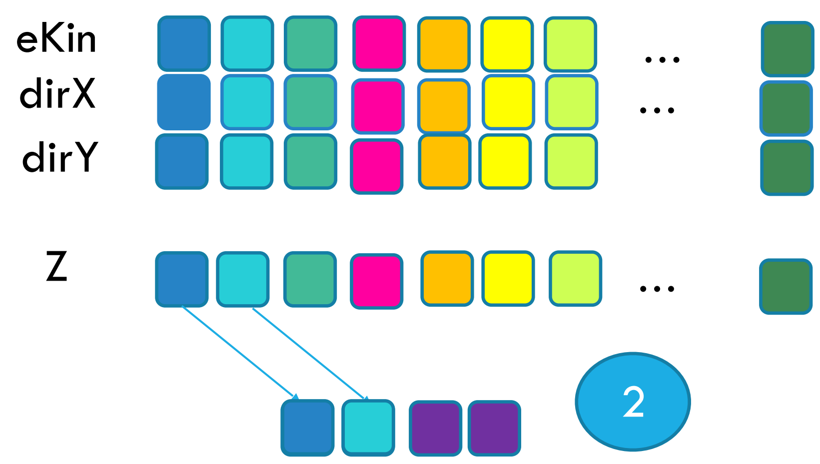


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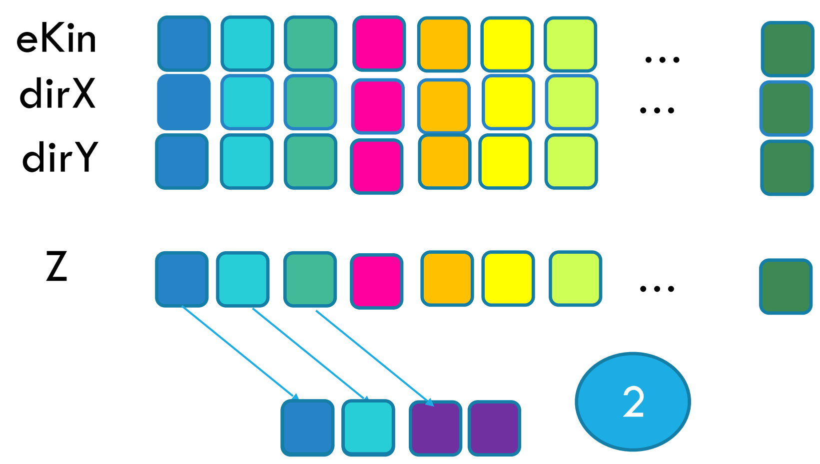


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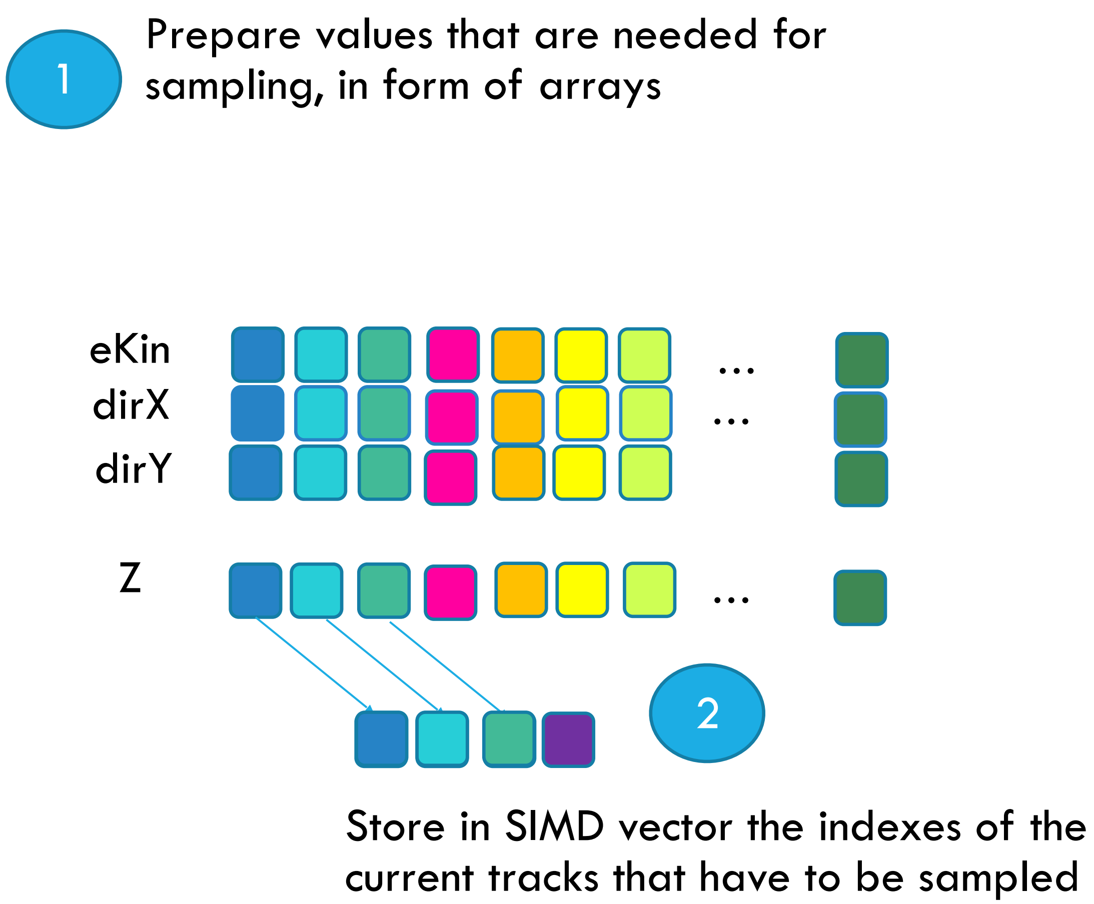



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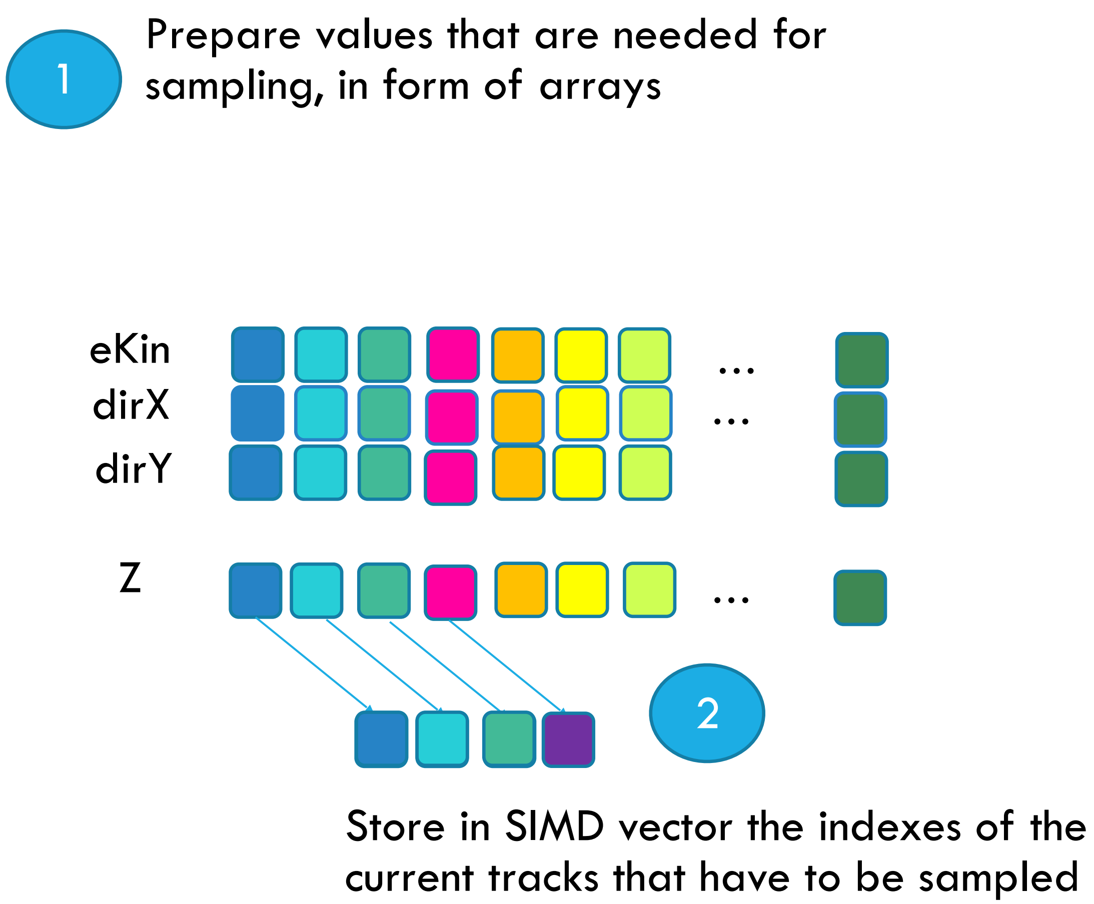



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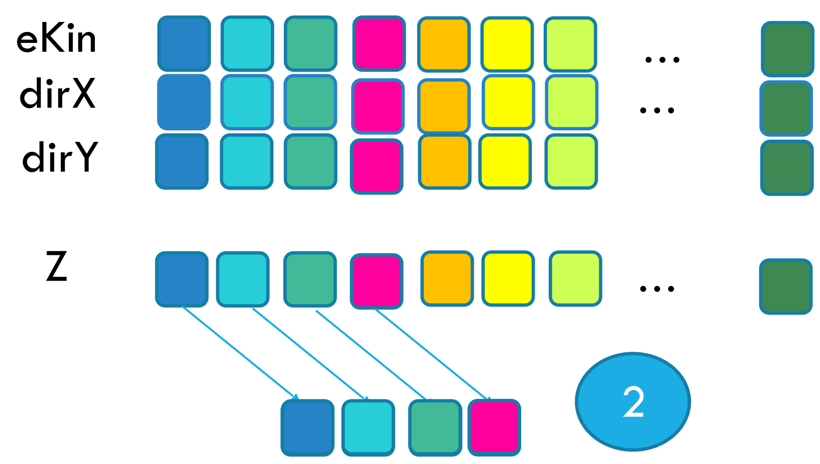


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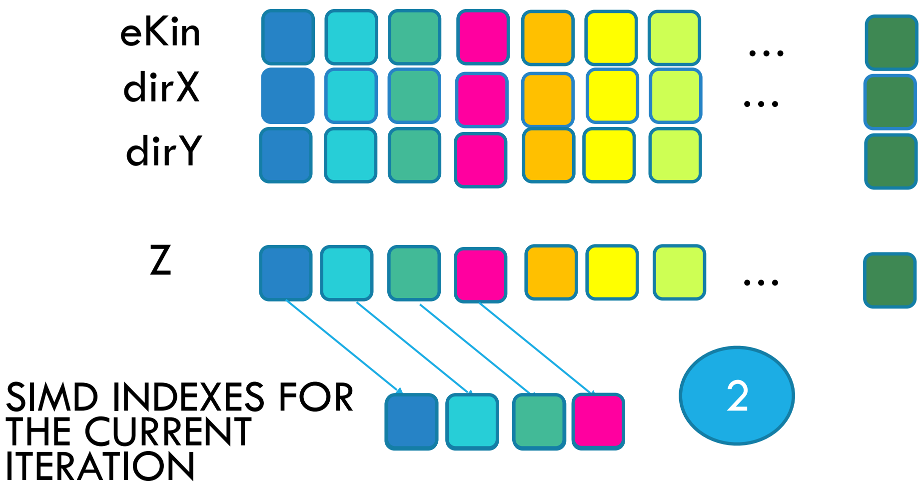


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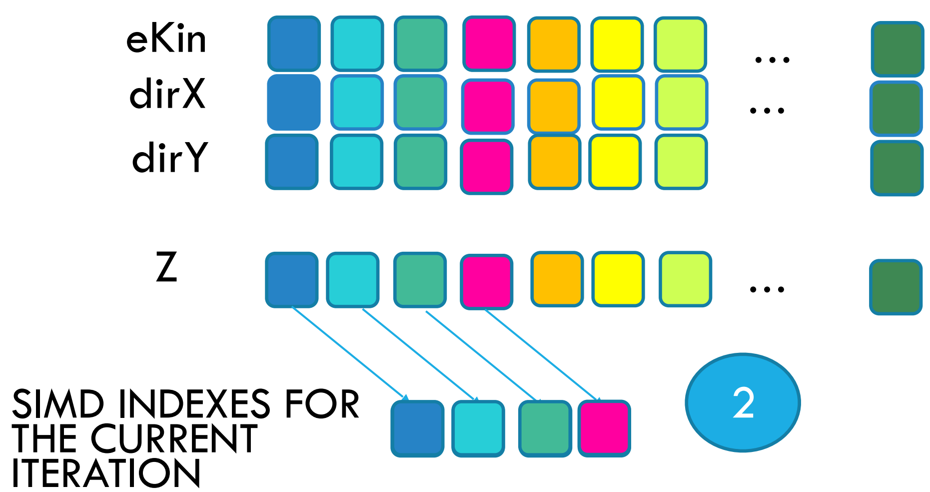


Store in SIMD vector the indexes of the current tracks that have to be sampled

3 Gather values from array using this indexes


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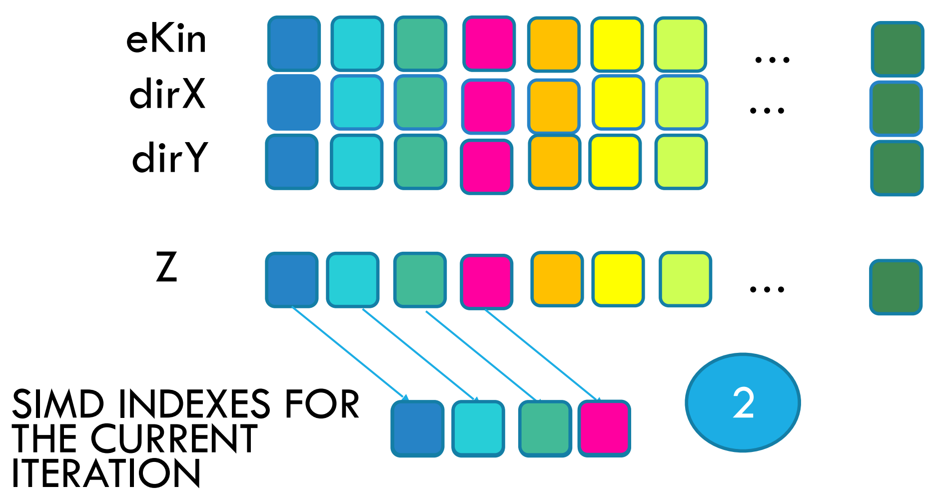


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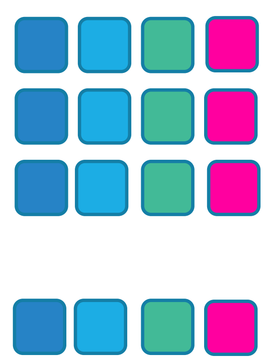



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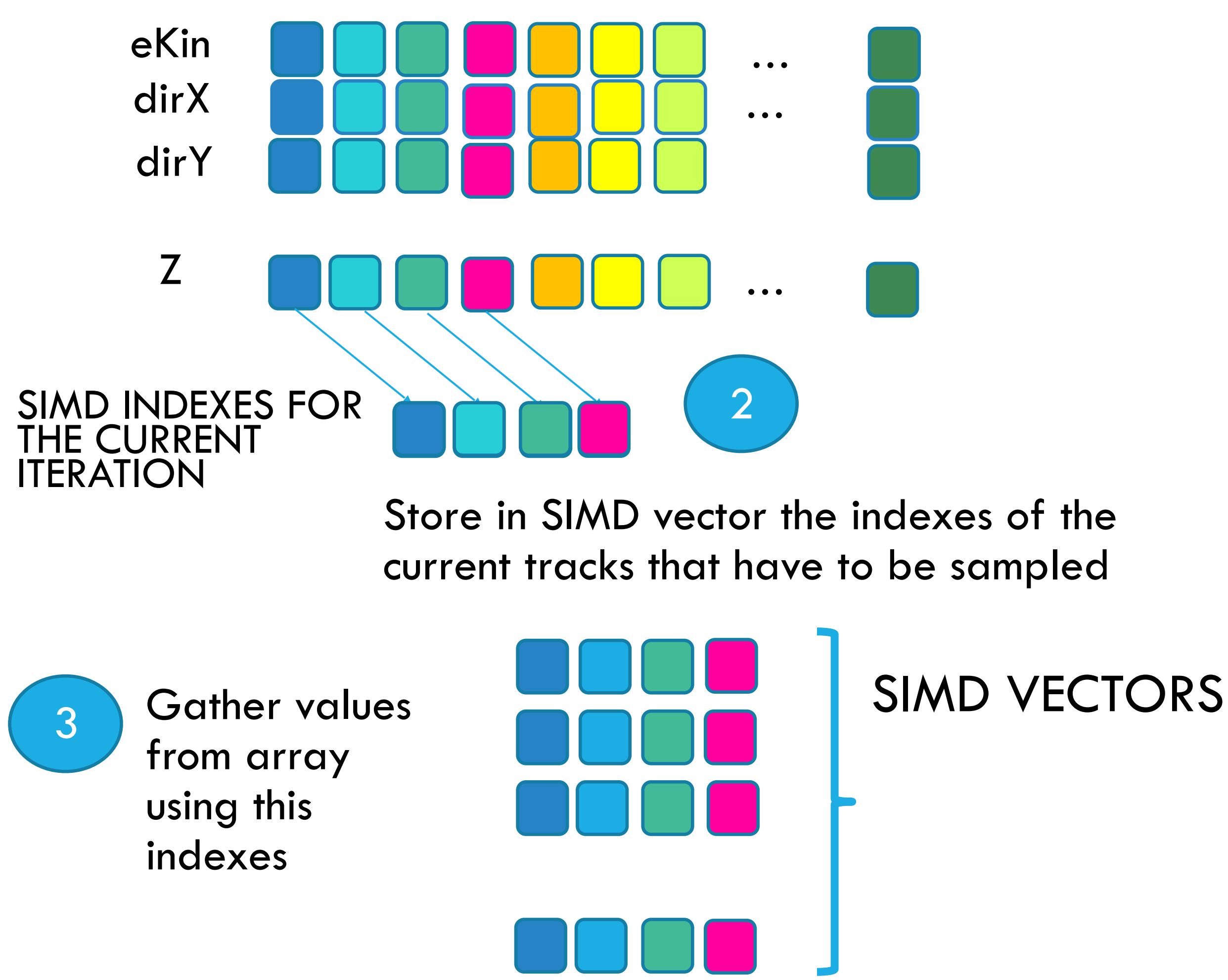



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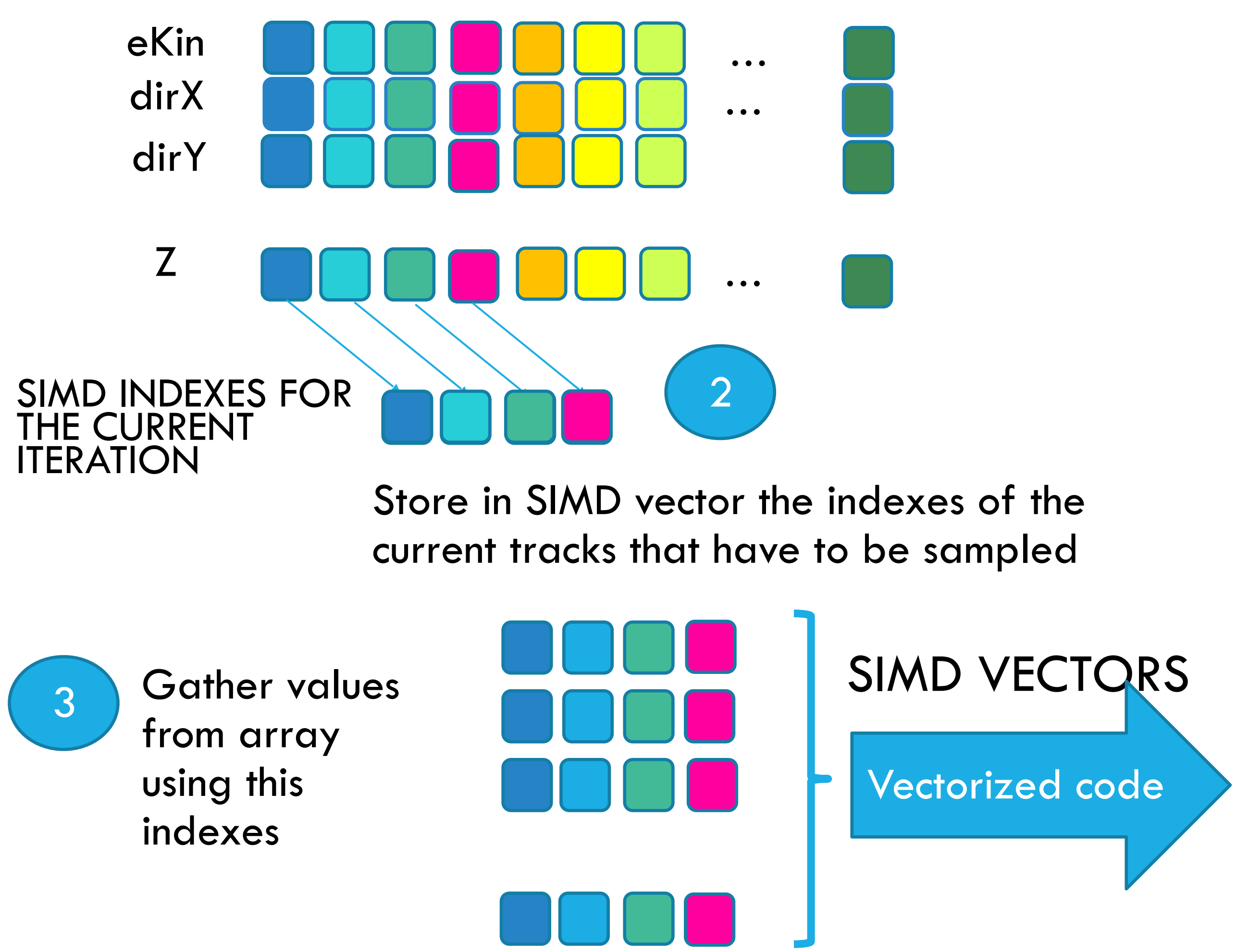



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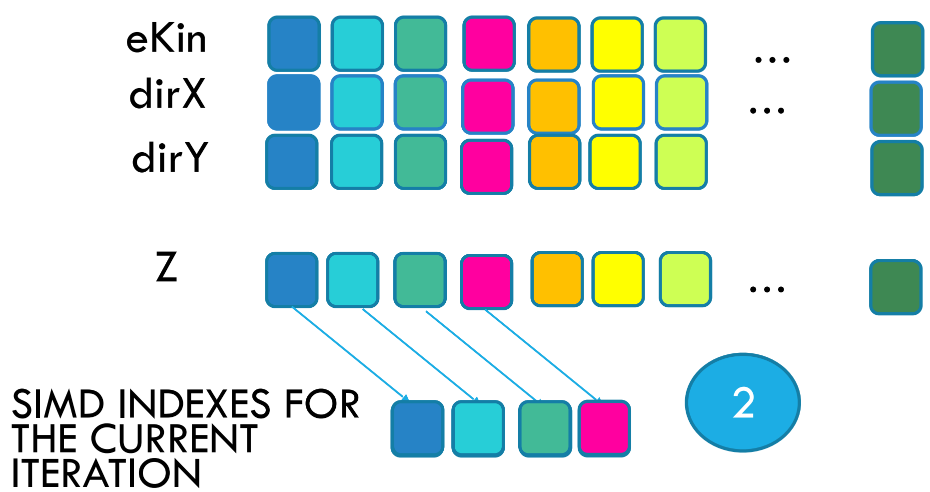
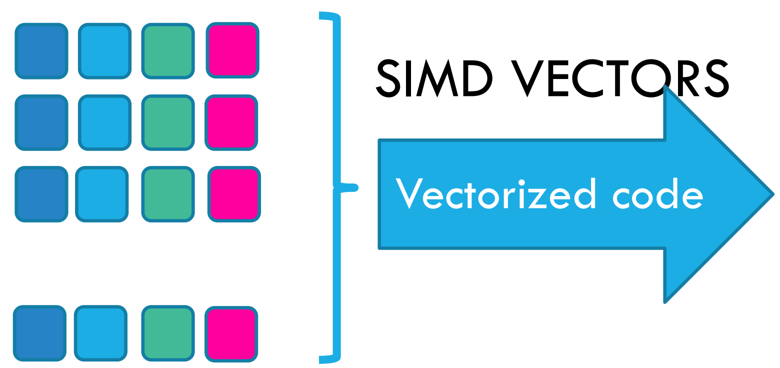



Store in SIMD vector the indexes of the current tracks that have to be sampled

3 Gather values from array using this indexes




4 Sample and if accepted, scatter back the resulting value to the array at the corresponding indexes



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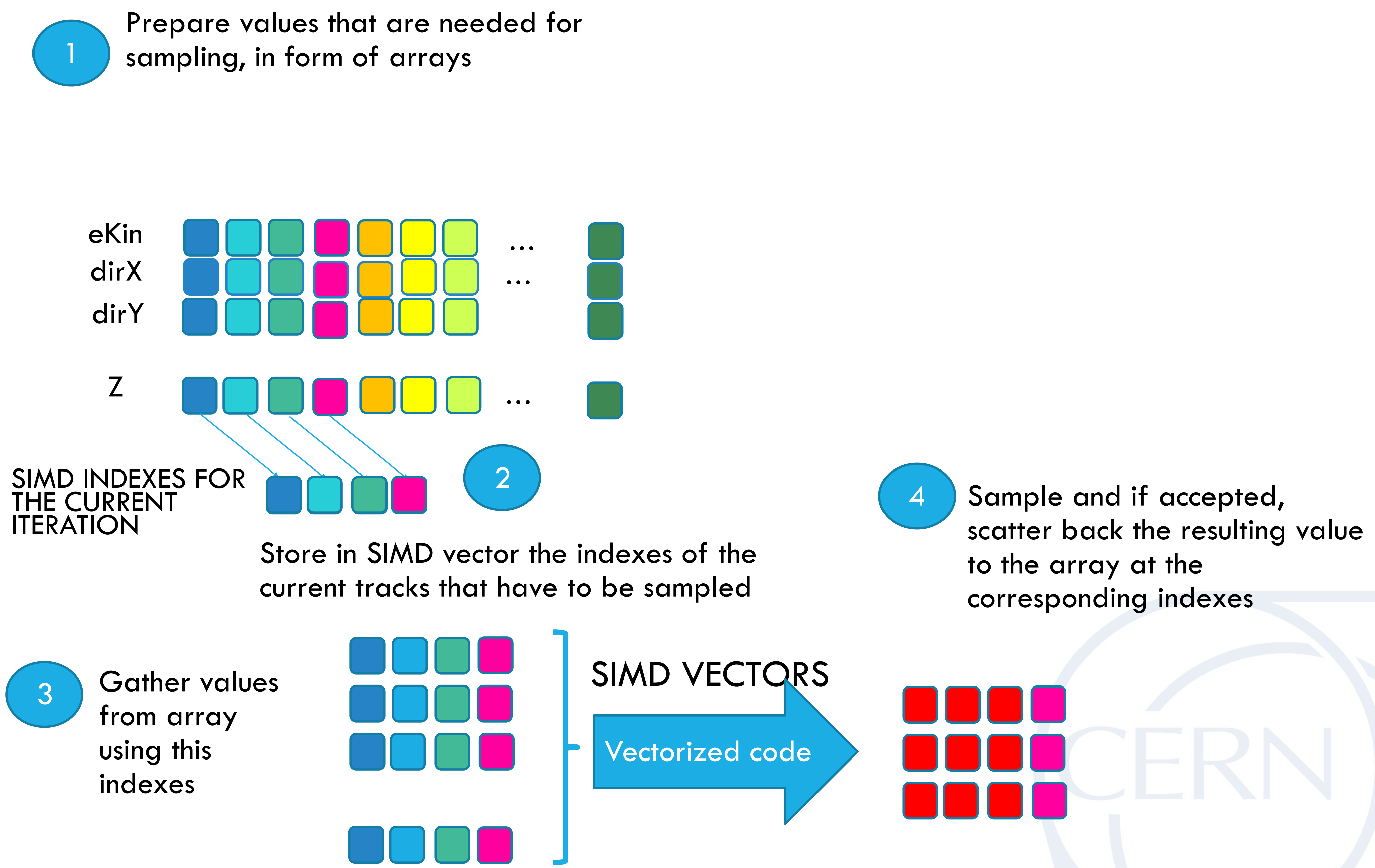




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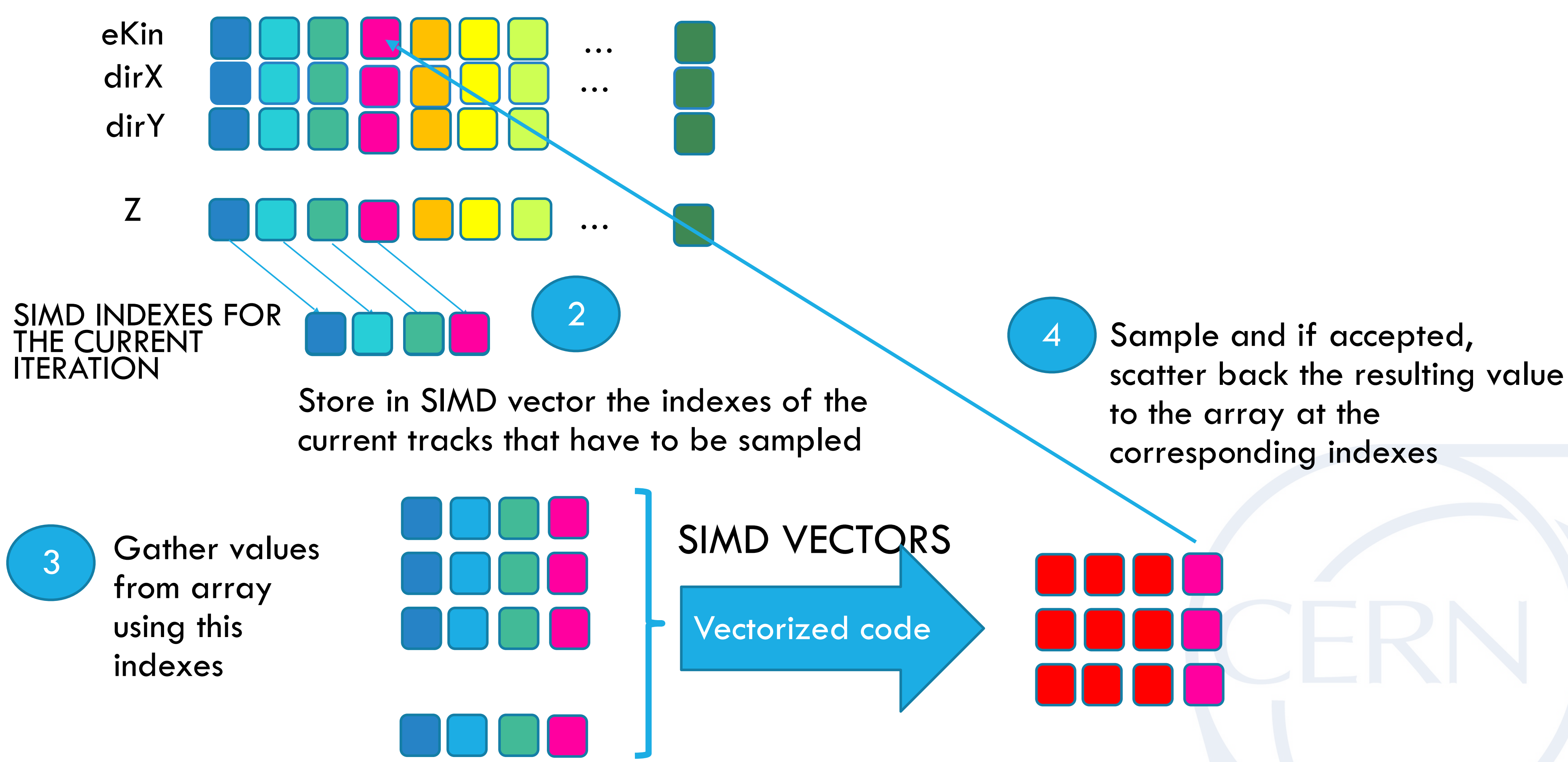



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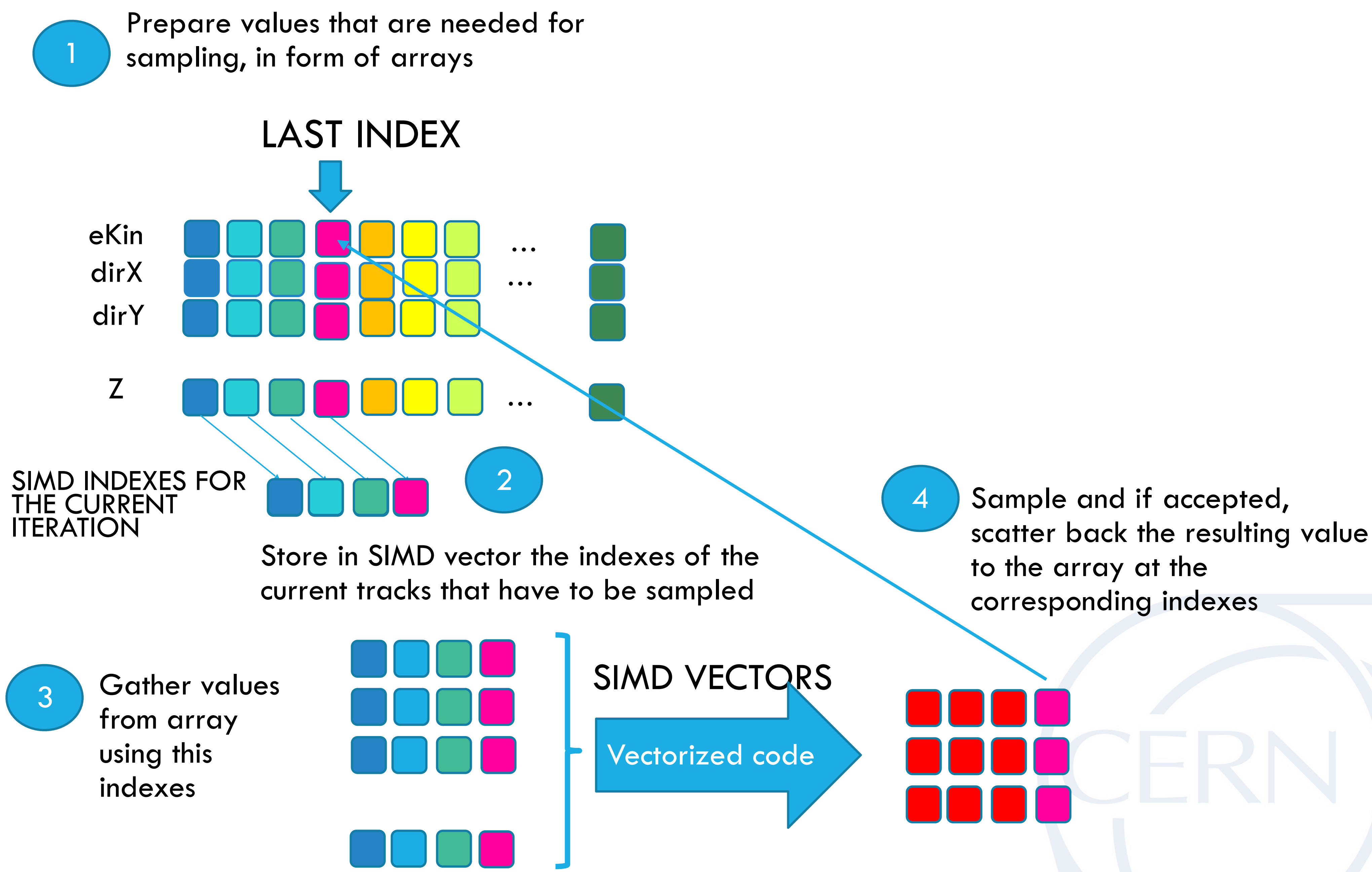



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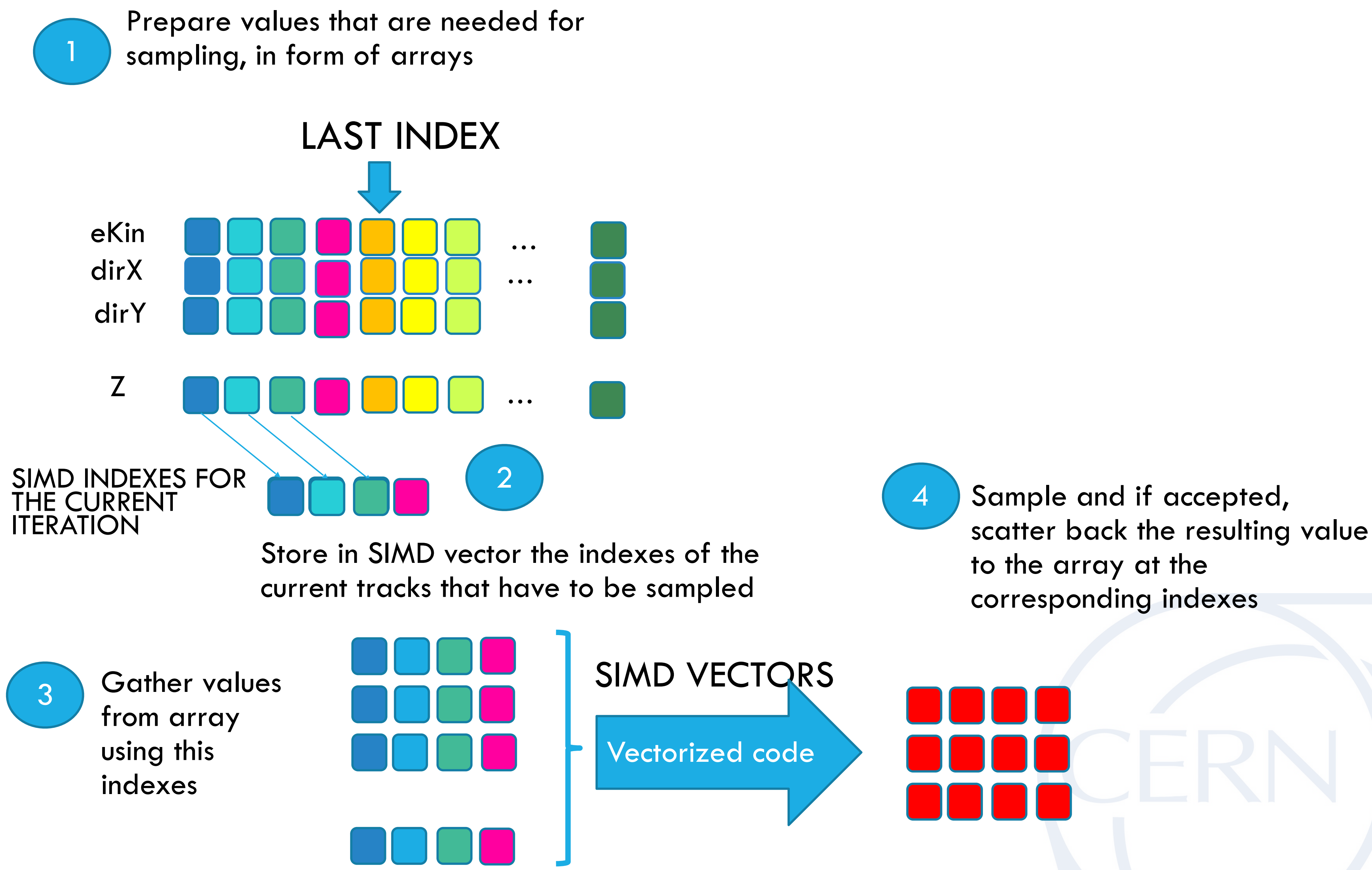



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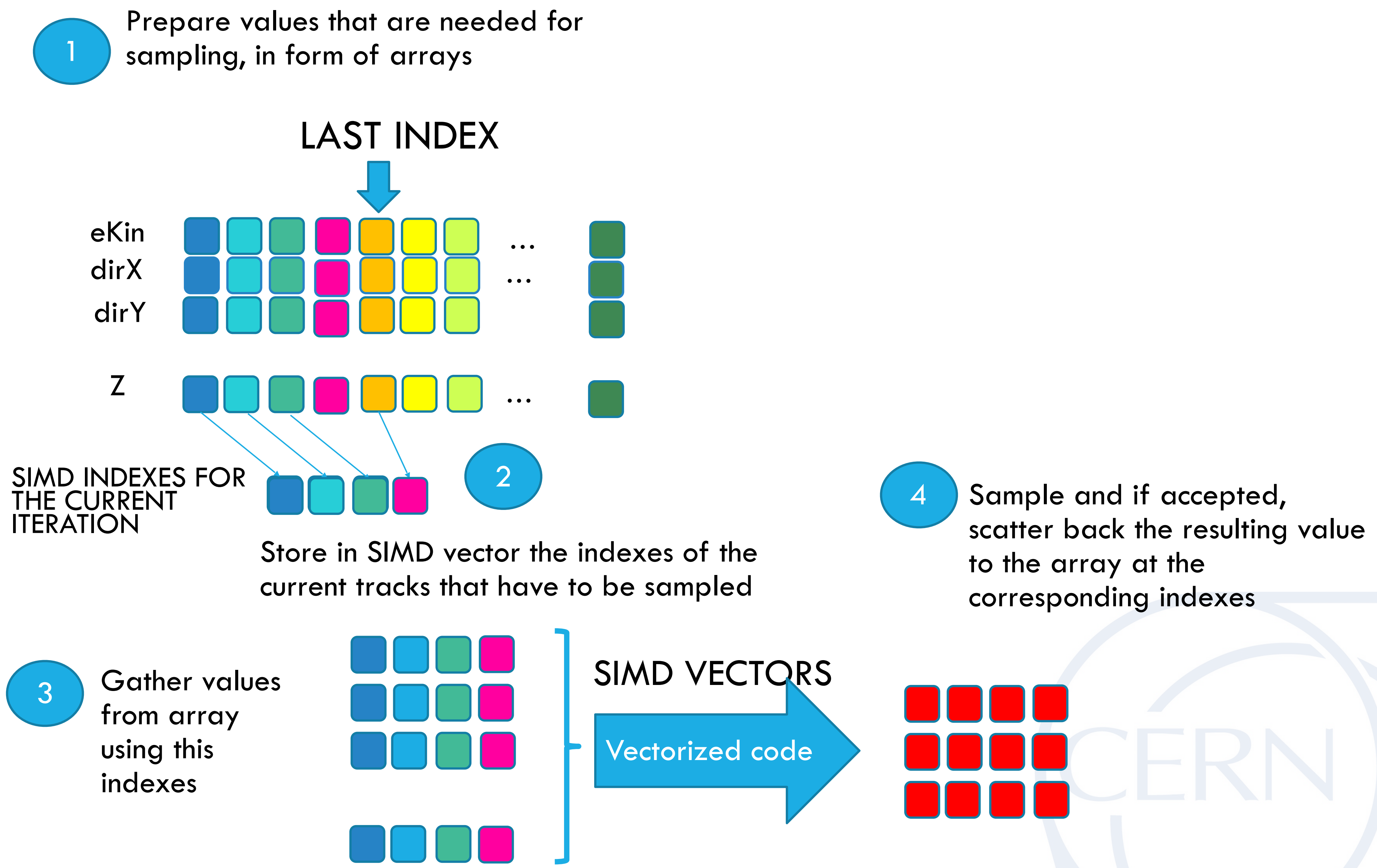




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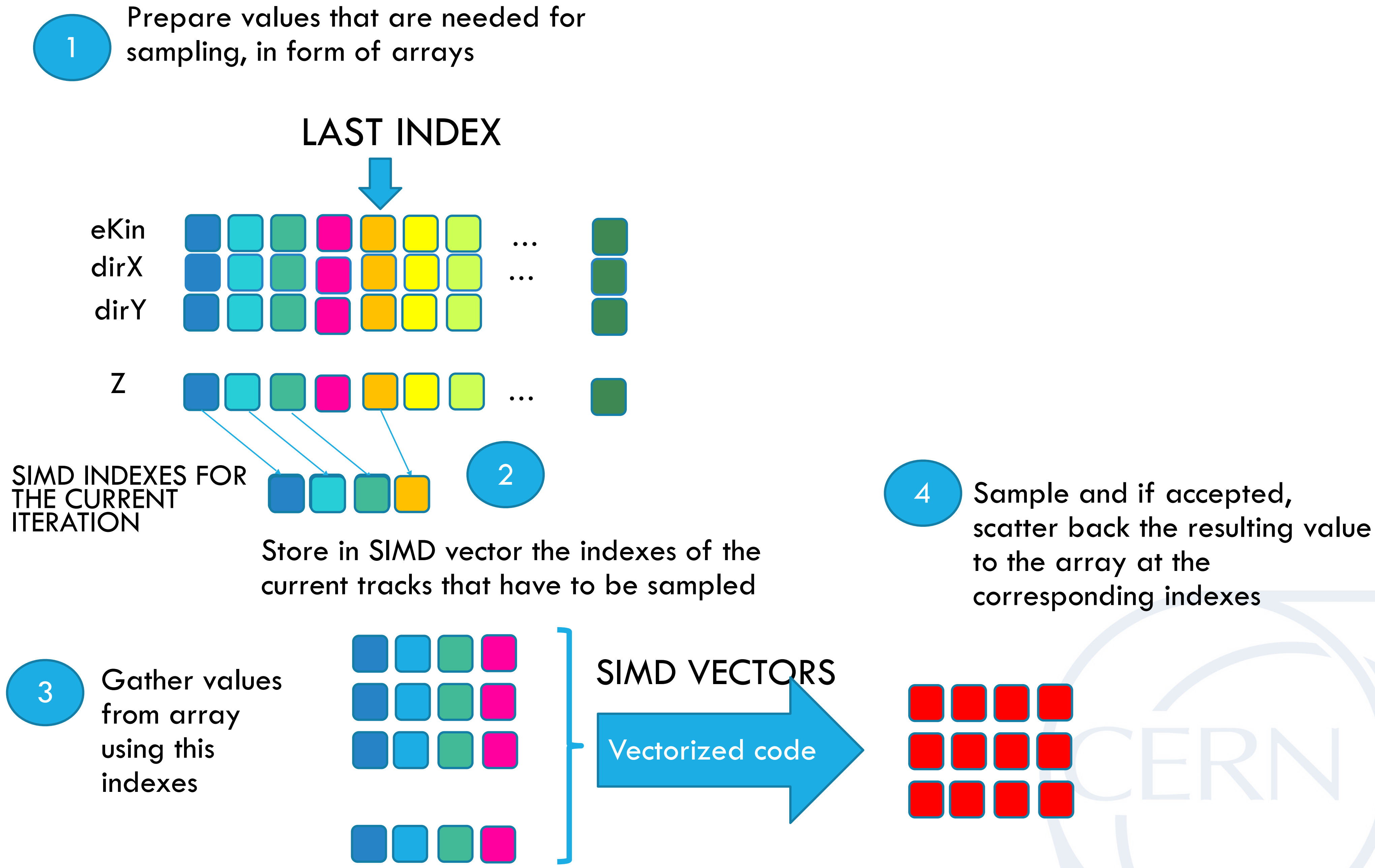



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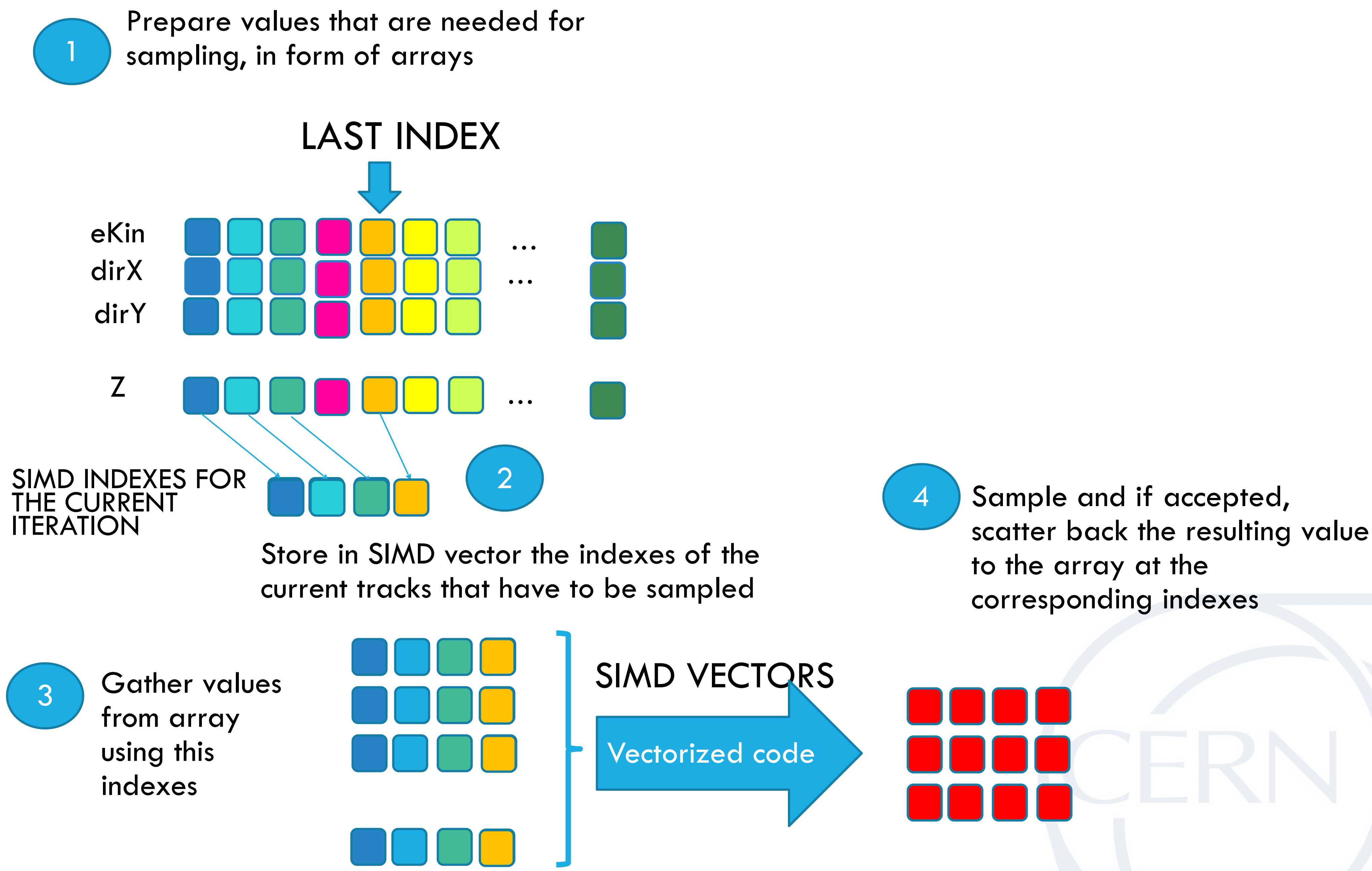



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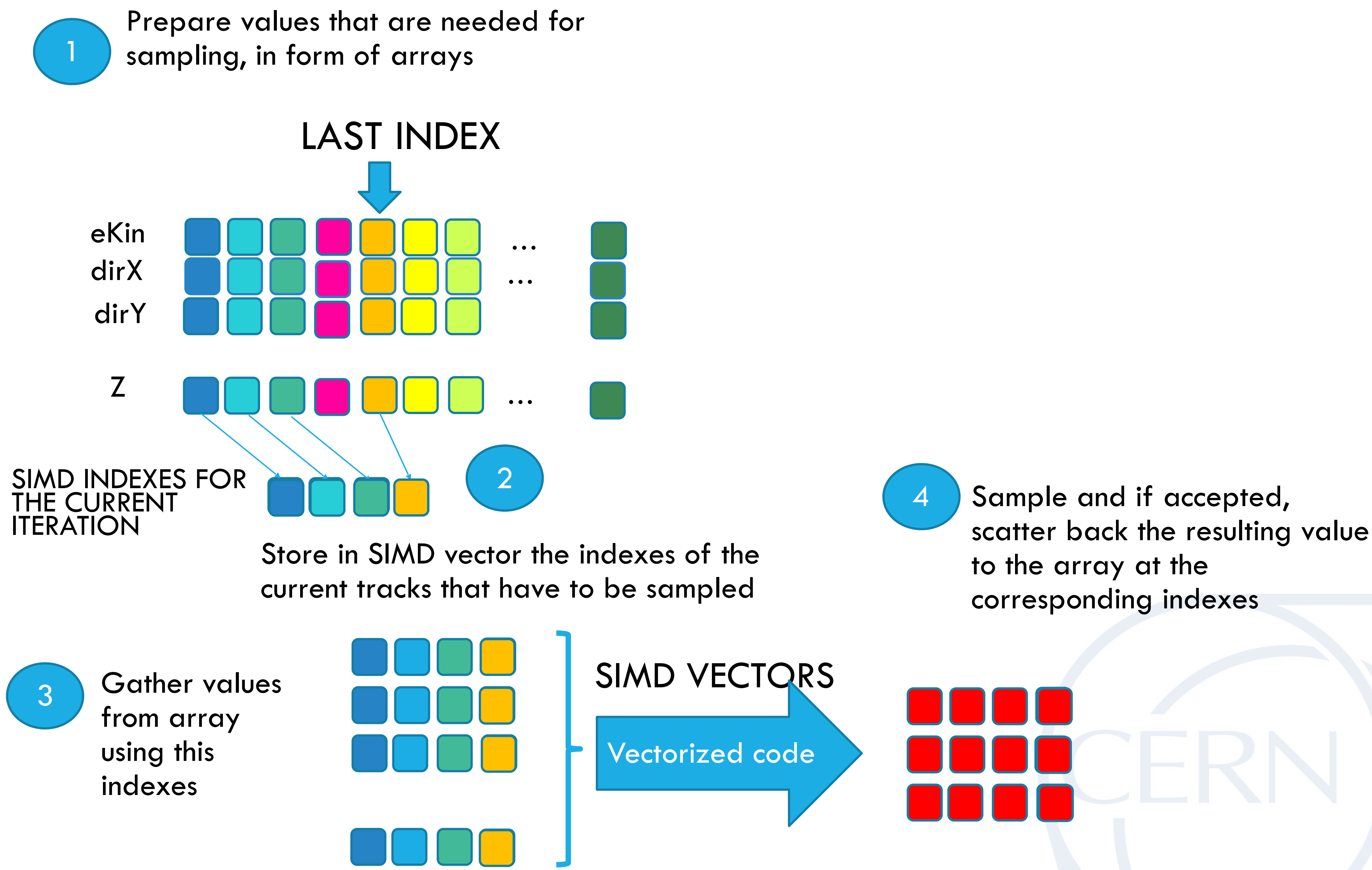



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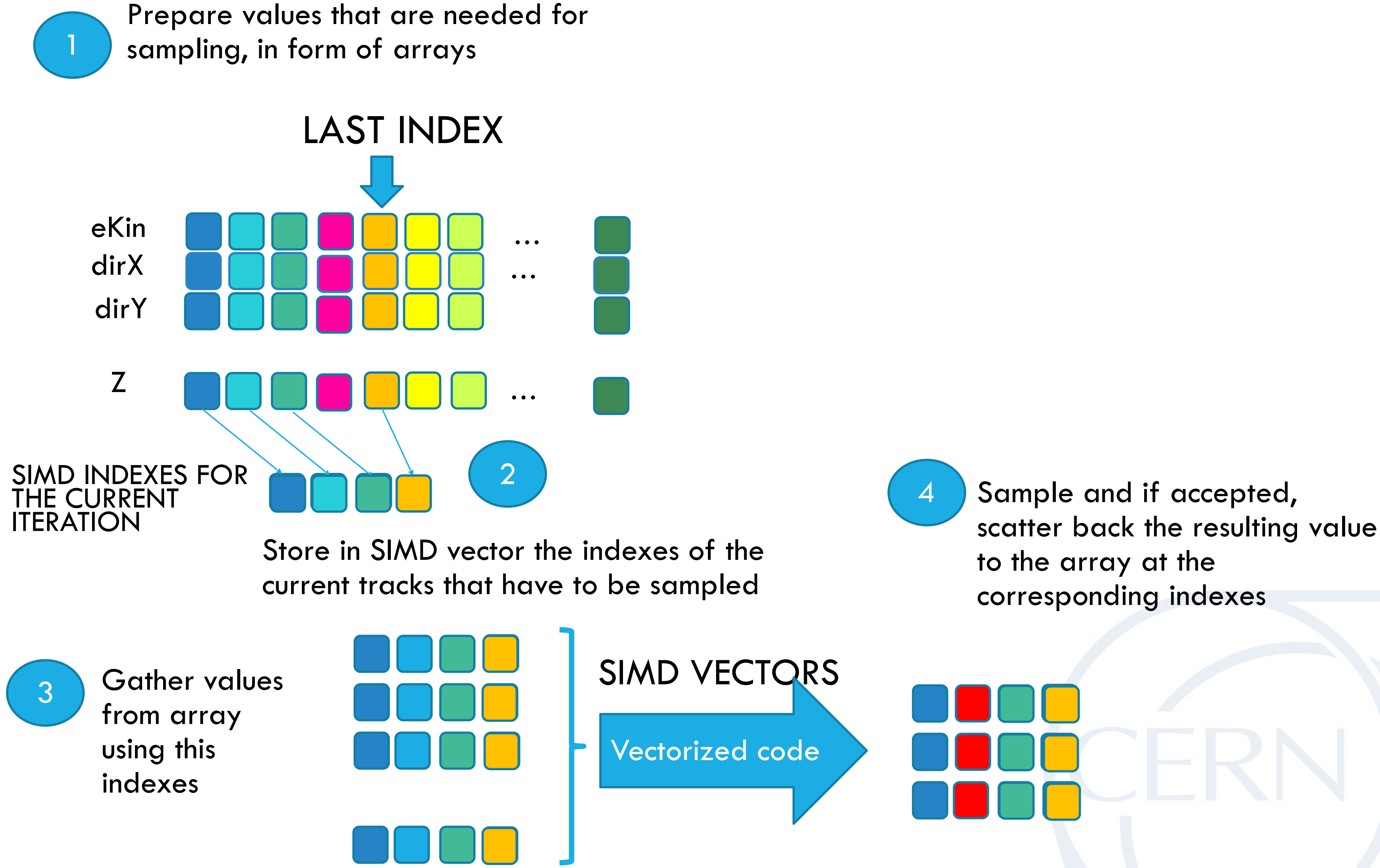



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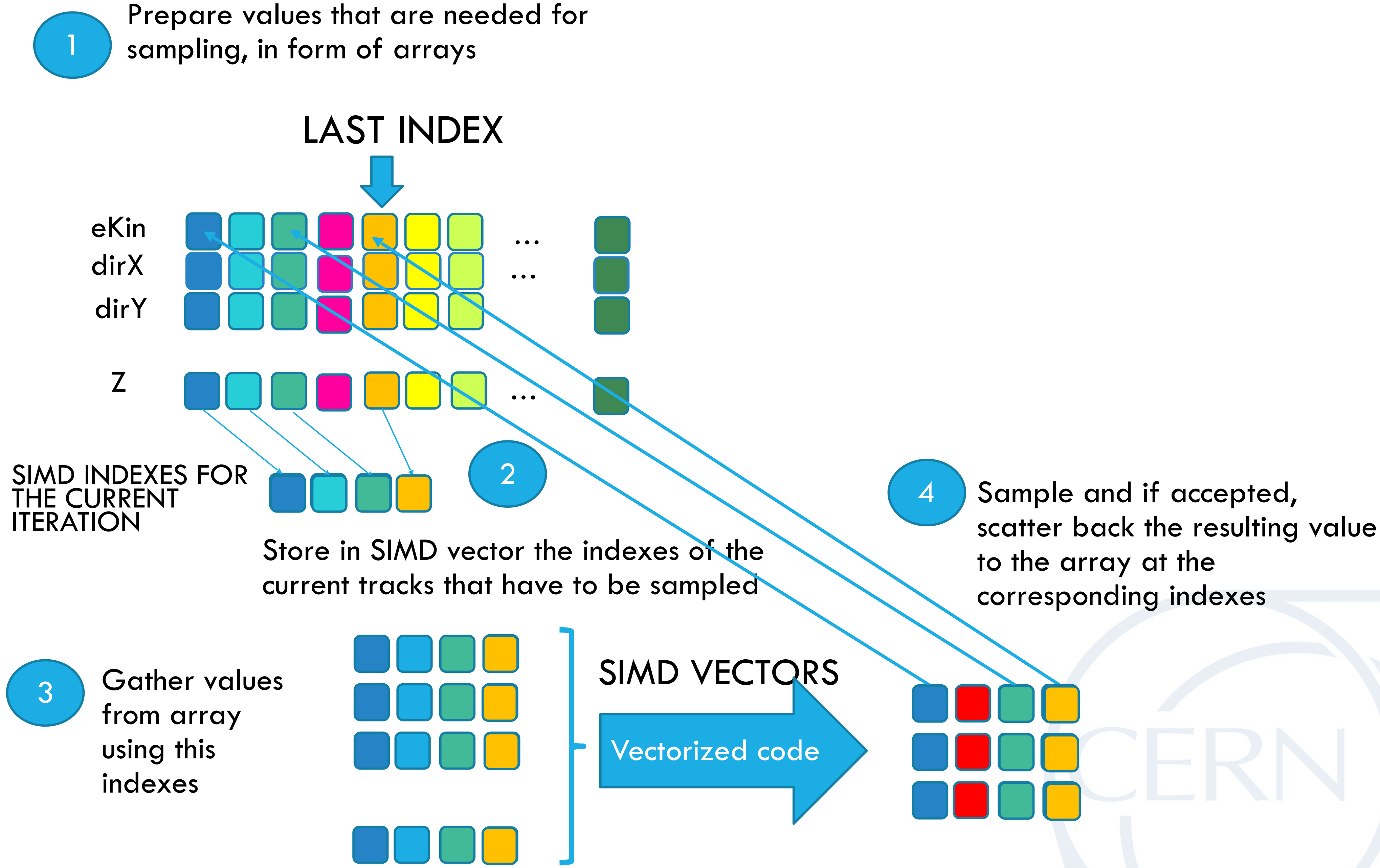



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