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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Sofia, Bulgaria

MOTIVATION

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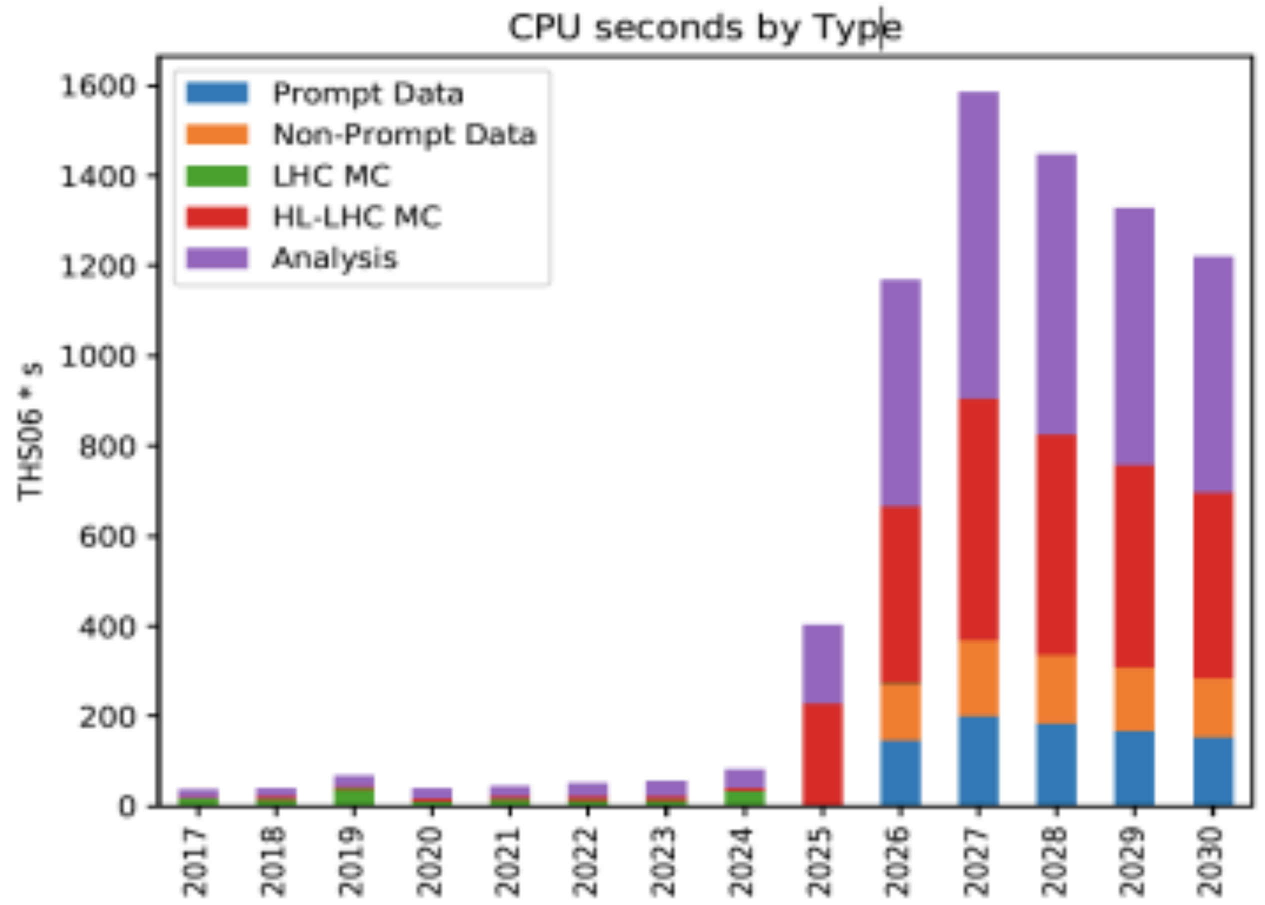
- Event simulation is one of the **most time consuming** parts of the workflow in the HEP sw ecosystem
  - For high-luminosity LHC phase (HL-LHC), the upgraded experiments expect to collect **150 times more data** than in Run 1
- The **GeantV R&D project** was launched in 2013, aiming at exploring emerging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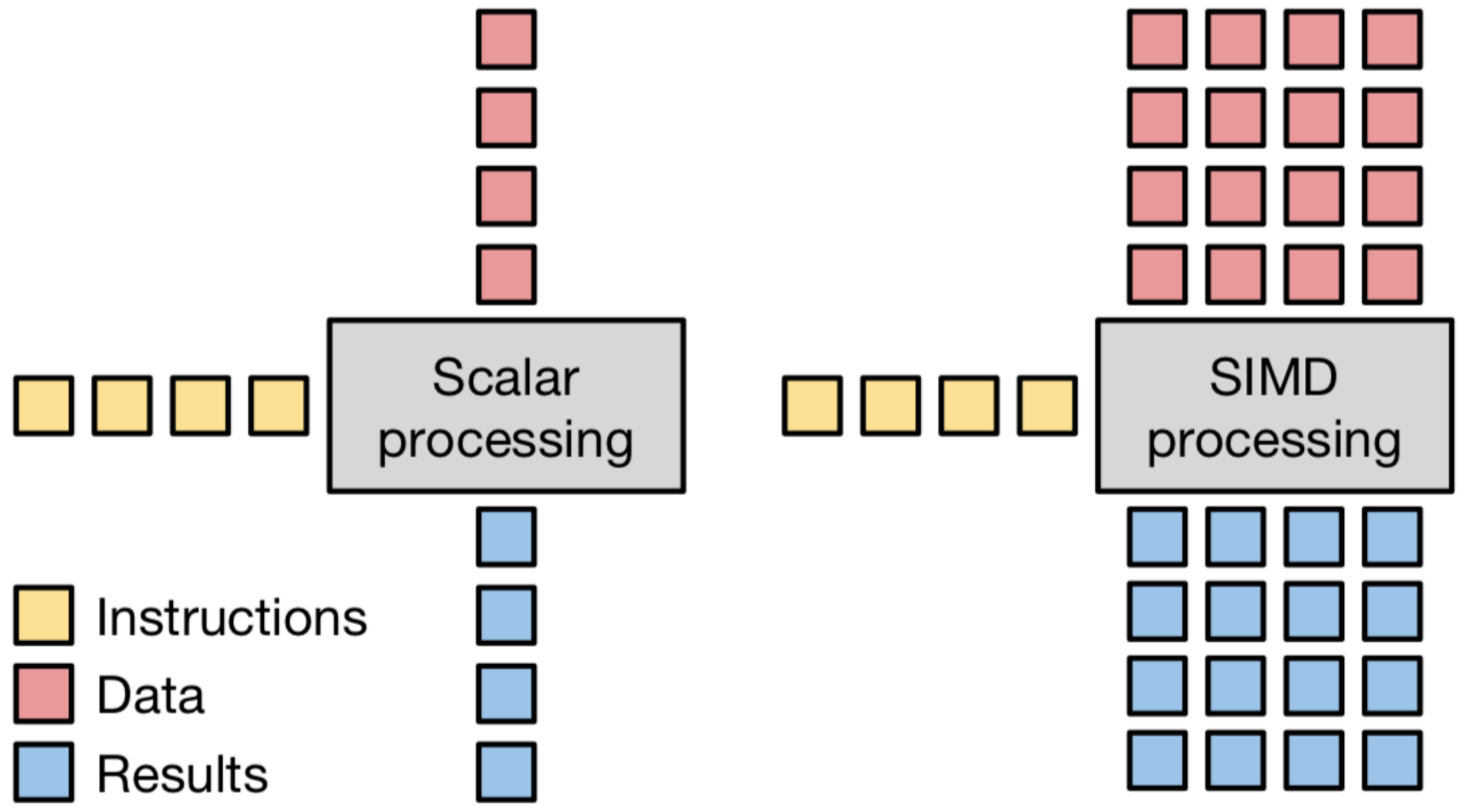
- The project studies performance gains when changing the classic particle transport approach, propagating **multiple tracks from multiple events in parallel**
  - improving code and data locality in the process
  - enabling SIMD/SIMT execution models: Vectorization+Multithreading
- **Vectorization of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



WHEN WE CAN PROFIT FROM VECTORIZATION

- Functions with many **math computations**, not bounded by **memory access**
  - Such as +, *, /, sqrt, sin, cos, exp, log (ordered according to approximate computation complexity)
  - Load 4 doubles into SIMD register is one instruction but it is not faster than loading values one by one
- 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  = Math::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));
}
```

GEANTV EM PHYSICS LIBRARY

Current State

particle	processes	model(s)	
		GeantV	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 [100 eV-100MeV]
			Mixed model [100 MeV-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 [100 eV-100MeV]
			Mixed model [100 MeV-100TeV]
	annihilation	Heitler (2γ) [0-100TeV]	Heitler (2γ) [0-100TeV]
γ	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

- When the particle undergoes a physics process, the **final state generation stage** occurs:

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Physics Stage

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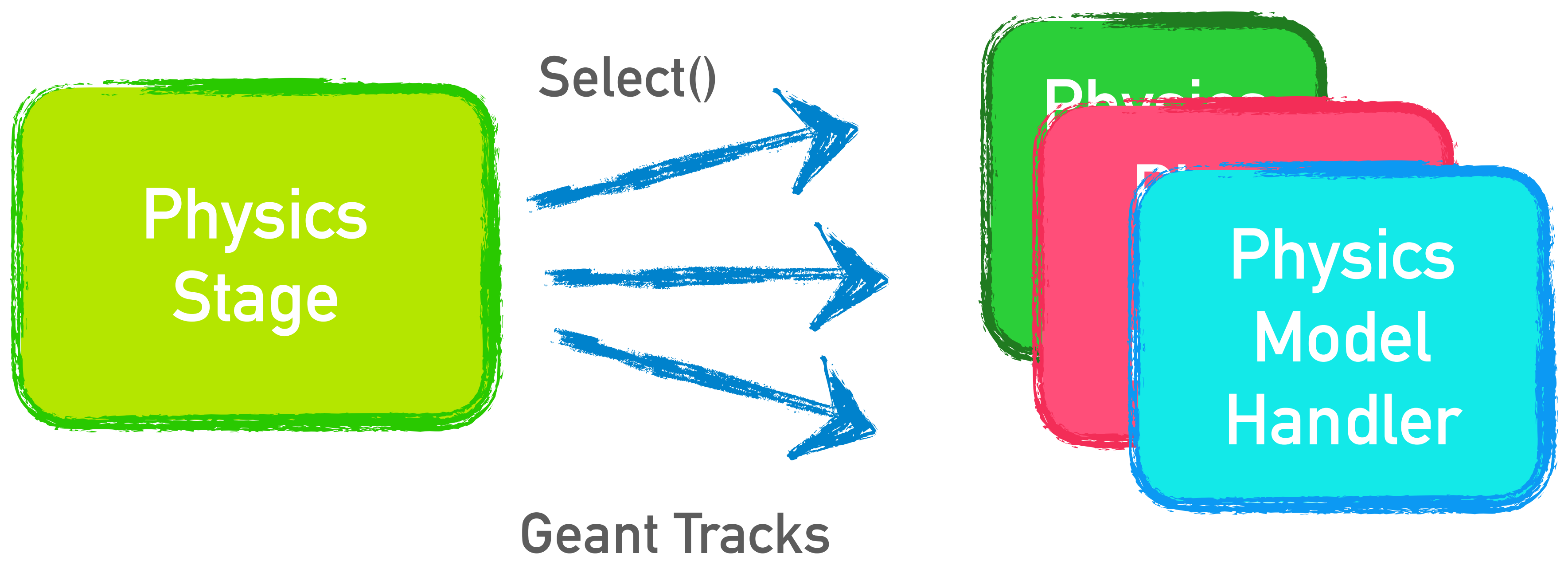

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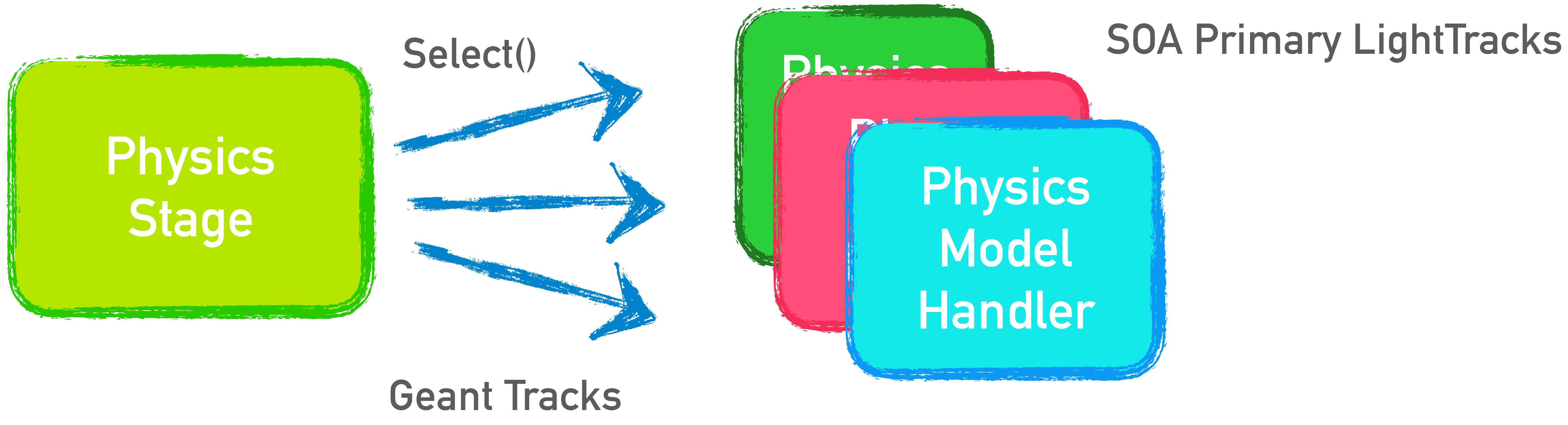

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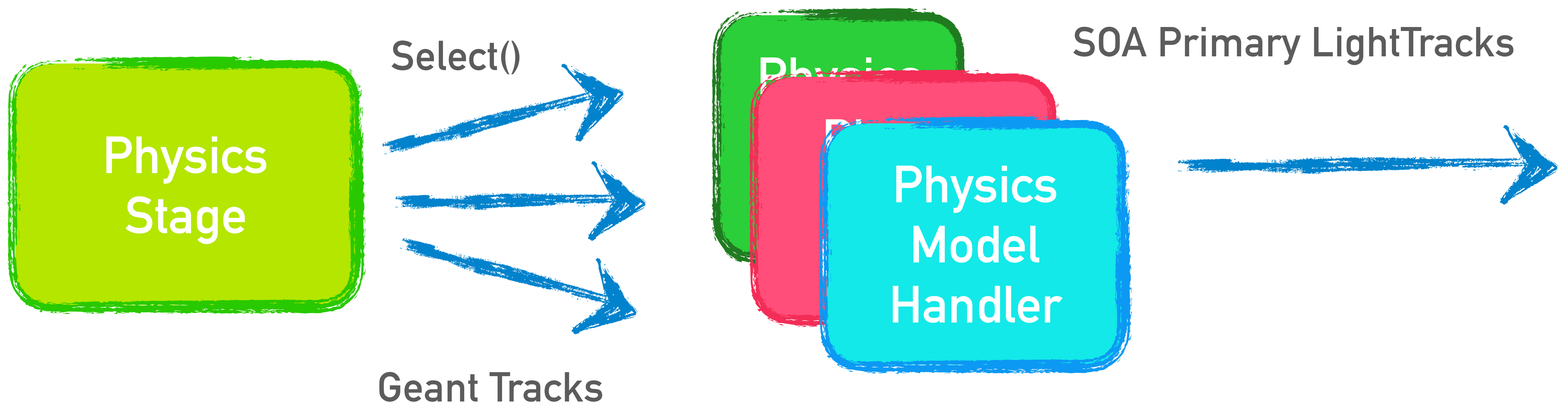

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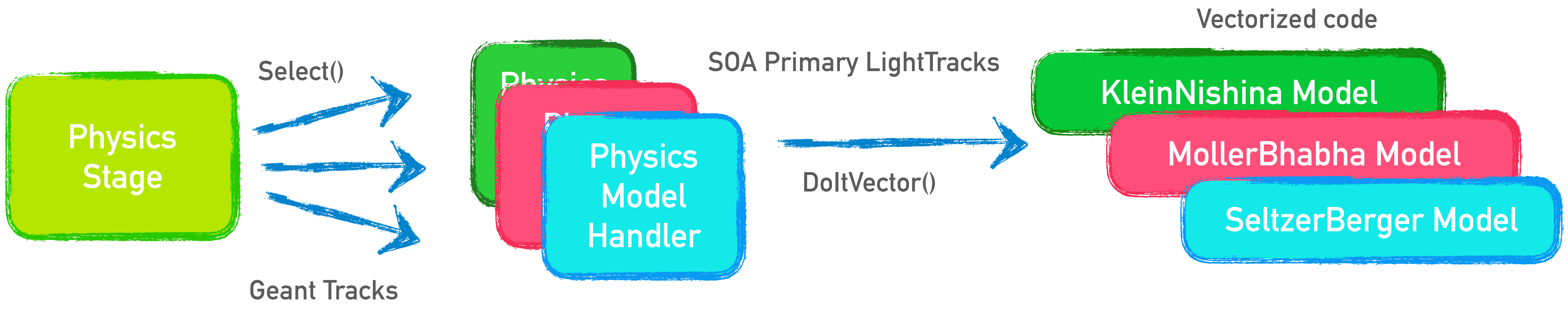

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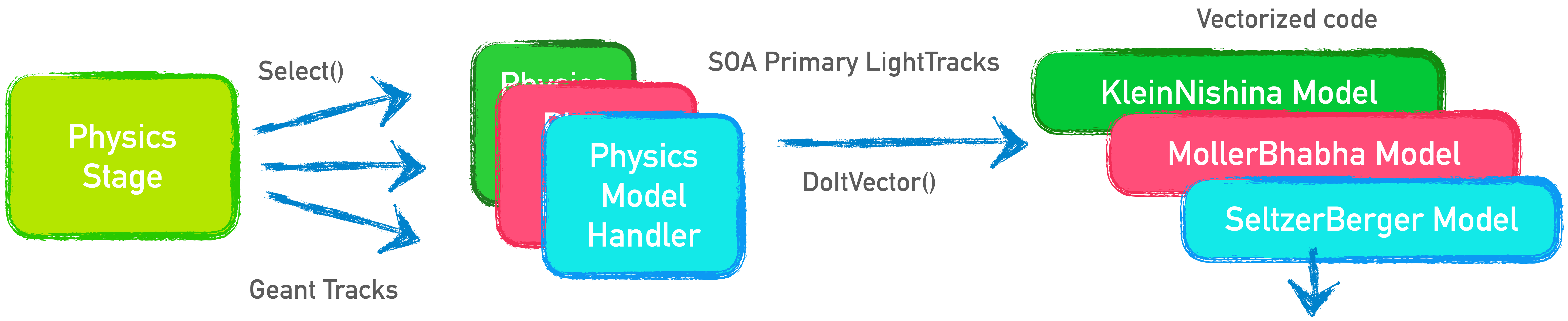

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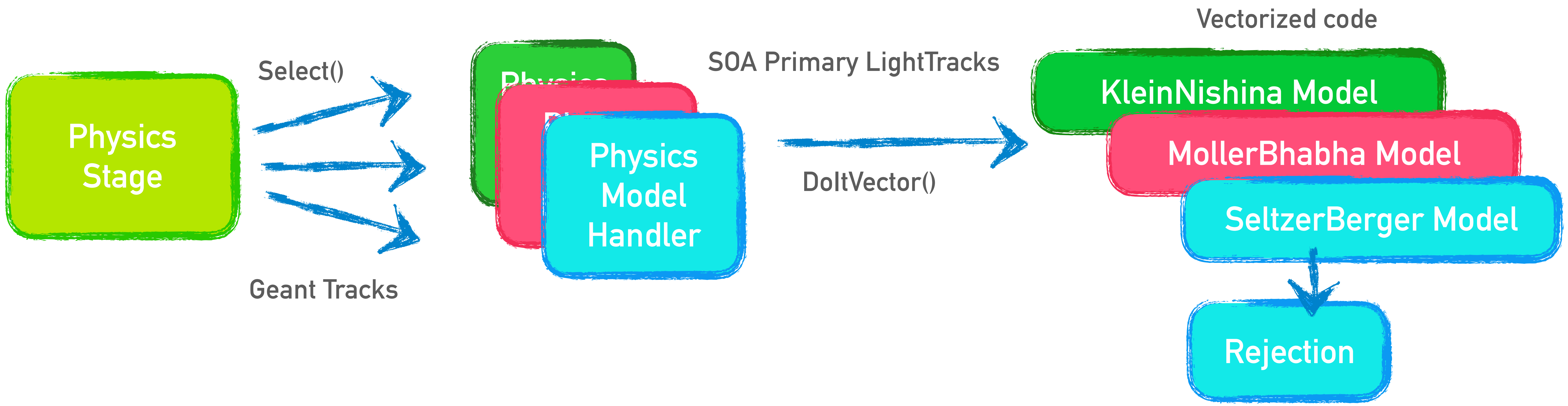

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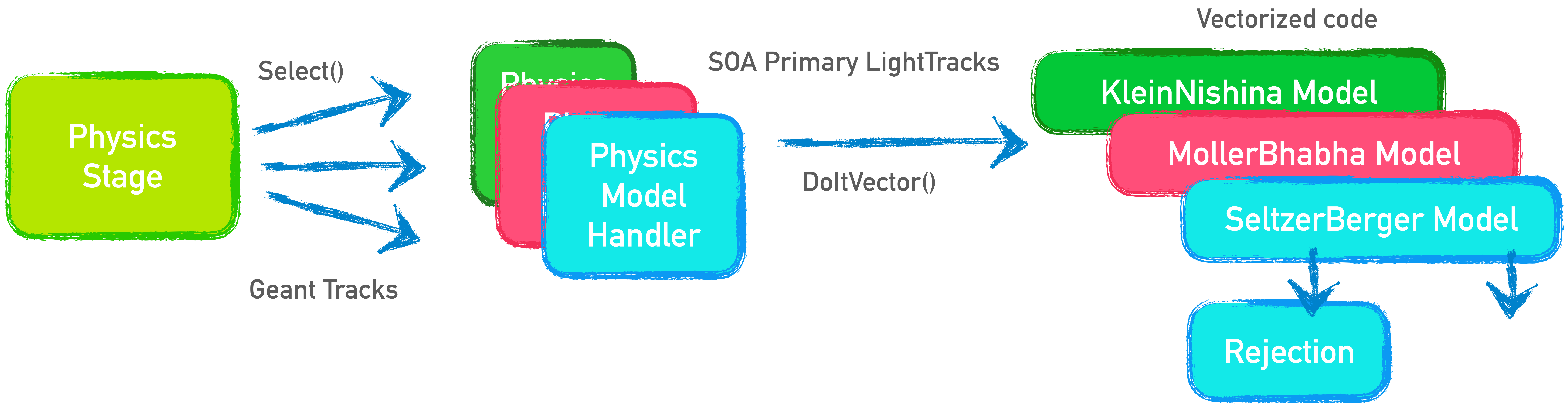

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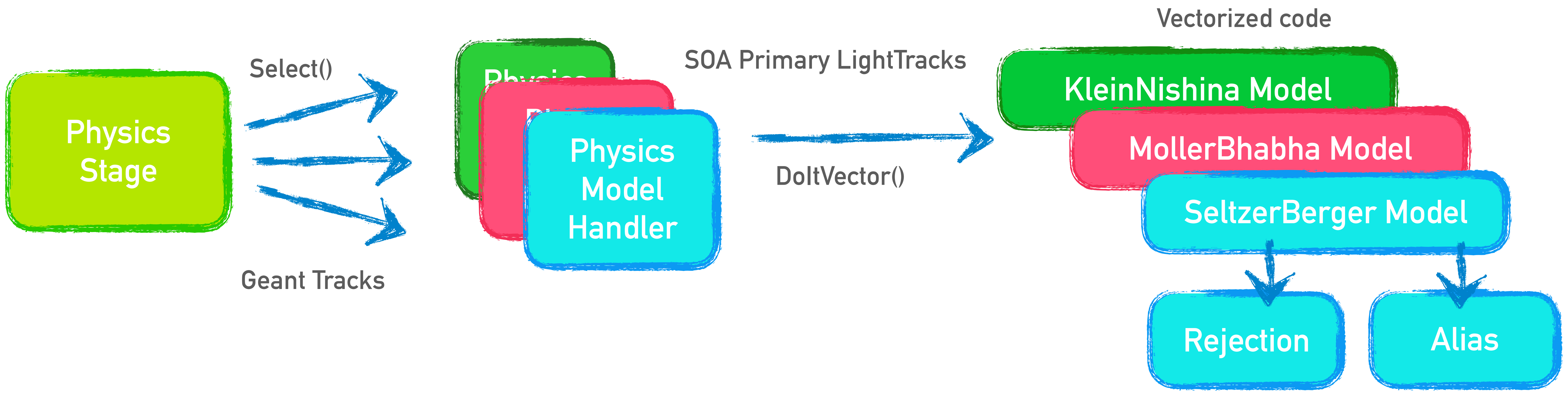

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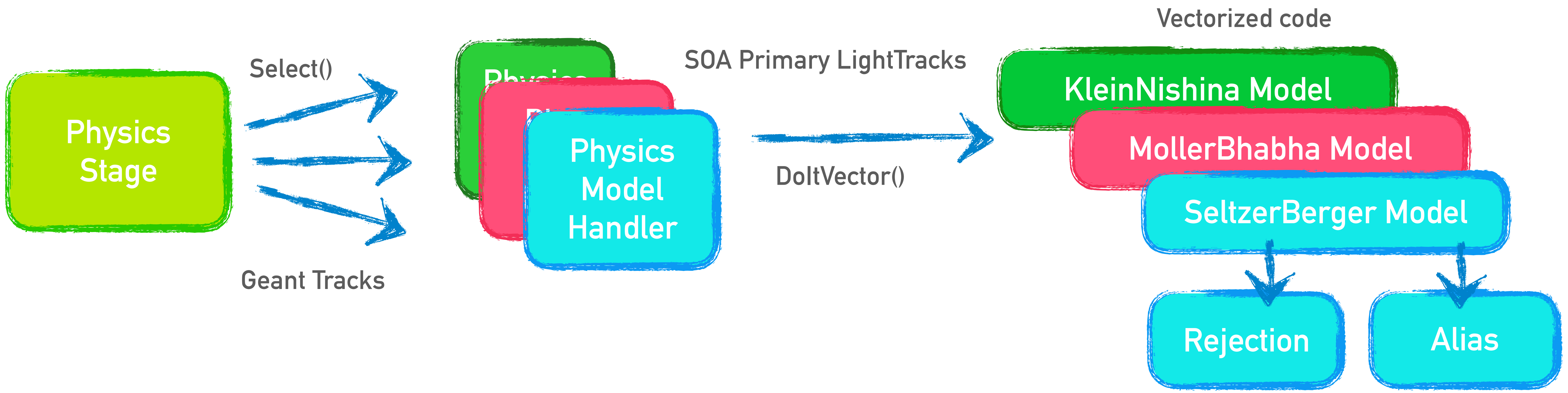

- Differential cross sections are used to update the **kinematic properties** of the primary particle and to **produce secondary particles** (if necessary)
  - Sampling with **Rejection:**
    - **pros:** fast if rejection rate is low, **cons:** unpredictable number of trials
  - Sampling with **Alias** tables + approximation
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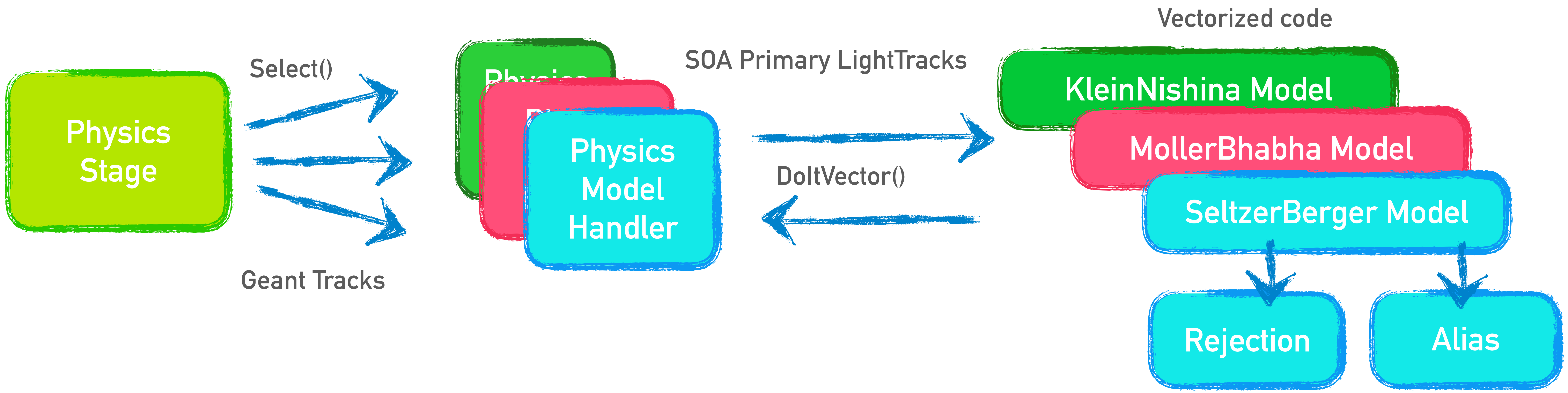

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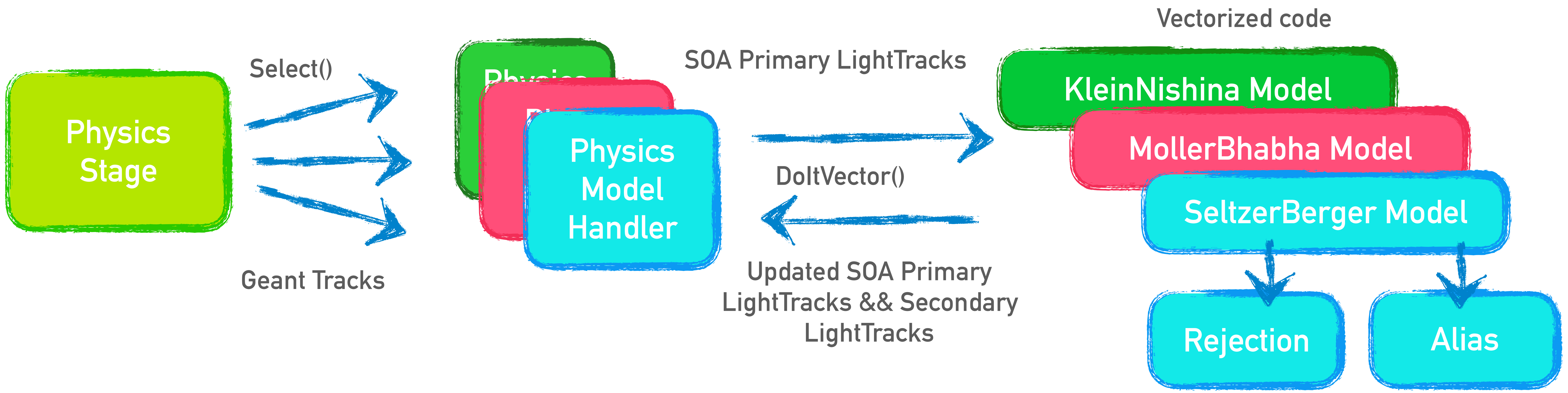

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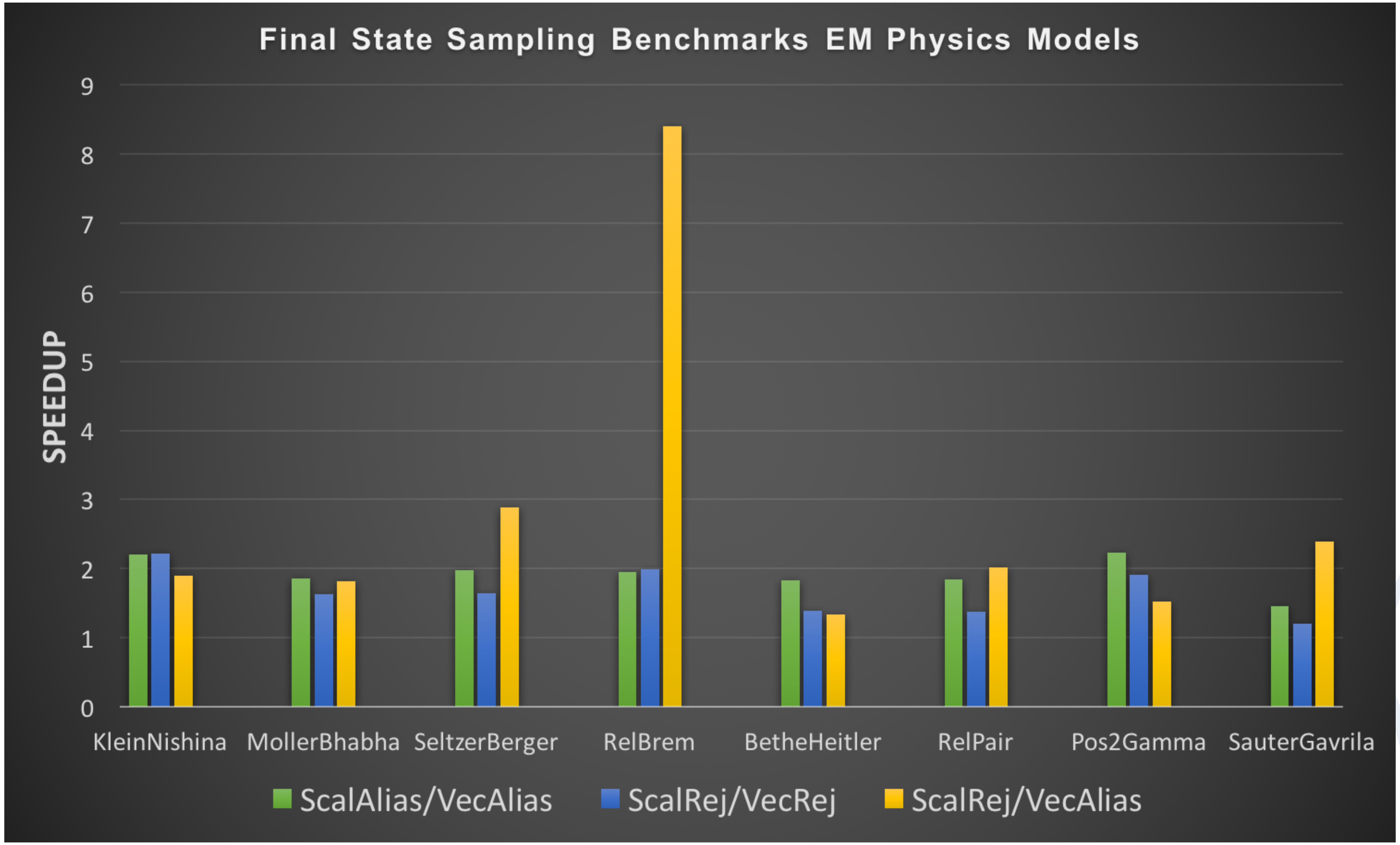
MODEL LEVEL TEST BENCHMARKS

- Specs: Haswell Core i7, AVX, Vc Backend - Detector: Lead - #baskets: 256 - Results with GoogleBenchmarks



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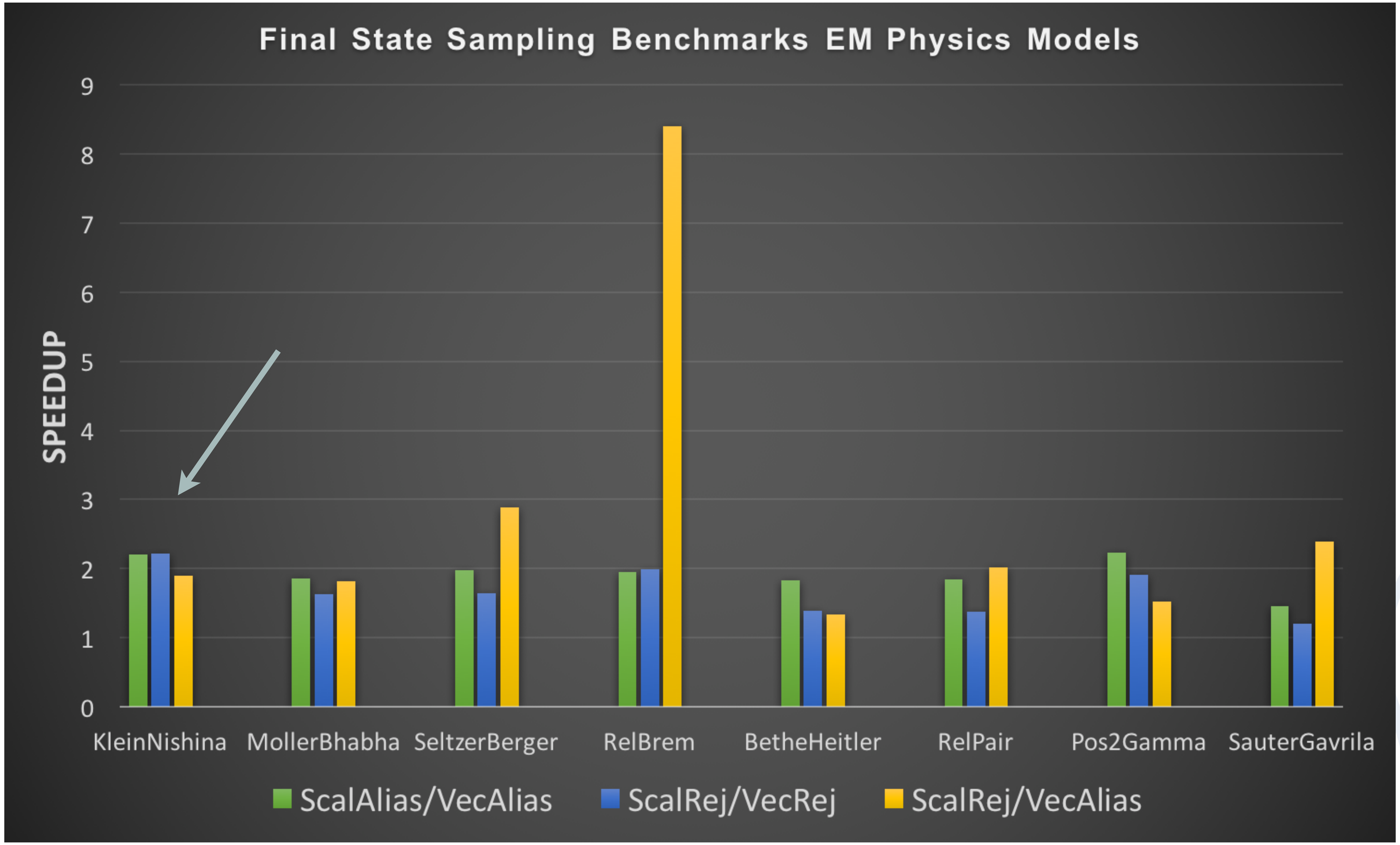

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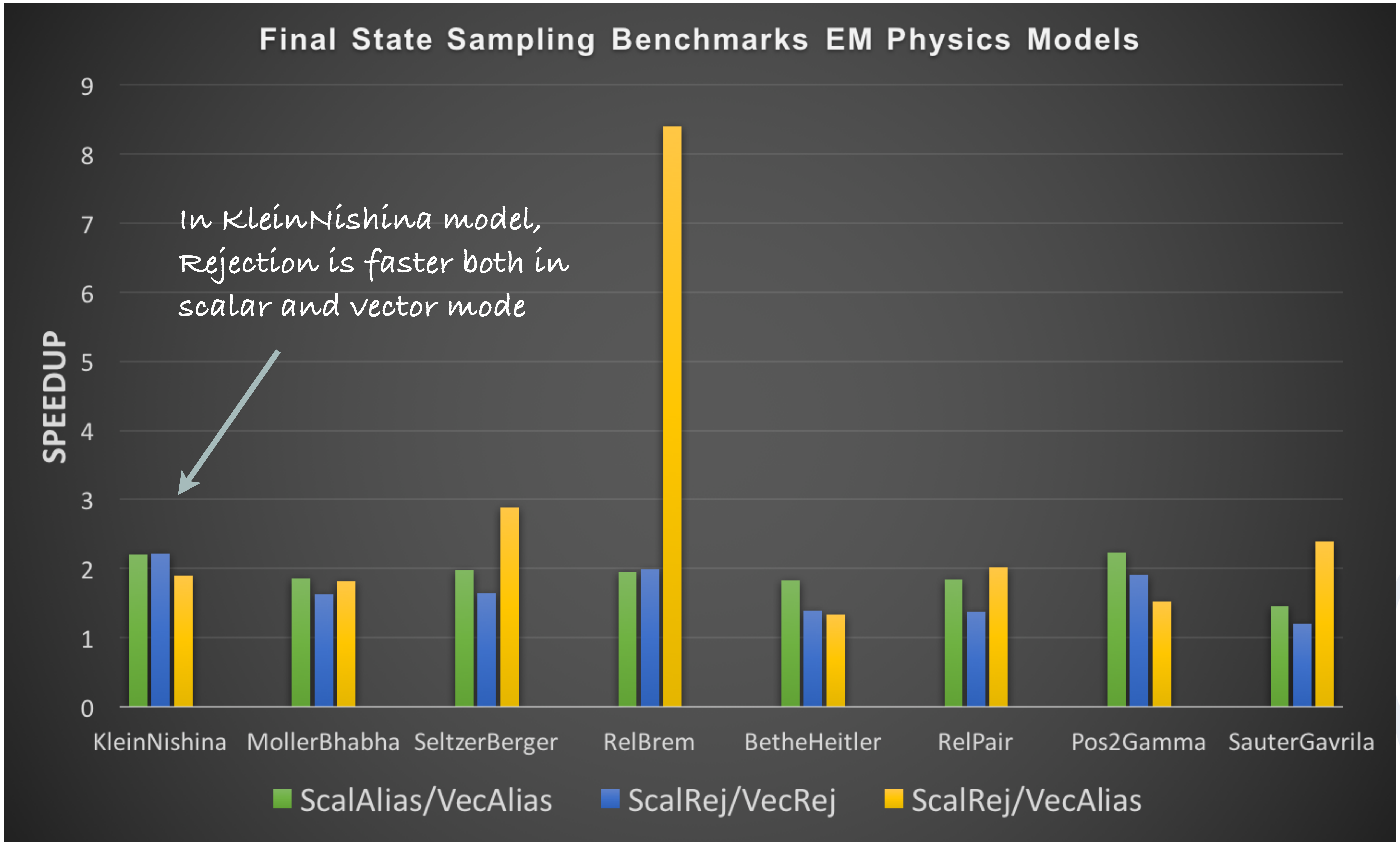

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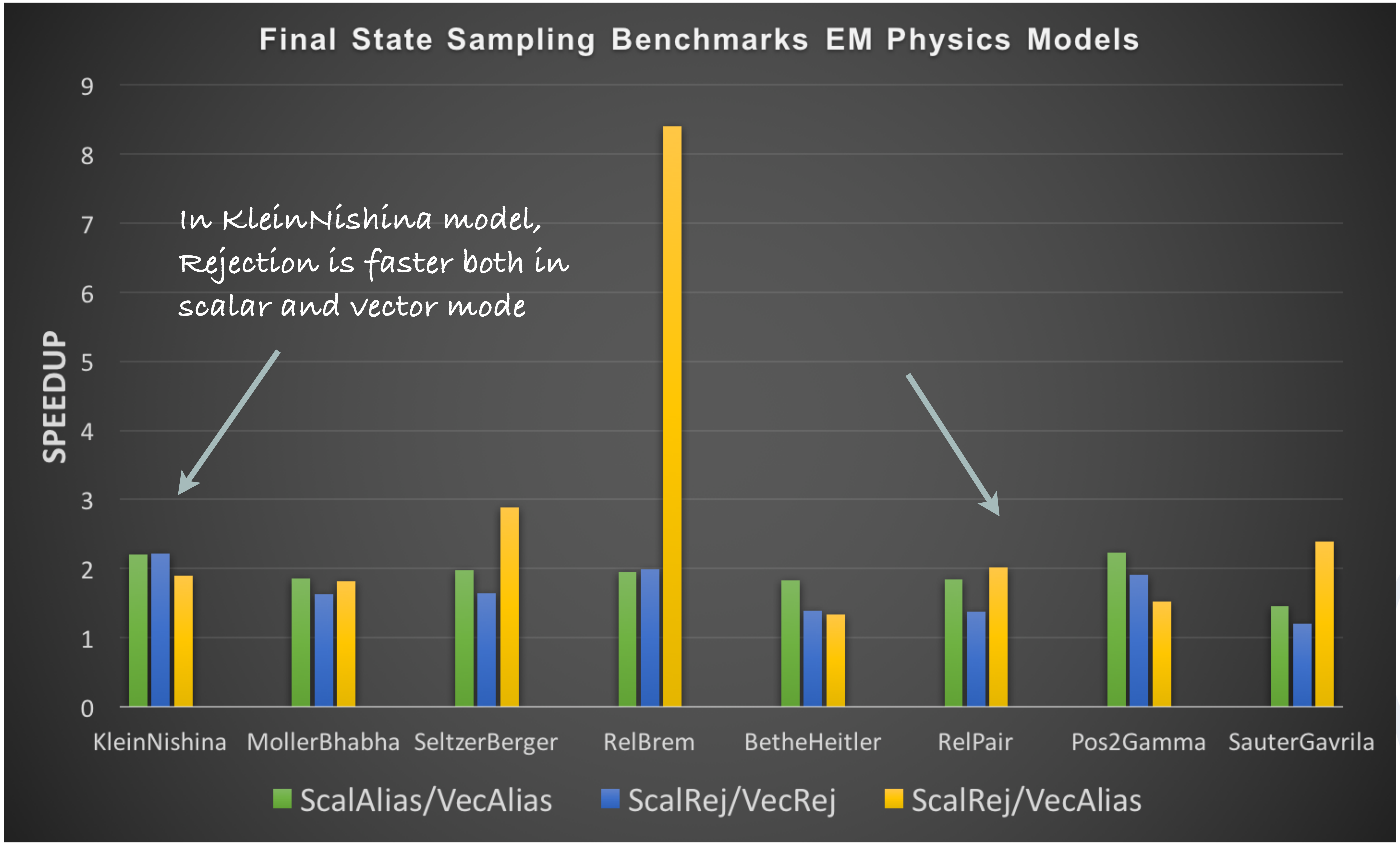

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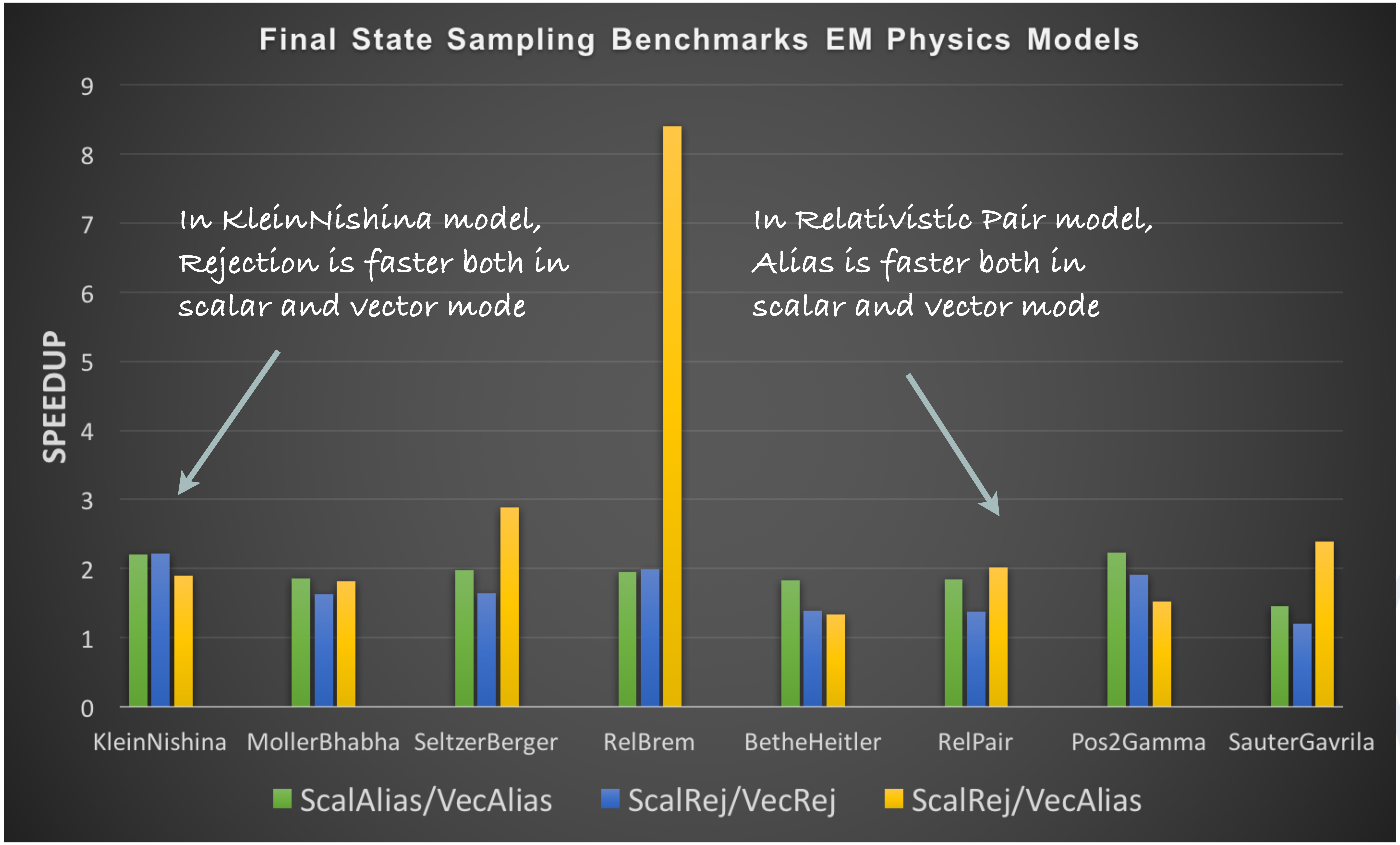

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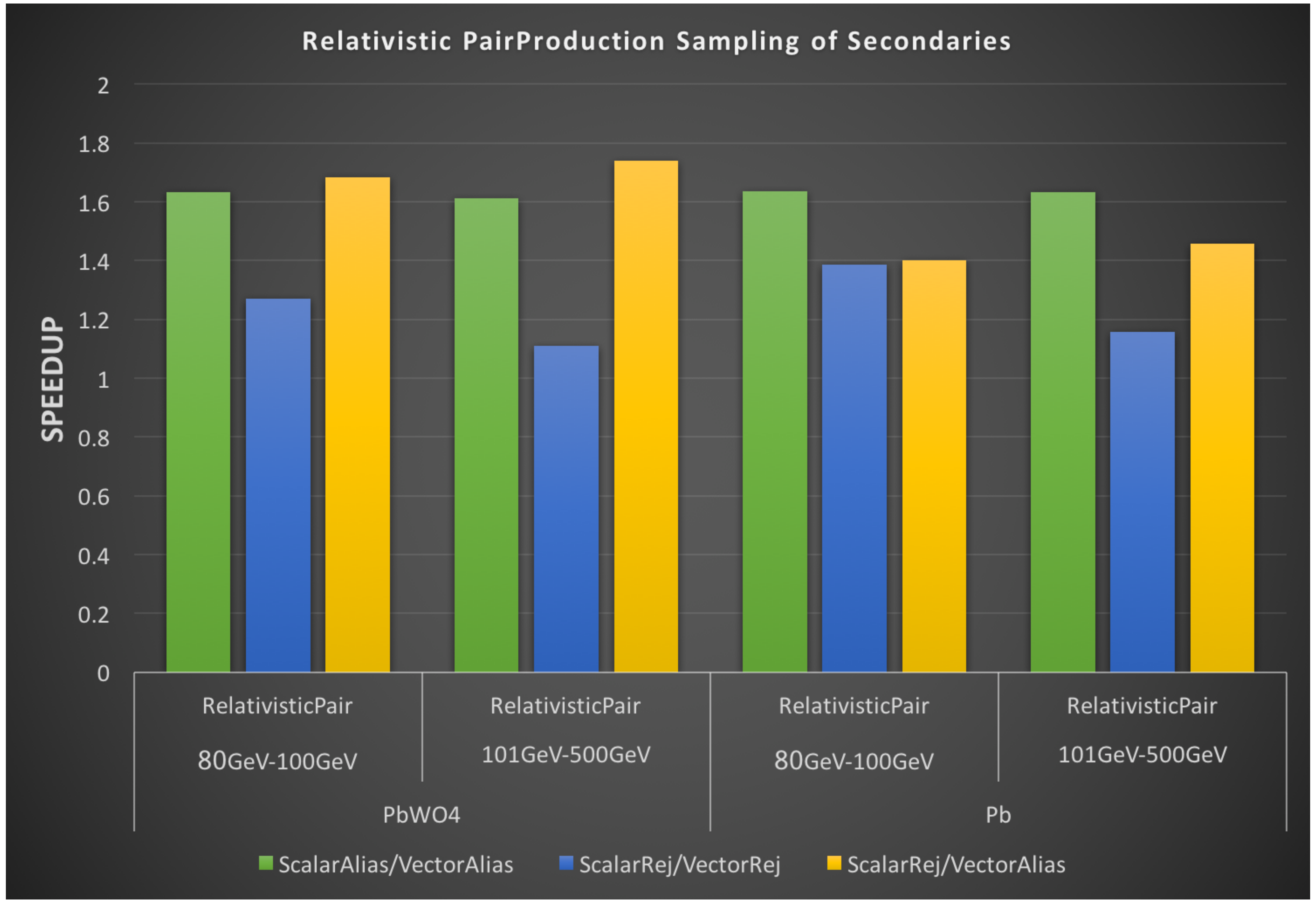
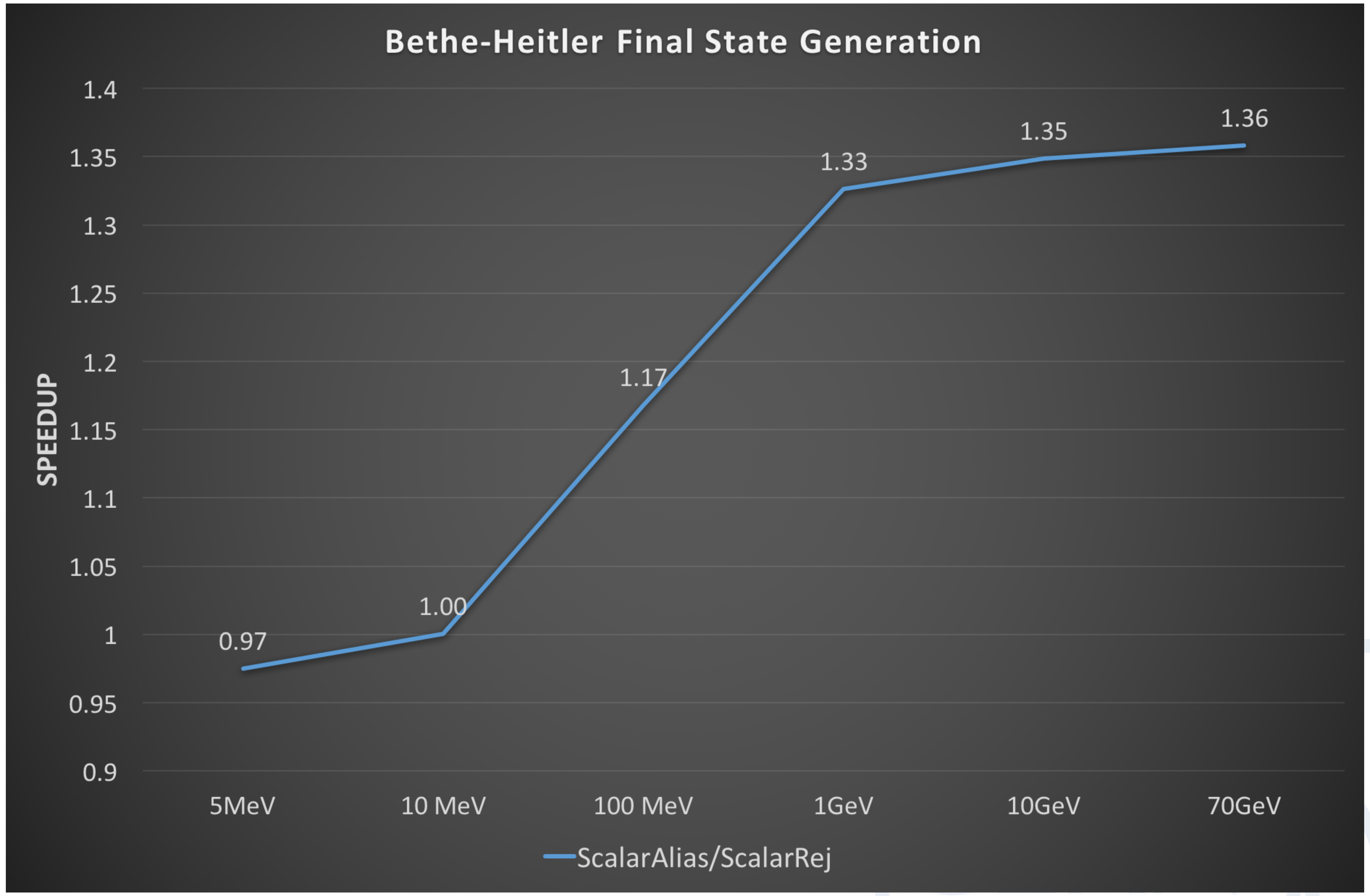
TUNING THE SIMULATION THROUGH MODELS





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Model for Energy Range [80GeV-100TeV]
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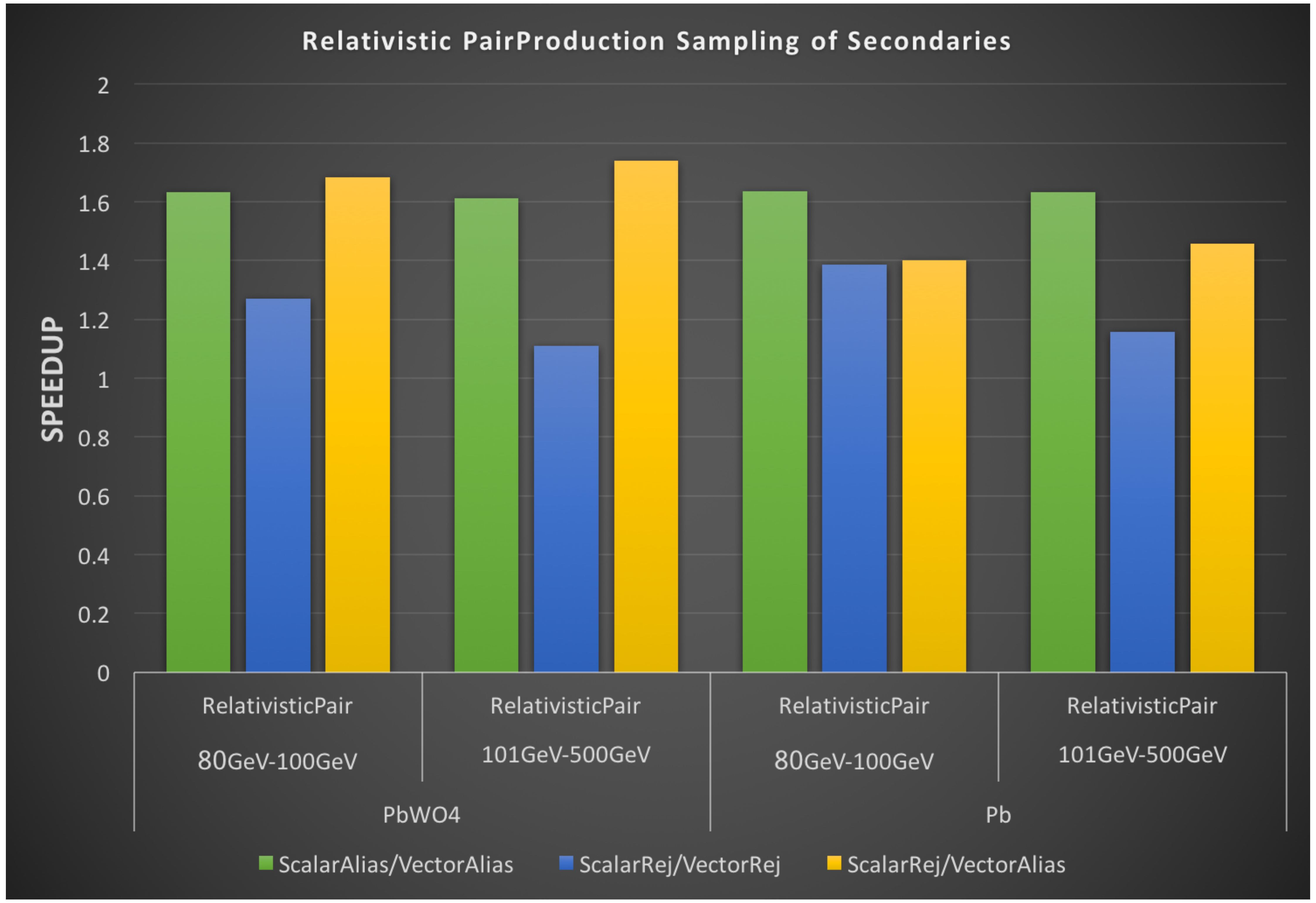

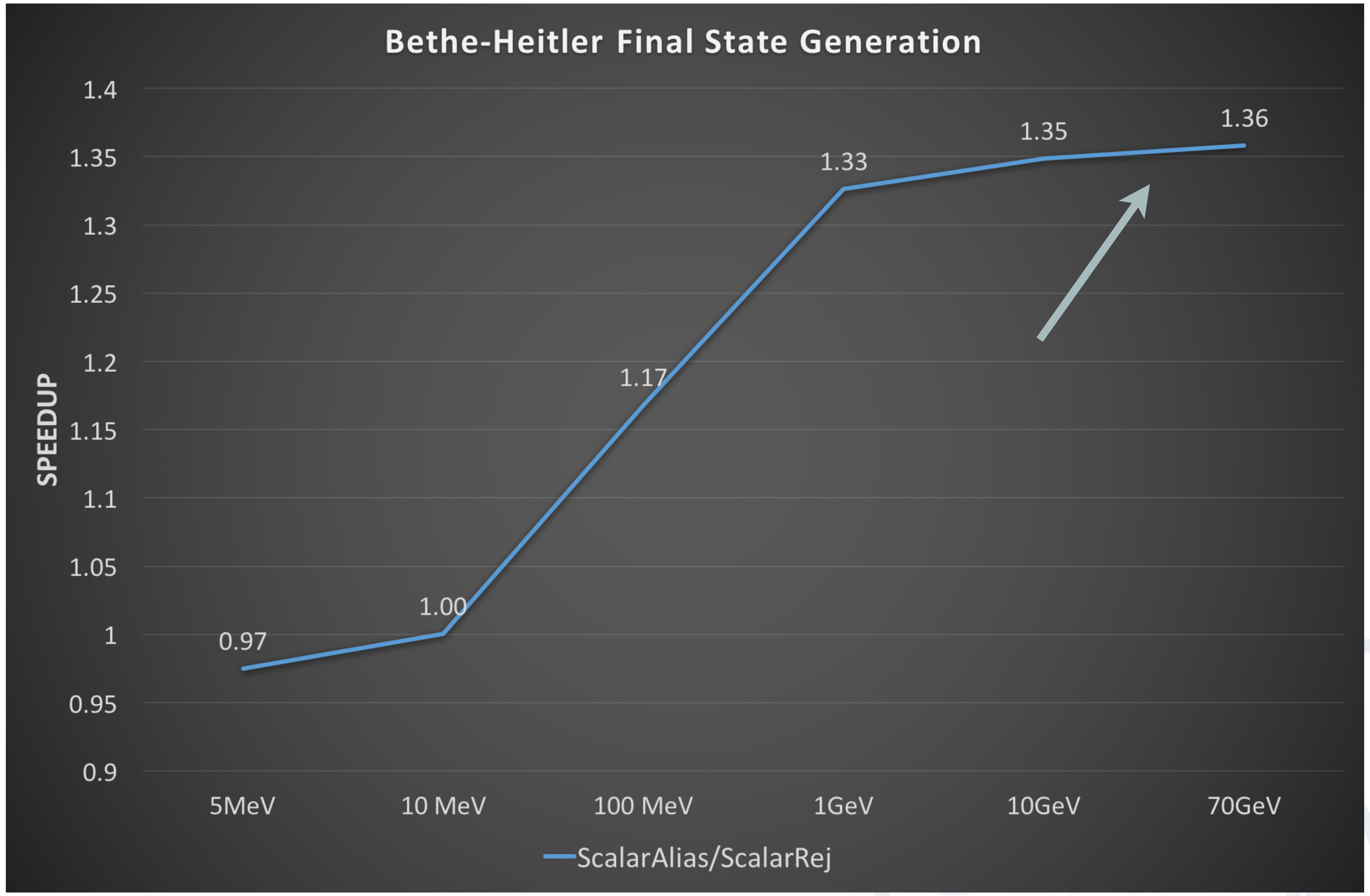

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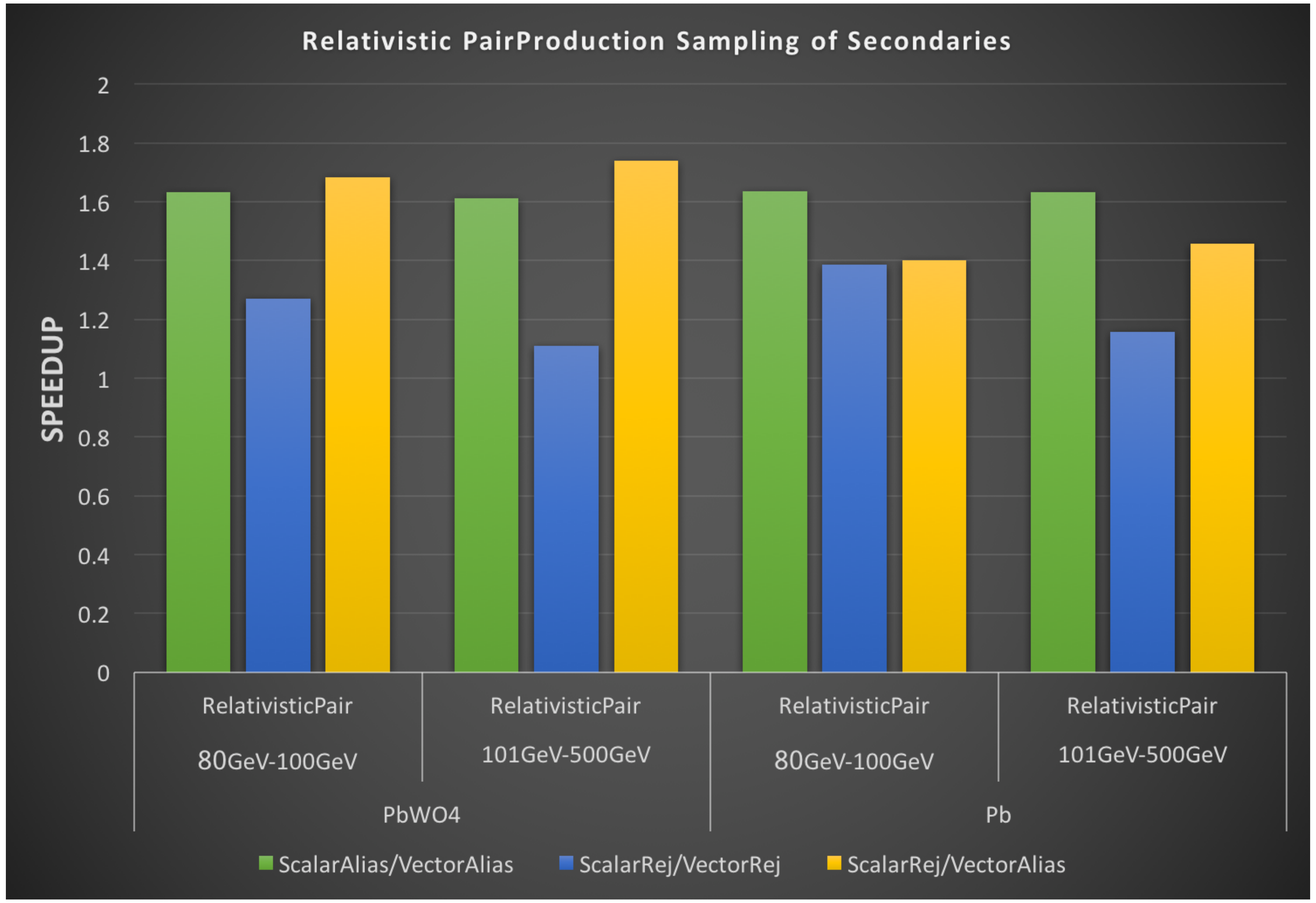

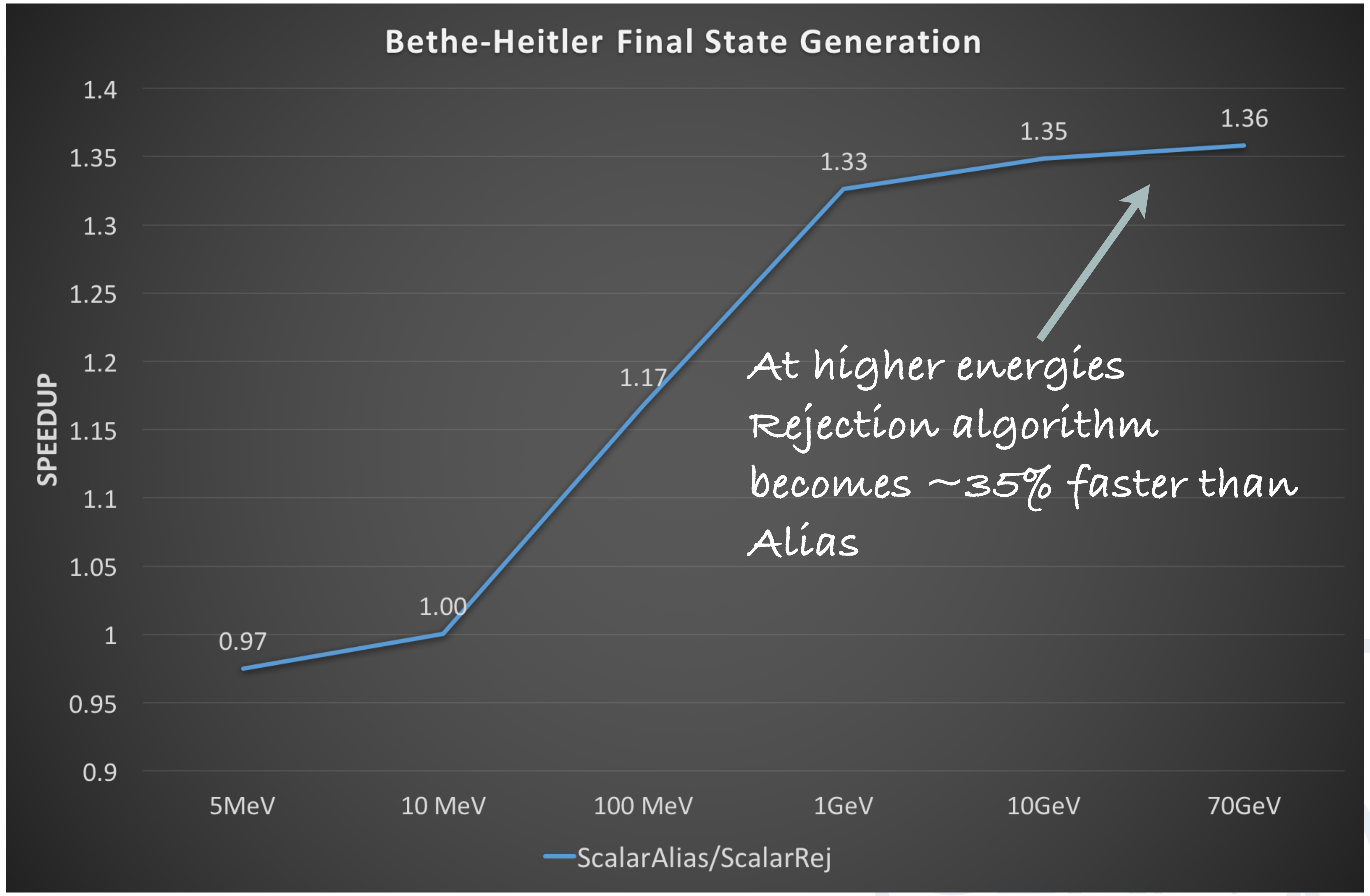

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- EM showers can be **fully simulated** in GeantV
  - Most of the EM models are now **vectorized** (work in progress on multiple scattering)
- **SpeedUp : there is no generic solution**
  - Final-state EM Model level: between **1.5-3** on Haswell, **2-4** on Skylake with AVX2
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- **VecMath library** and **Vectorized pRNG** (handling reproducibility issues)
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GeantV website: http://geant.cern.ch

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- **CERN**: G. Amadio, J. Apostolakis, M. Bandieramonte, R. Brun, F. Carminati, G. Cosmo, A. Gheata, M. Gheata, I. Goulas, V. Ivantchenko, F. Hariri, P.R. Karpinski, G.R. Khattak, D. Konstantinov, P. Mato, P. Mendez, K.Nikolics, M. Novak, W. Pokorski, A. Ribon, O. Shadura, S. Vallecorsa, S. Wenzel
- **CIC-IPN (Mexico)**: J. Martínez Castro, A. Miranda Aguillar
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alpha release is out!

THANKS FOR THE ATTENTION!

QUESTIONS?

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BACKUP

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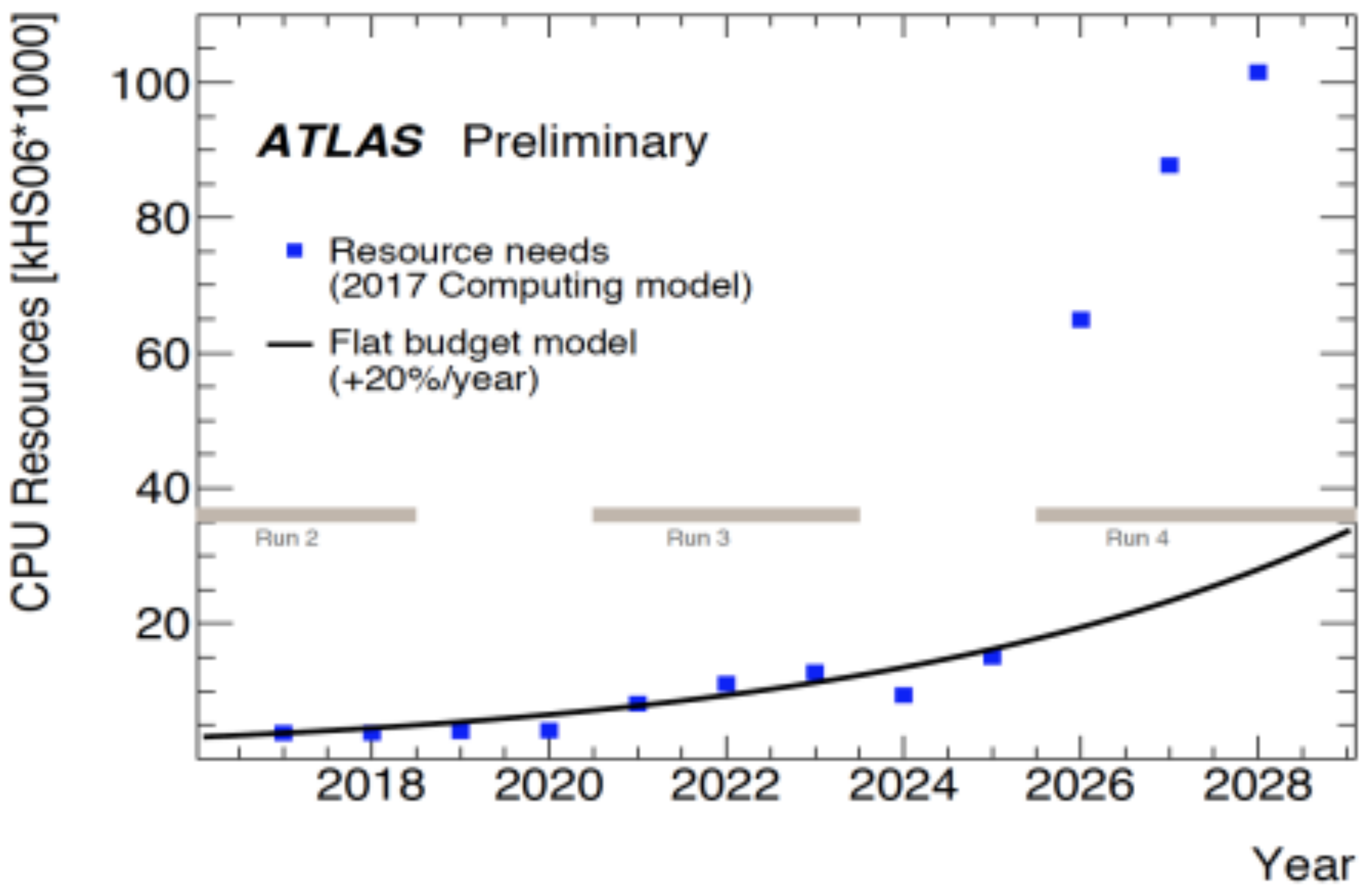
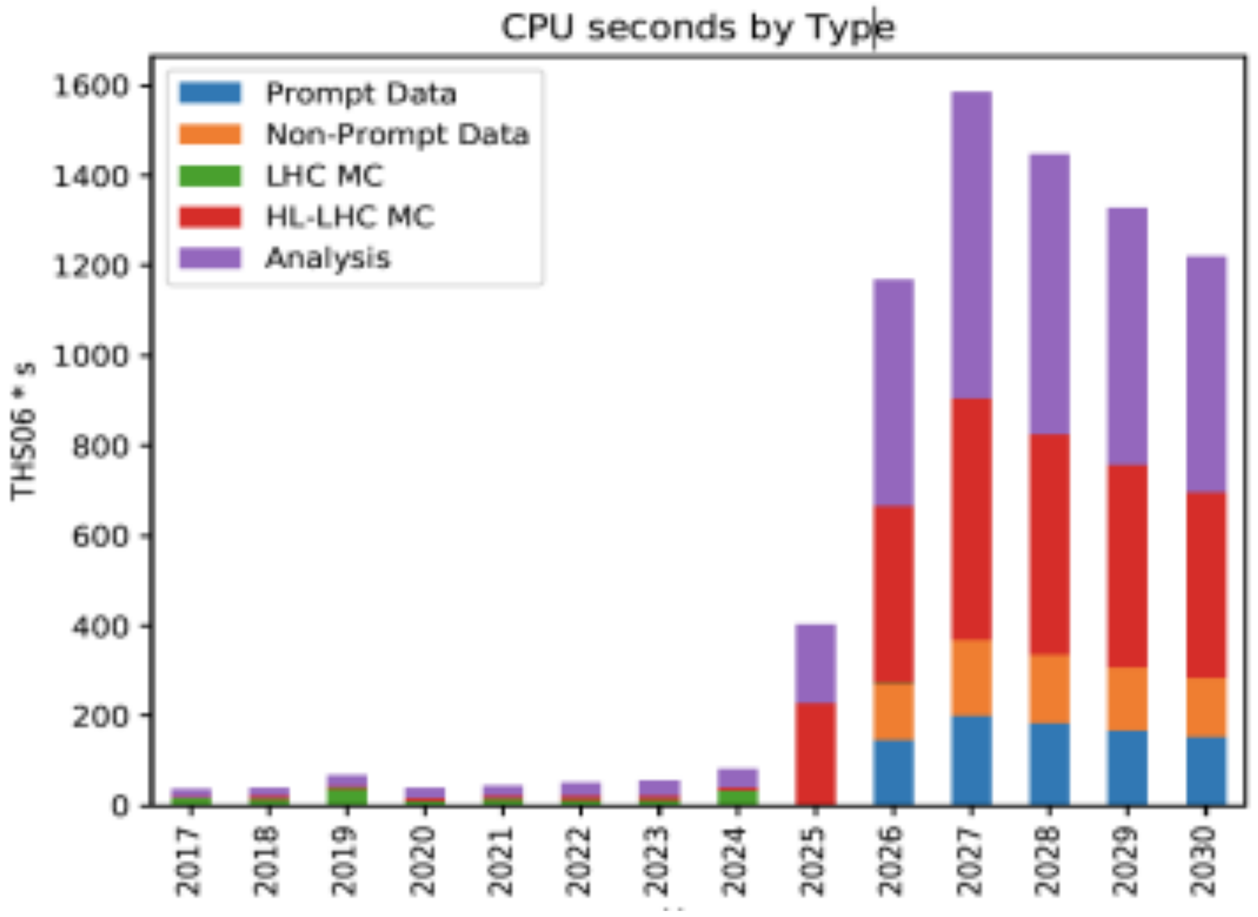
NEED FOR FASTER SIMULATION CODE FOR HEP COMMUNITY

- 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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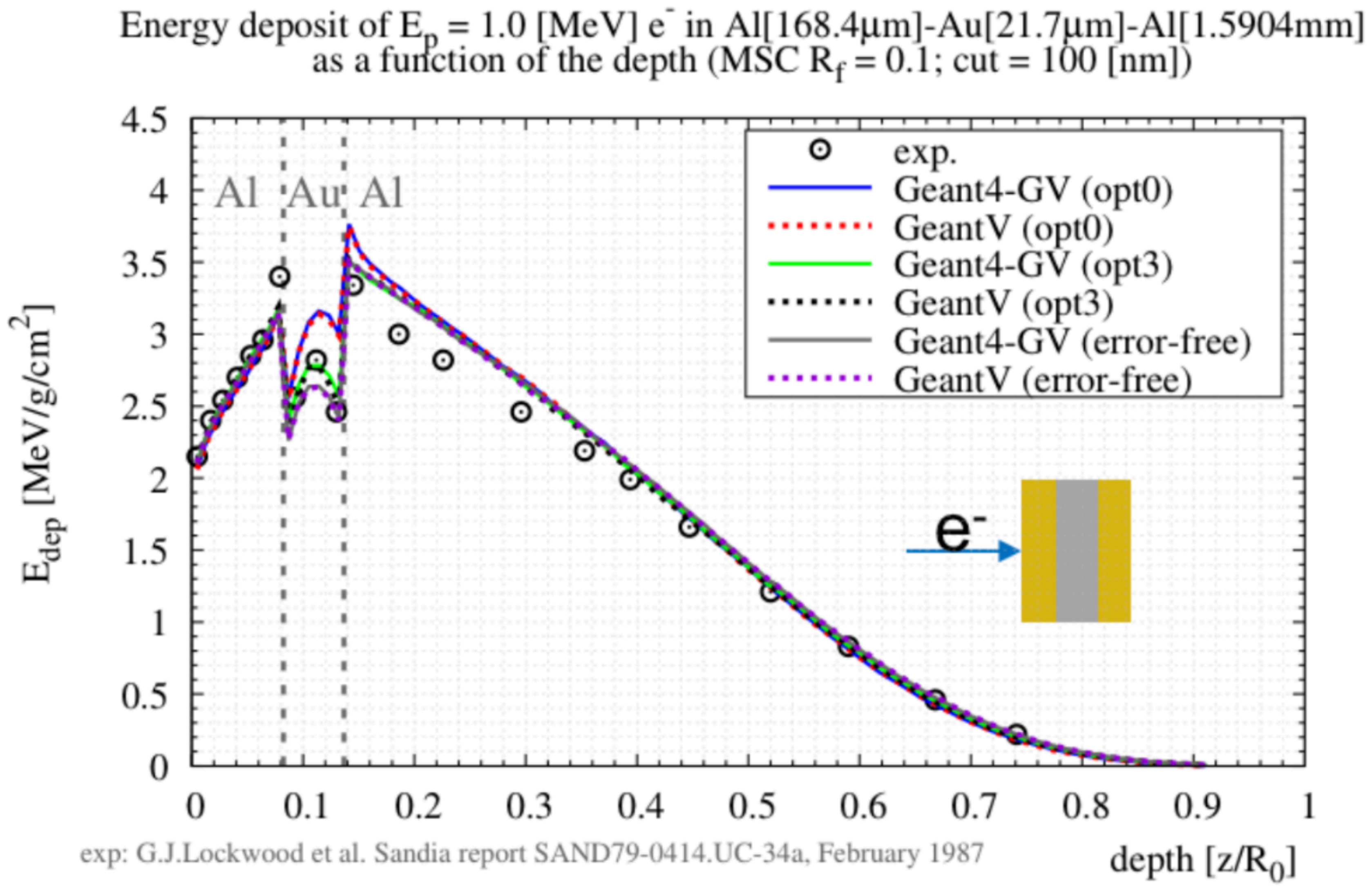
EM PHYSICS MODELS VALIDATION



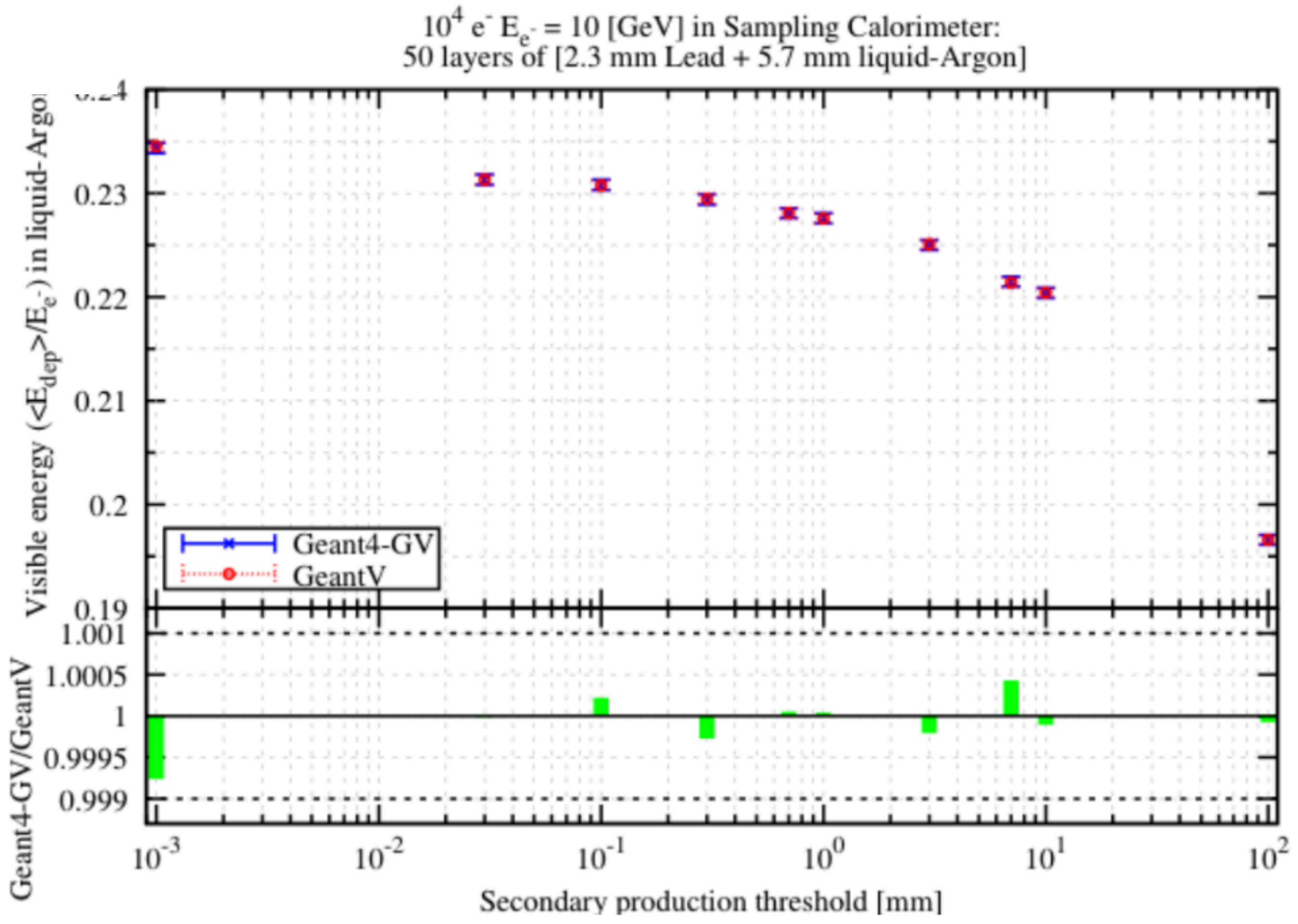
Multi-layered target

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; γ: 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

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



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

ATLAS simplified sampling calorimeter

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.

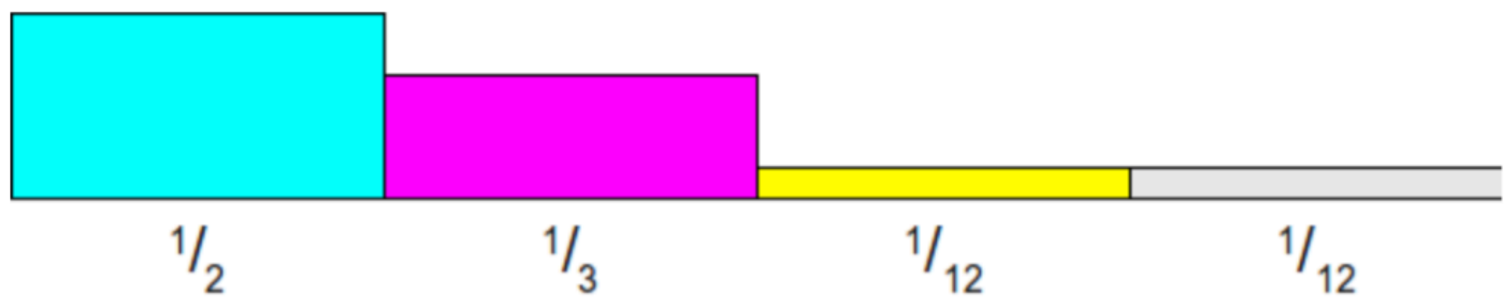
**

RESULTS: MODEL LEVEL TEST BENCHMARKS

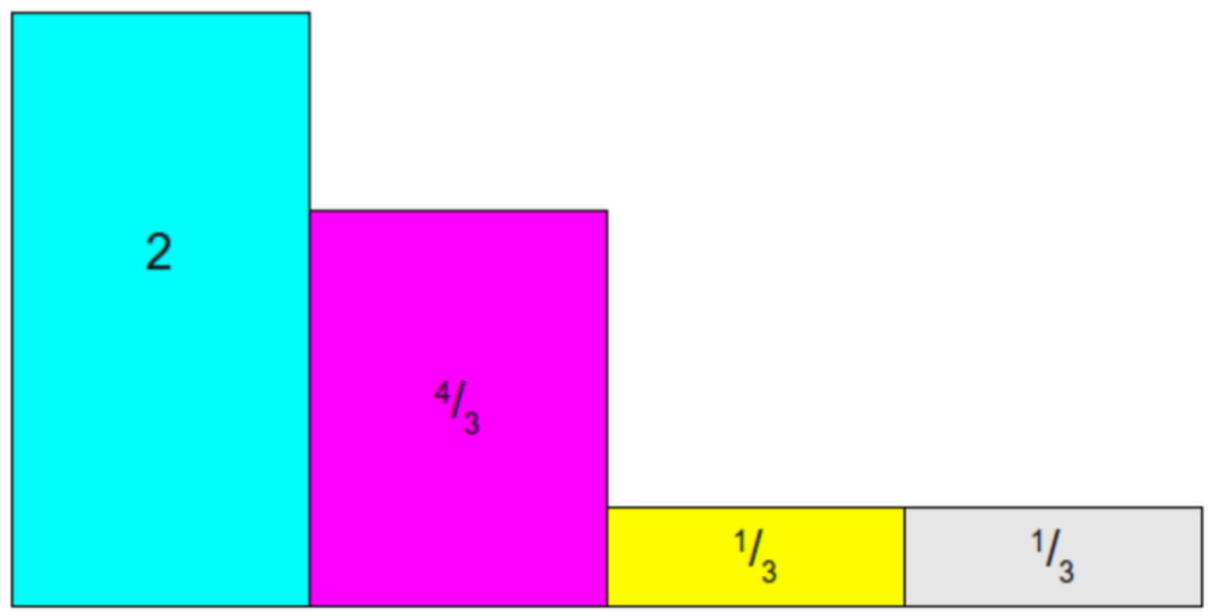
Model	Haswell (avx)	
	Scalar Time [ms]	SpeedUp
Klein-Nishina alias	56.4	2.2
Klein-Nishina rej	48.37	2.21
Moller-Bhabba alias	51.32	1.85
Moller-Bhabba rej	50.21	1.62
Seltzer-Berger brems alias	73.19	1.98
Seltzer-Berger brems rej	106.63	1.64
Relativistic brems alias	76.96	2
Relativistic brems rej	330.57	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

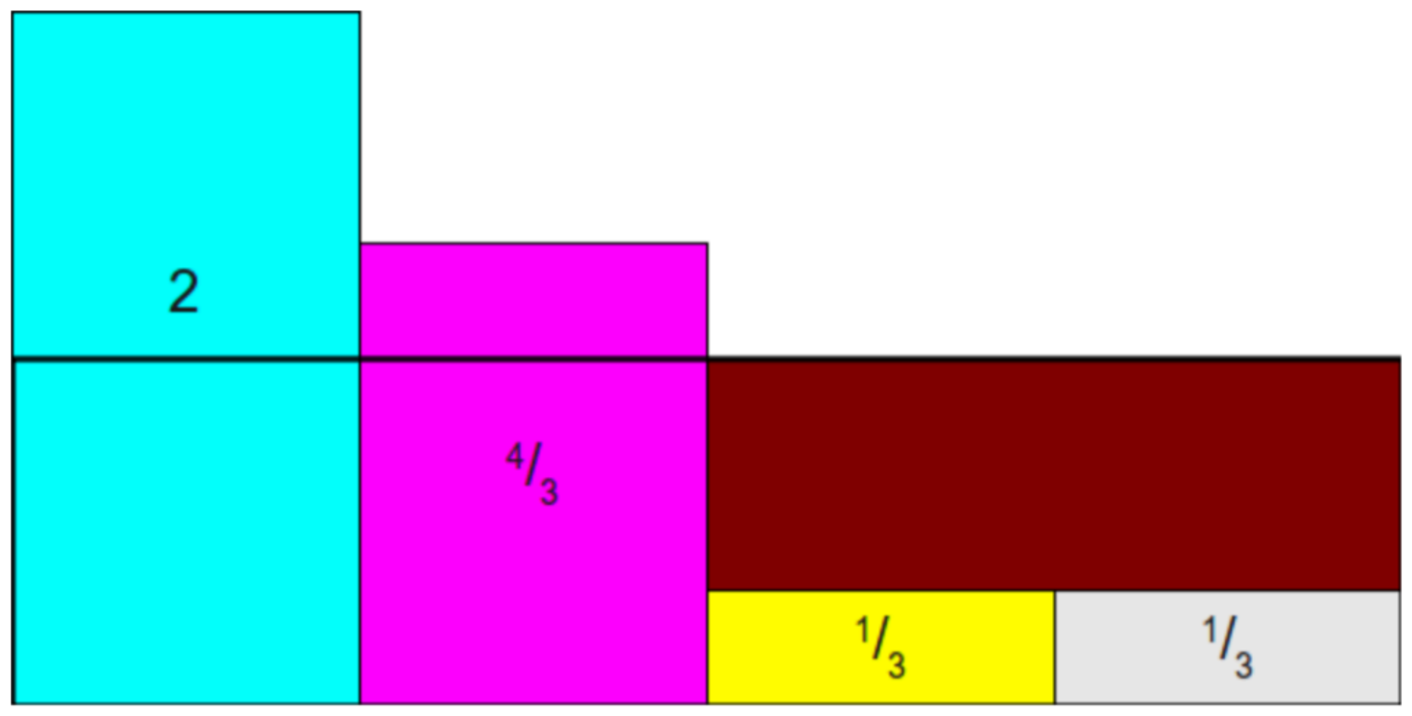
ALIAS SAMPLING



Initial pdf (equal likelihood=1/4)



Scaled probabilities so that a prob of 1/4 would weight 1



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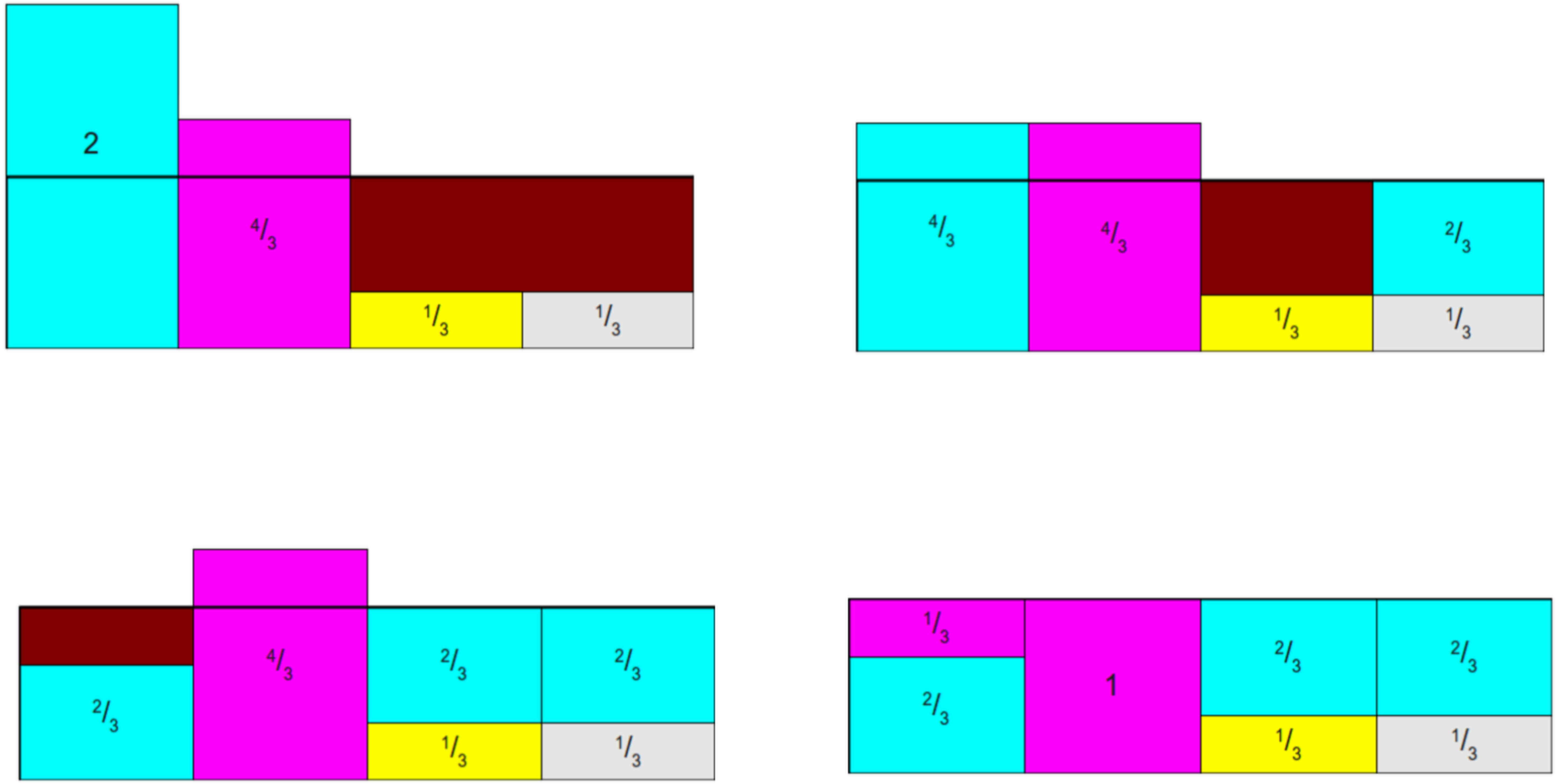

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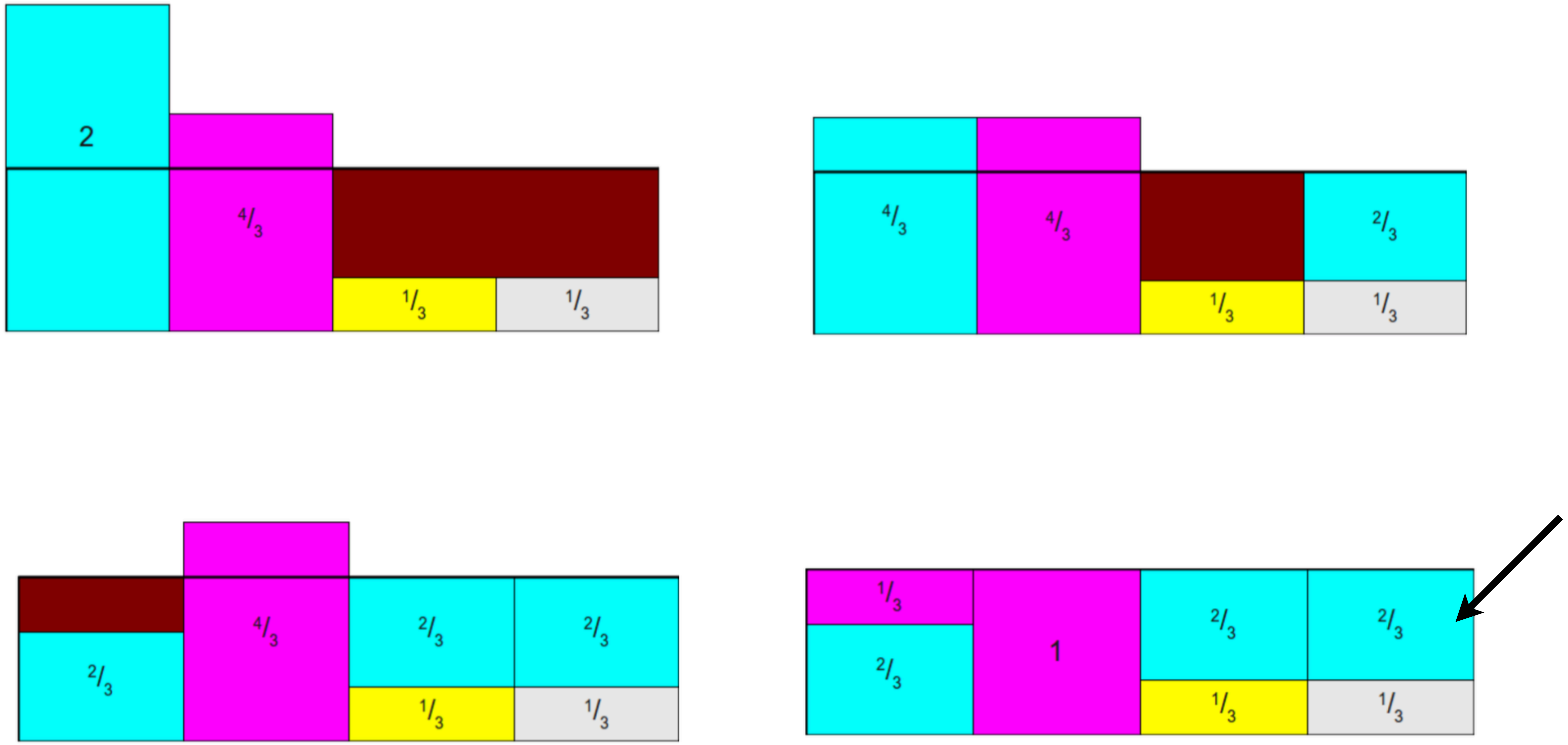
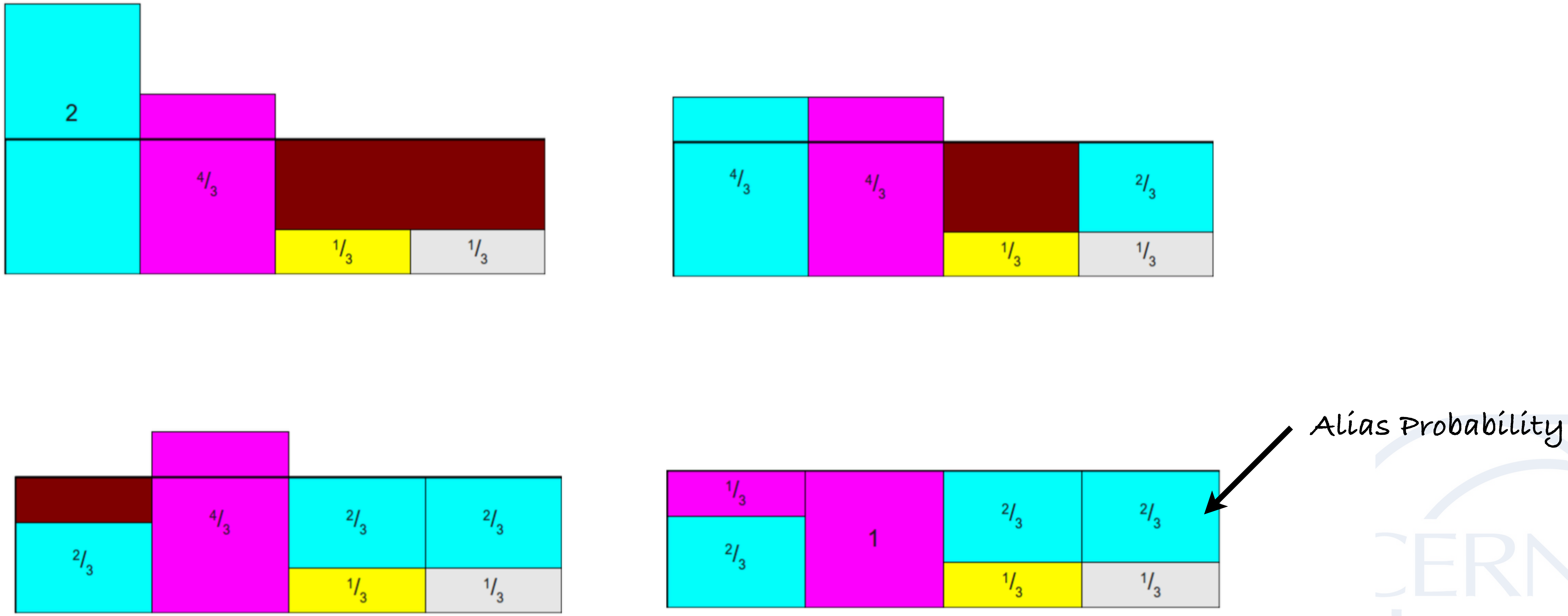
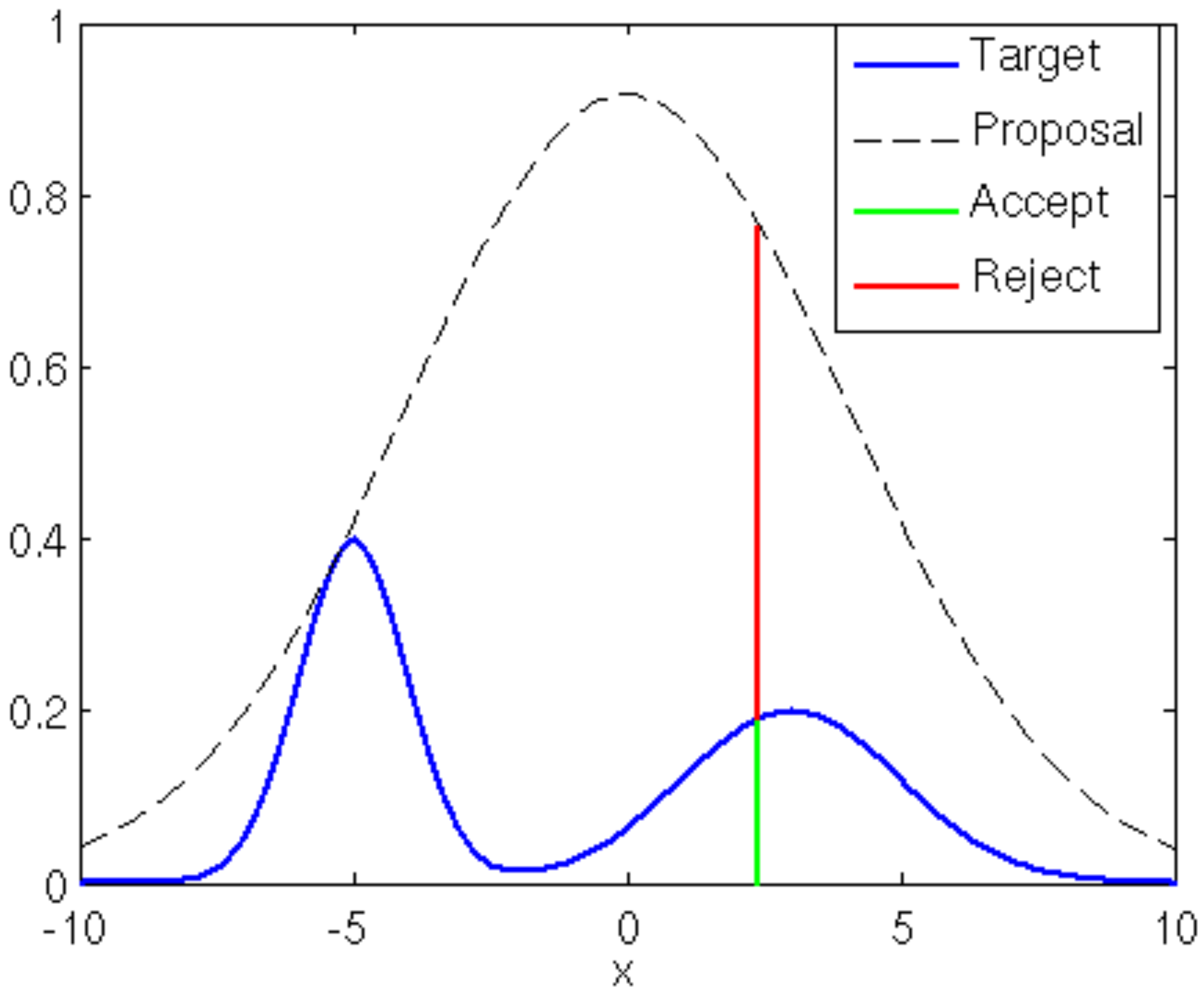


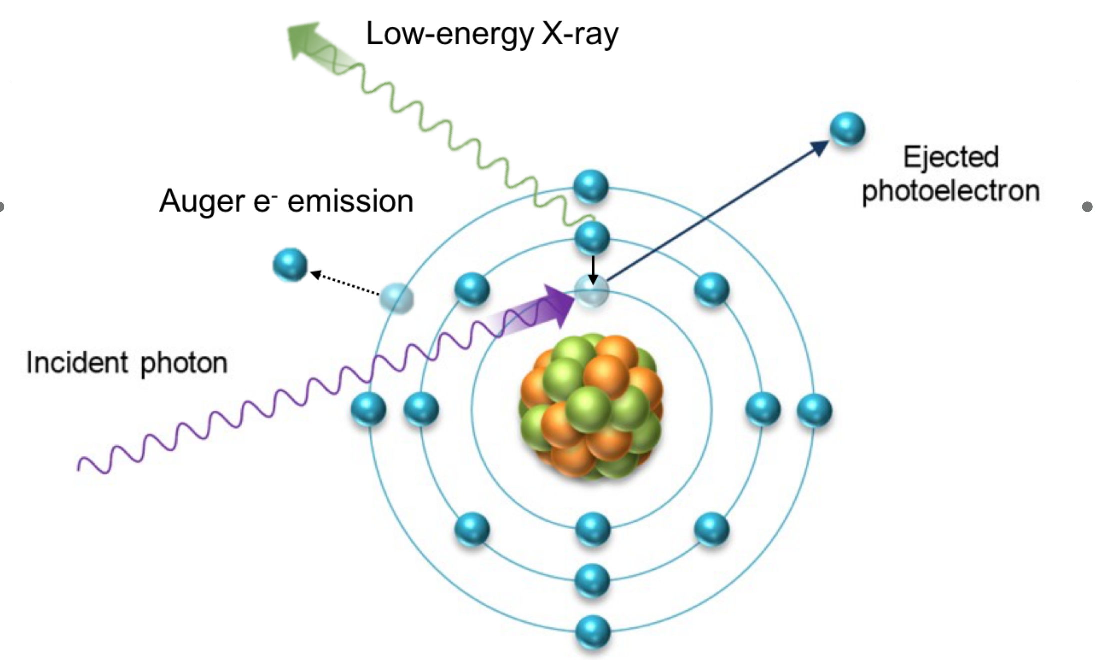
ALIAS SAMPLING



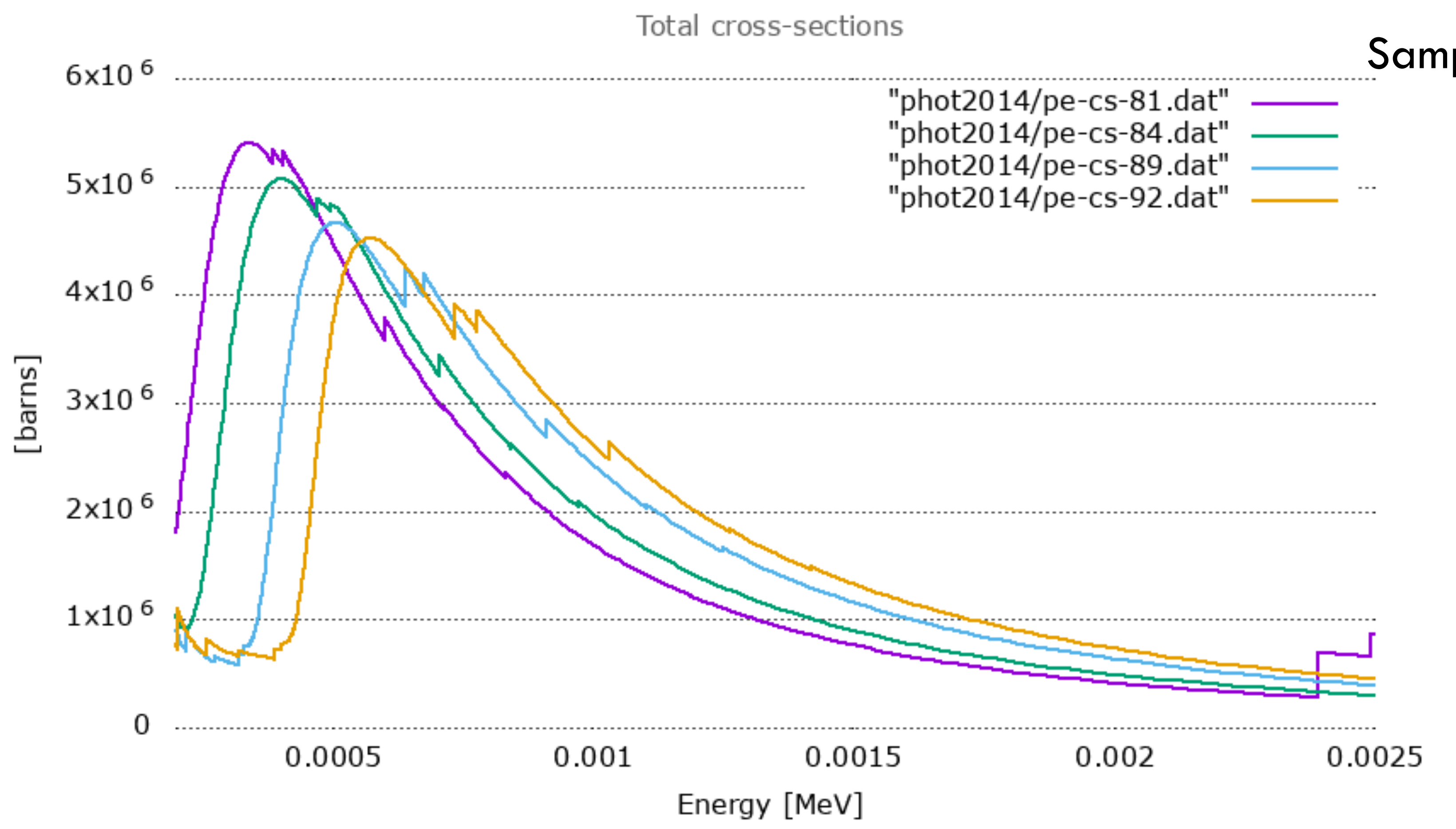
REJECTION SAMPLING

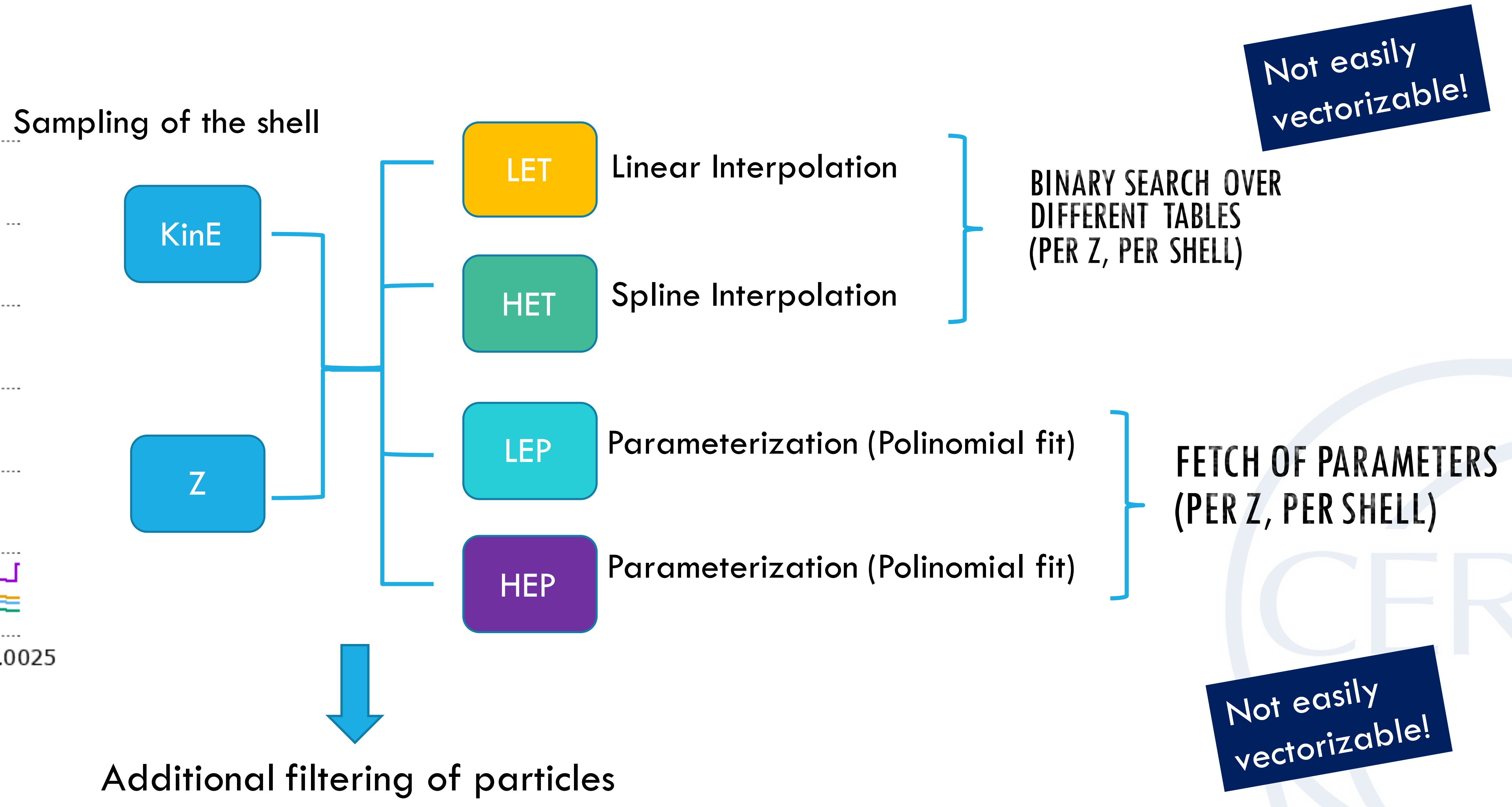


EXAMPLE: PE EFFECT

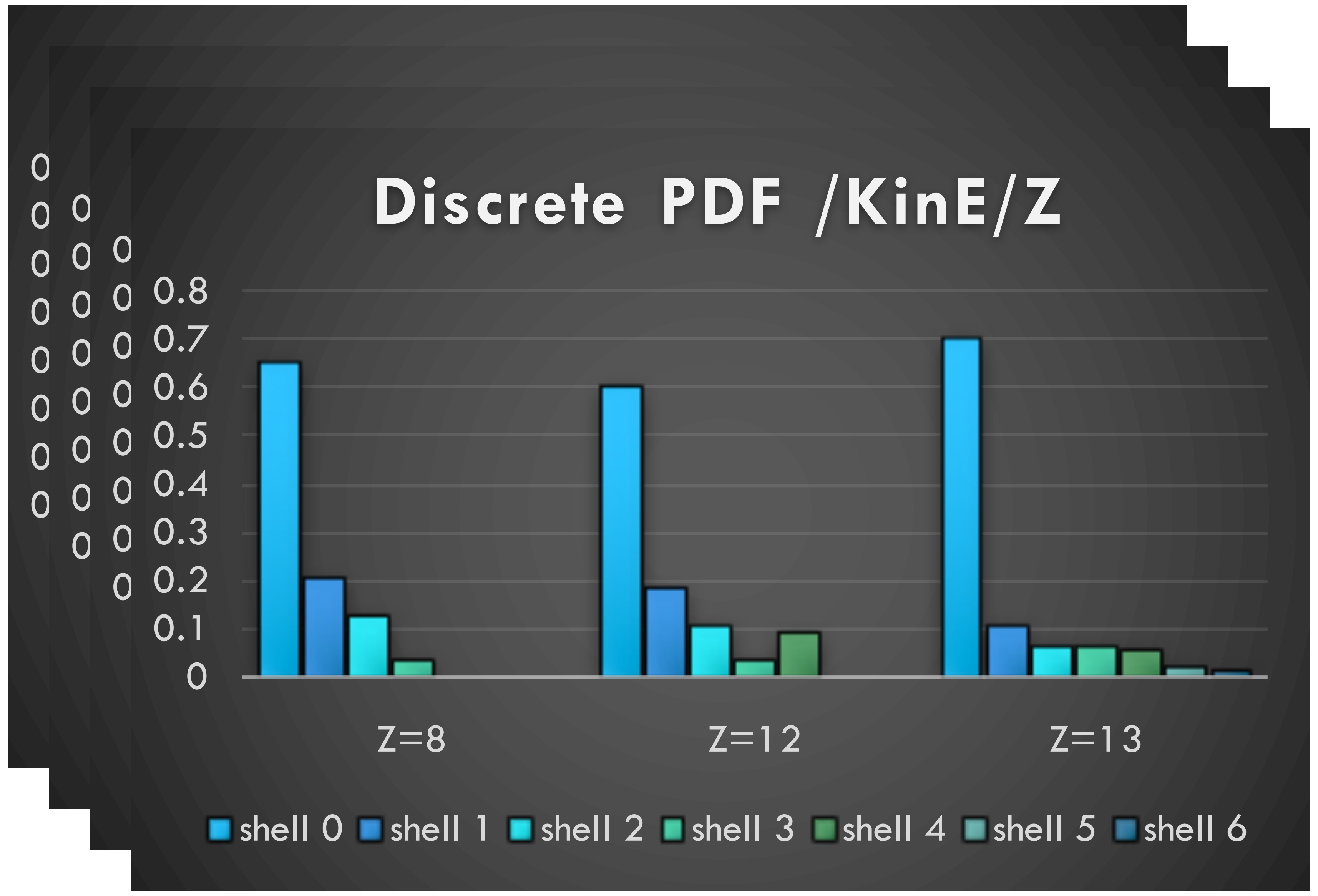


- Photoelectric effect total cross-section is not an easy function
- Fit in two different energy ranges, but not below k-shell binding energy
  - Tabulated cross-sections left for low energies
- For the final state sampling one need to sample
  - the angle: described by the SauterGavrila differential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

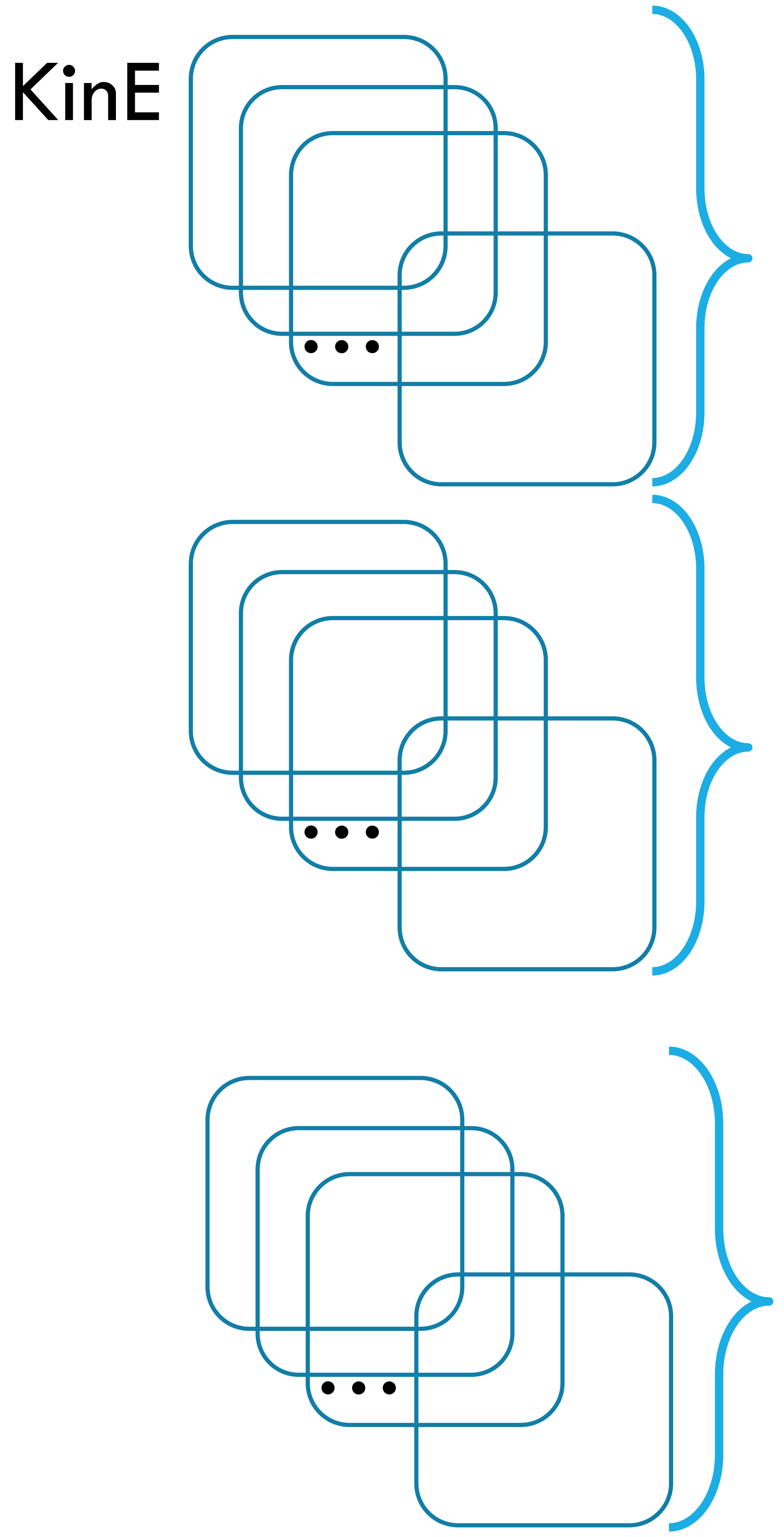




VECTORIZATION WITH DISCRETE ALIAS TABLES



ALIAS TABLE FOR DISCRETE DISTRIBUTION



- 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

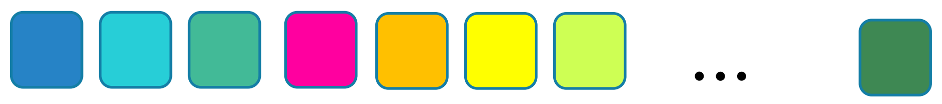
VECTORIZATION OF REJECTION SAMPLING

VECTORIZATION OF REJECTION SAMPLING

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

VECTORIZATION OF REJECTION SAMPLING

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

eKin 

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VECTORIZATION OF REJECTION SAMPLING

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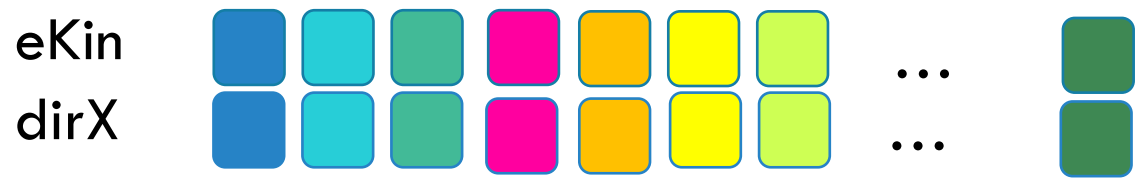

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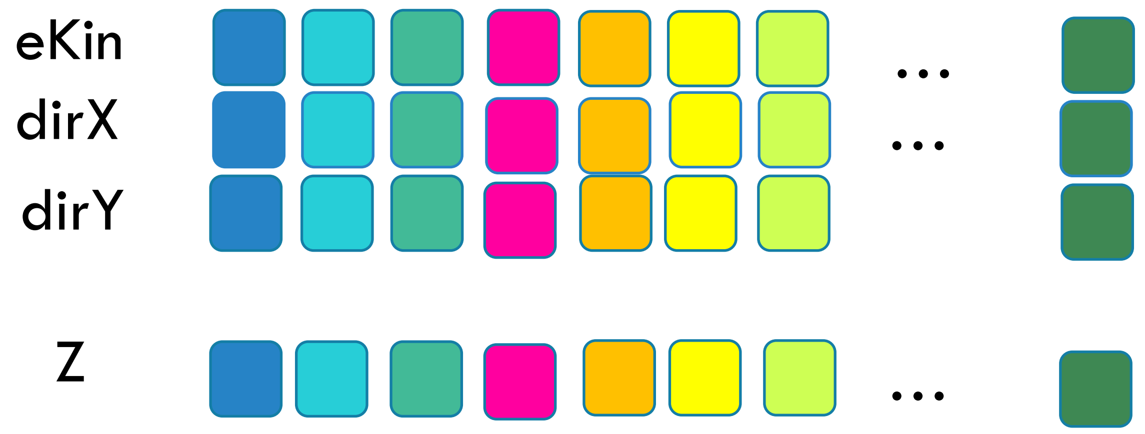

VECTORIZATION OF REJECTION SAMPLING

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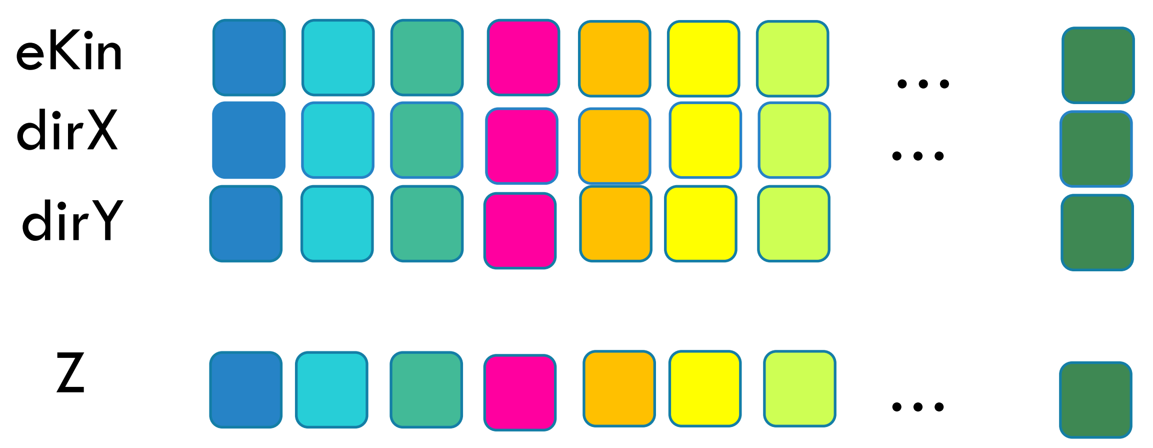
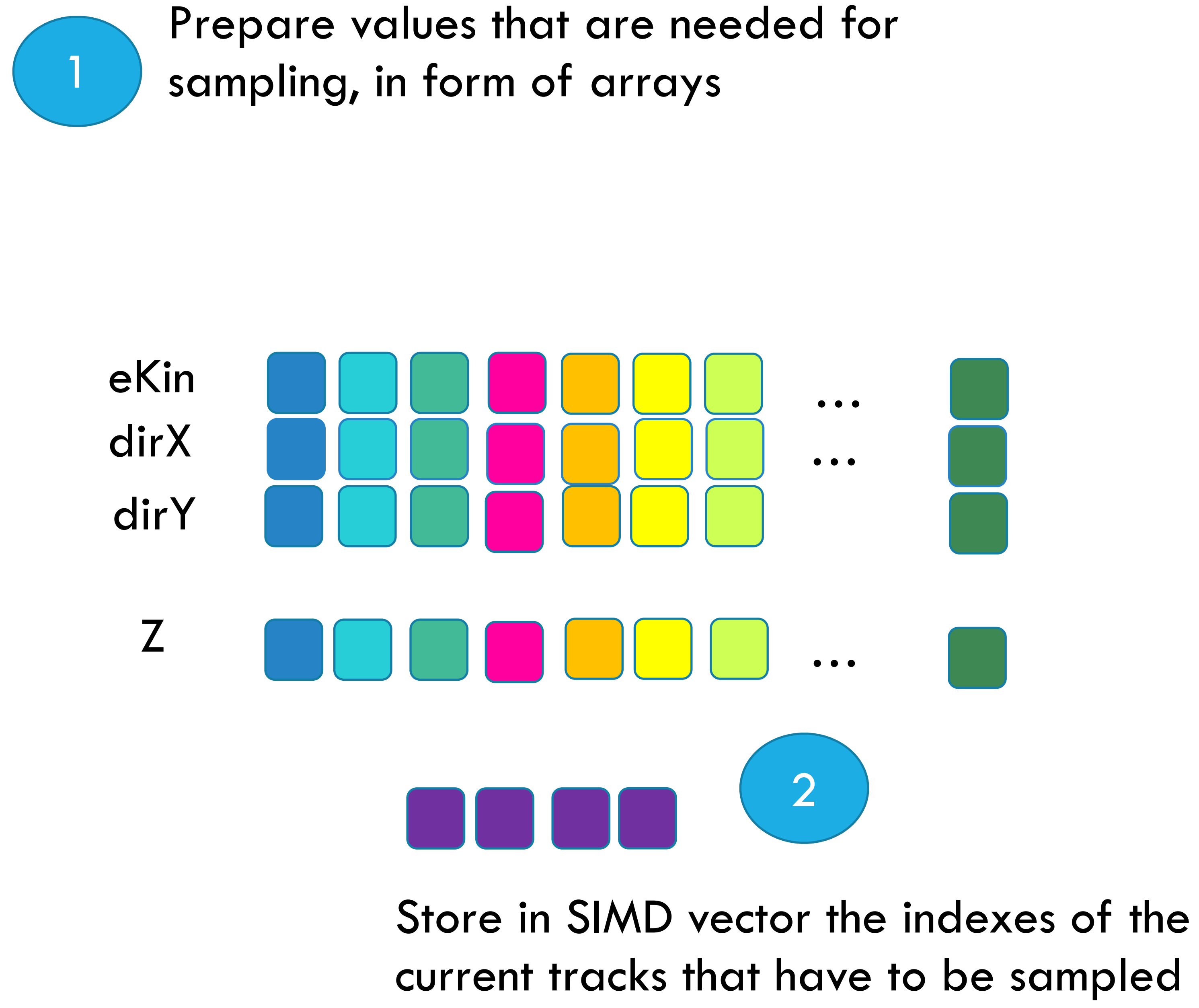


2 Store in SIMD vector the indexes of the current tracks that have to be sampled

VECTORIZATION OF REJECTION SAMPLING



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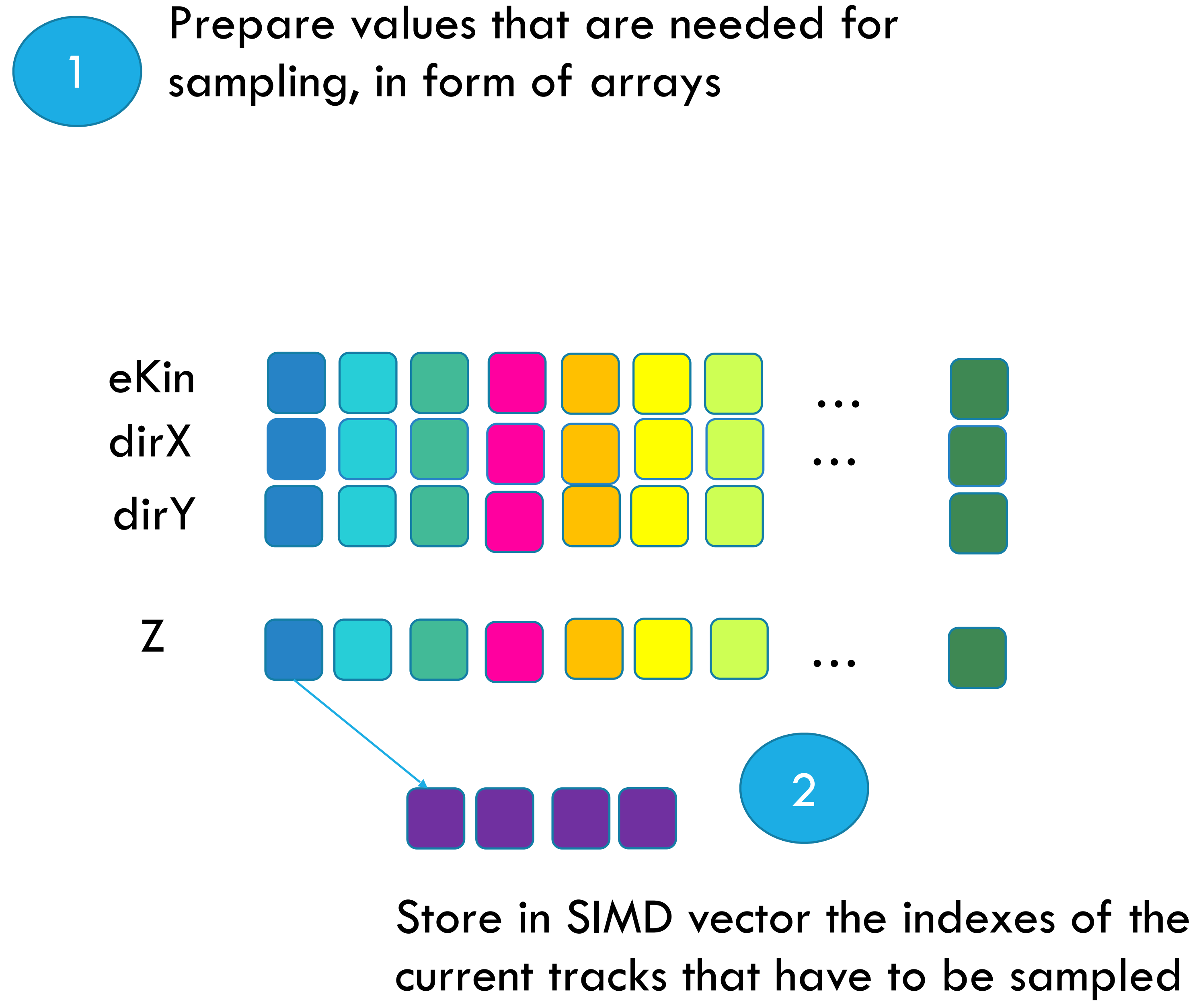

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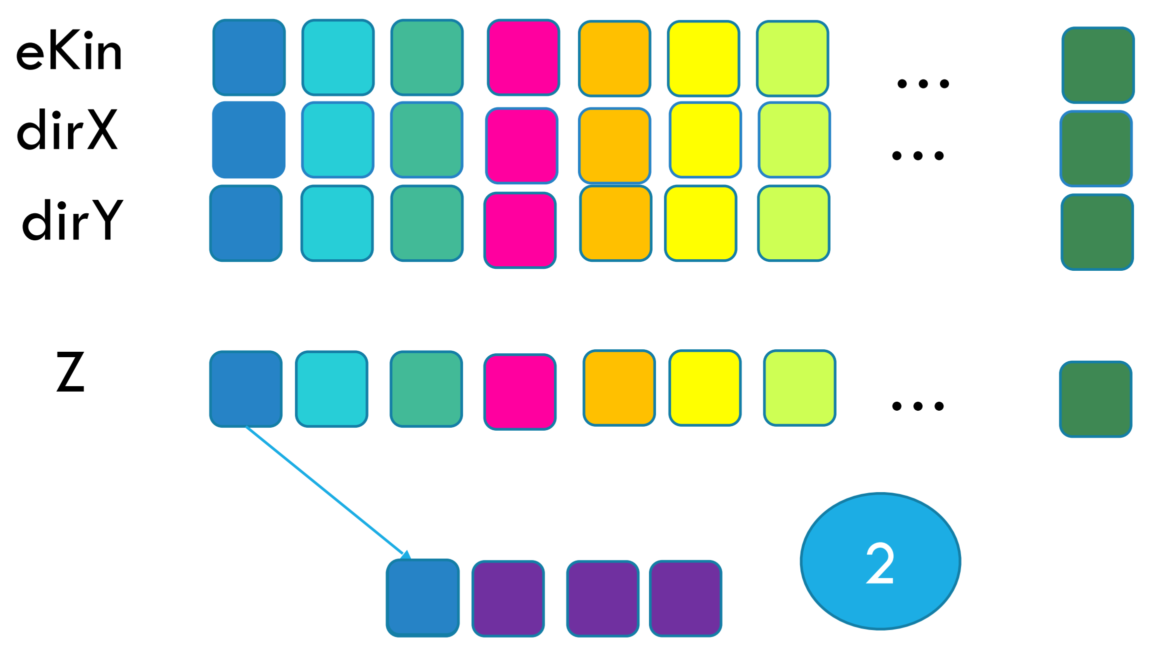

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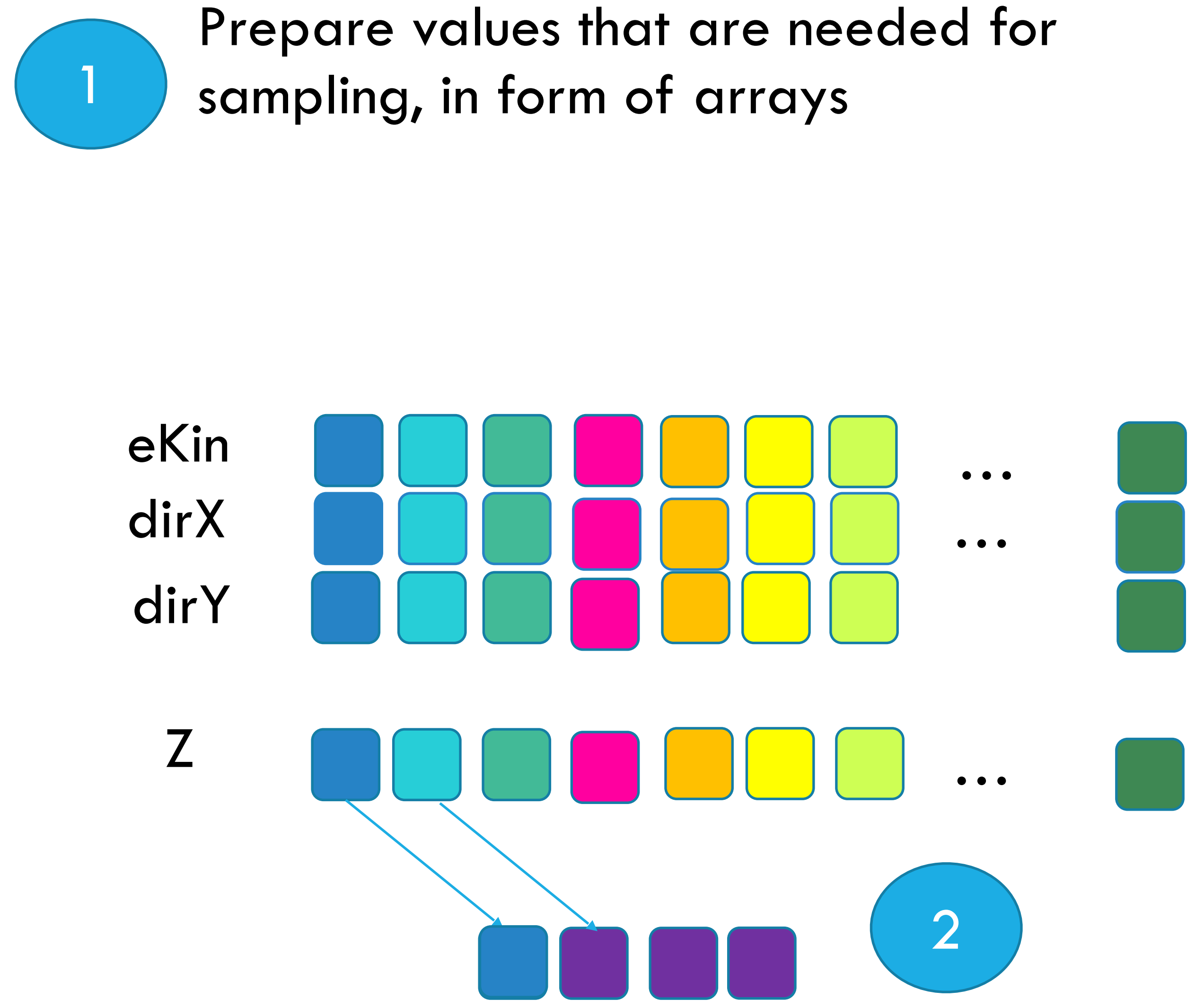
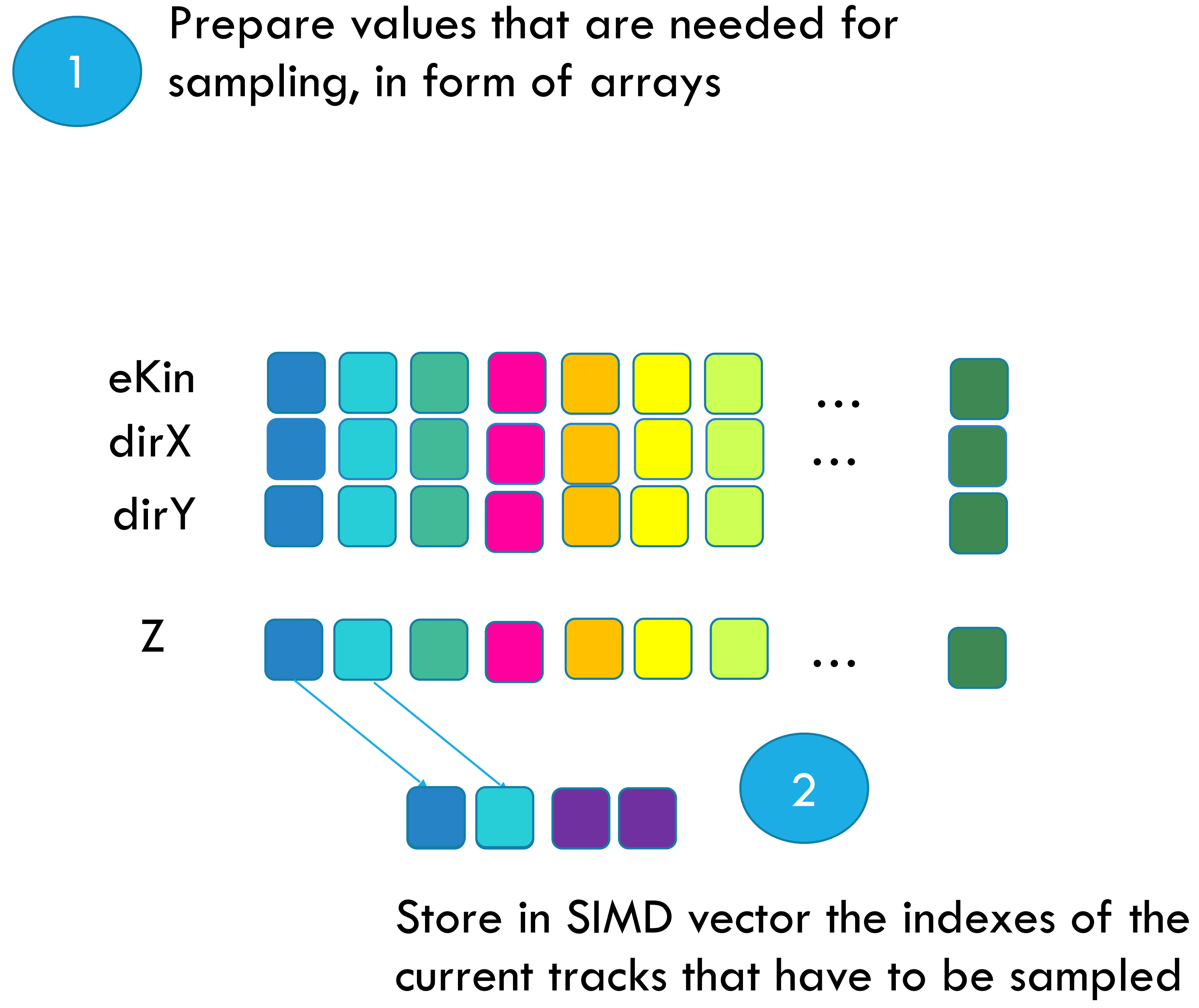


Prepare values that are needed for sampling, in form of arrays

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

VECTORIZATION OF REJECTION SAMPLING



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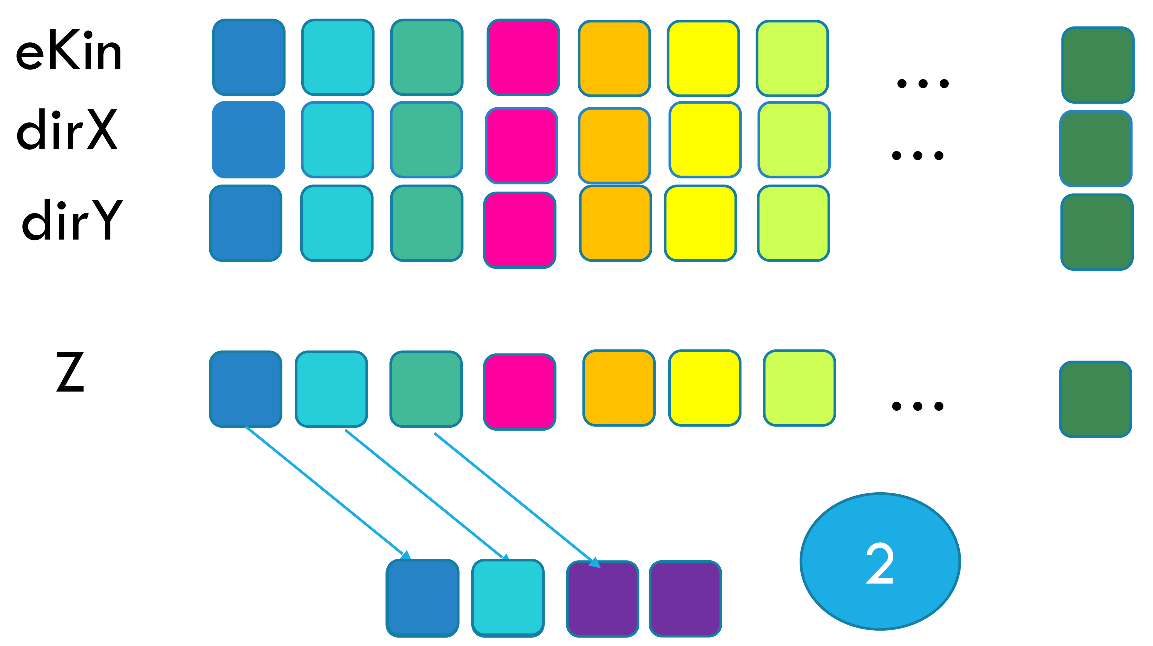

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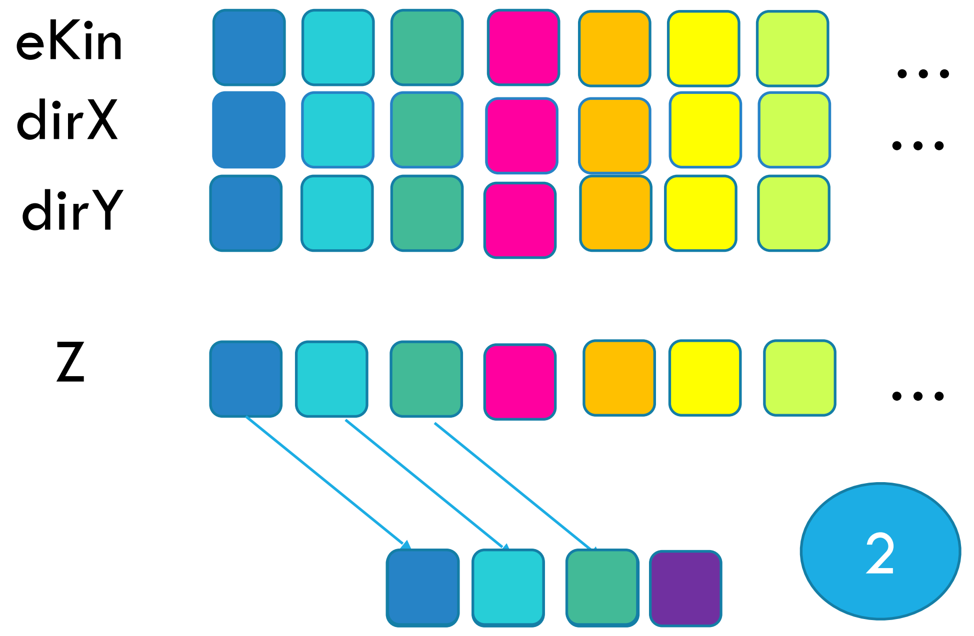

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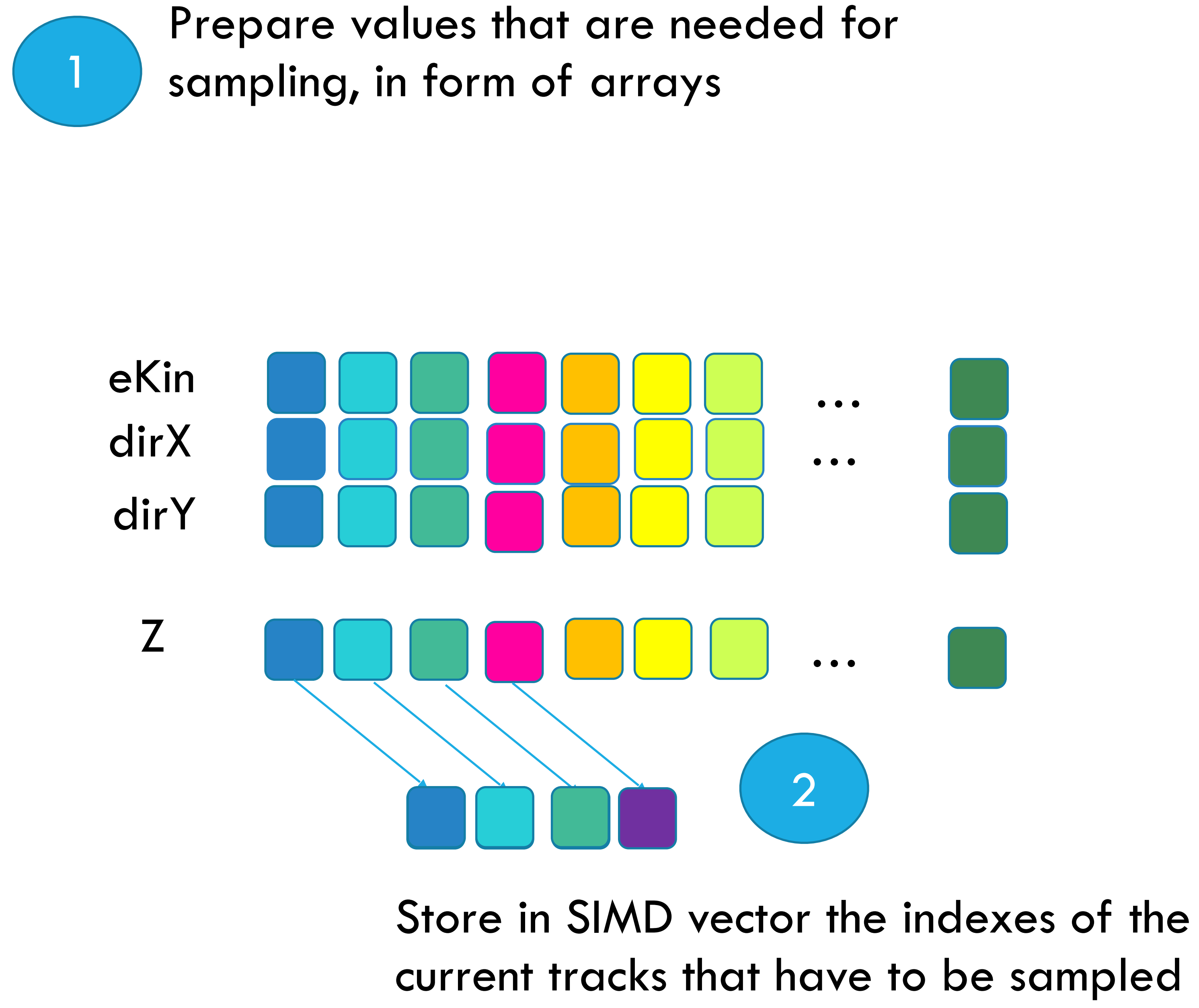

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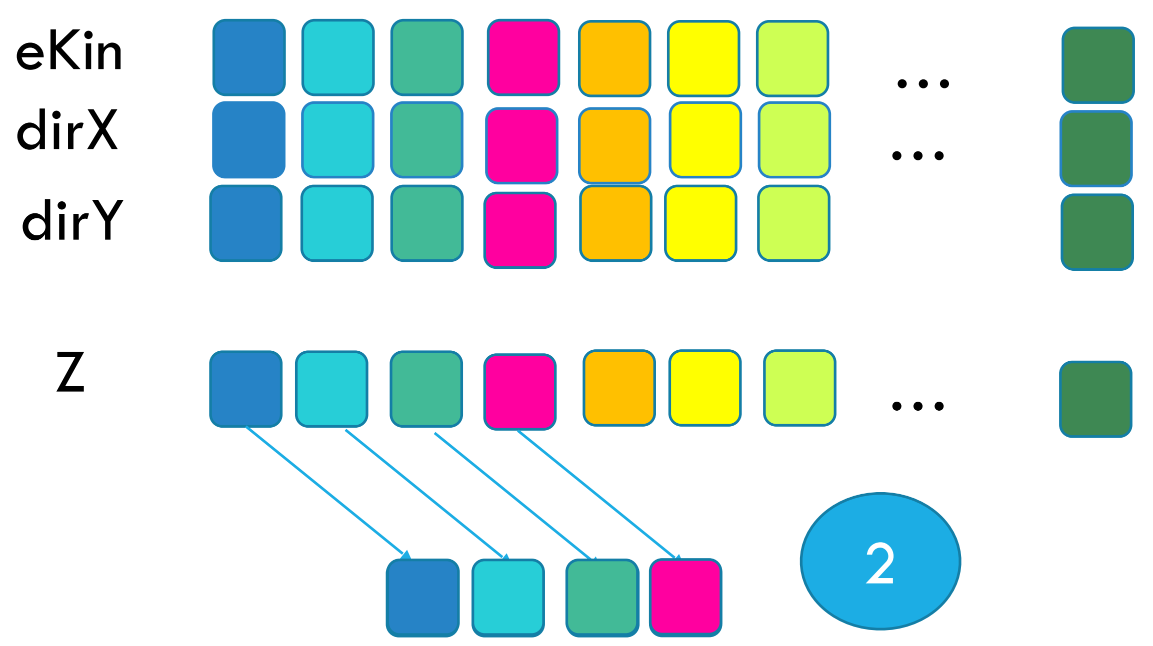
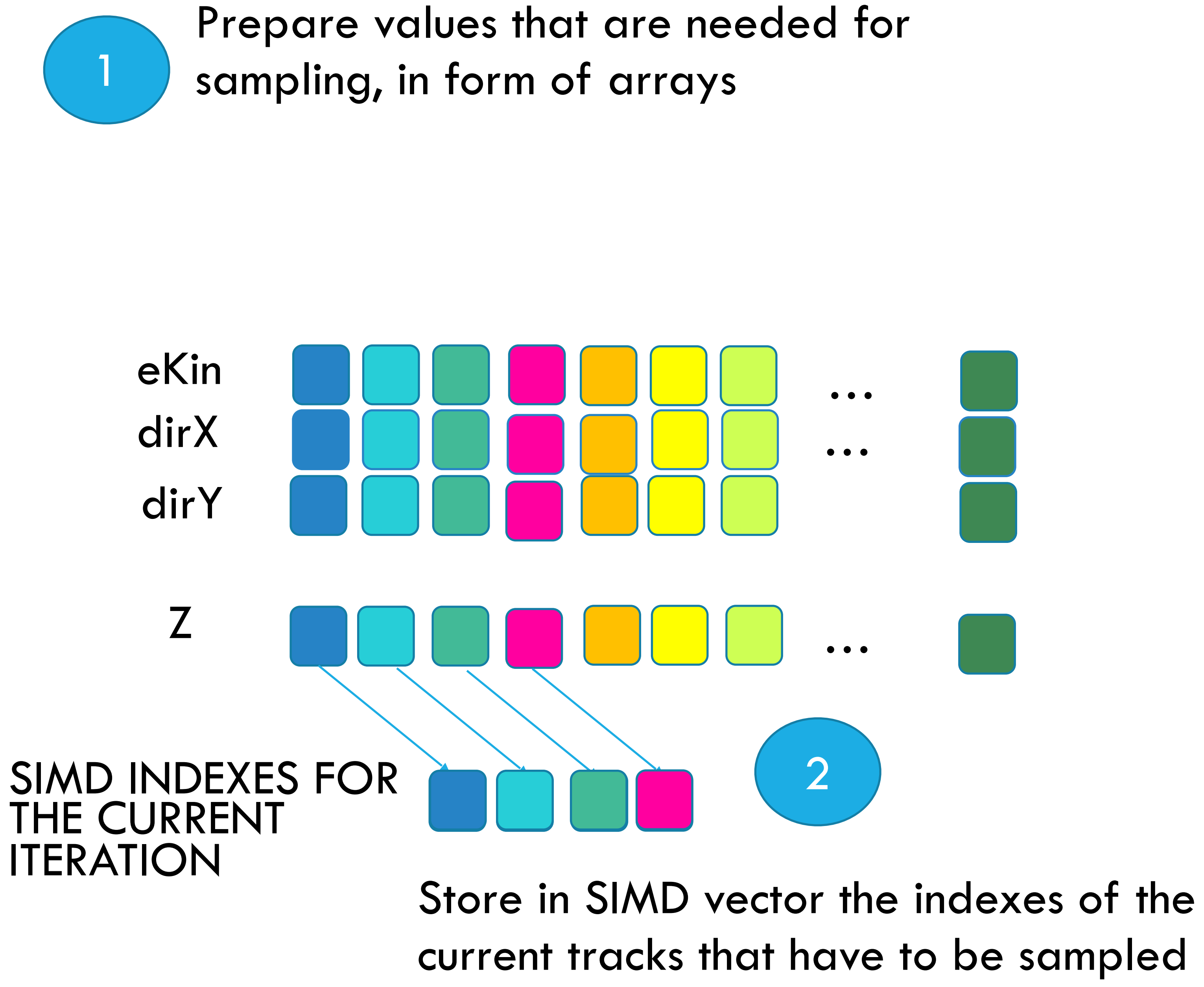


Store in SIMD vector the indexes of the current tracks that have to be sampled

VECTORIZATION OF REJECTION SAMPLING



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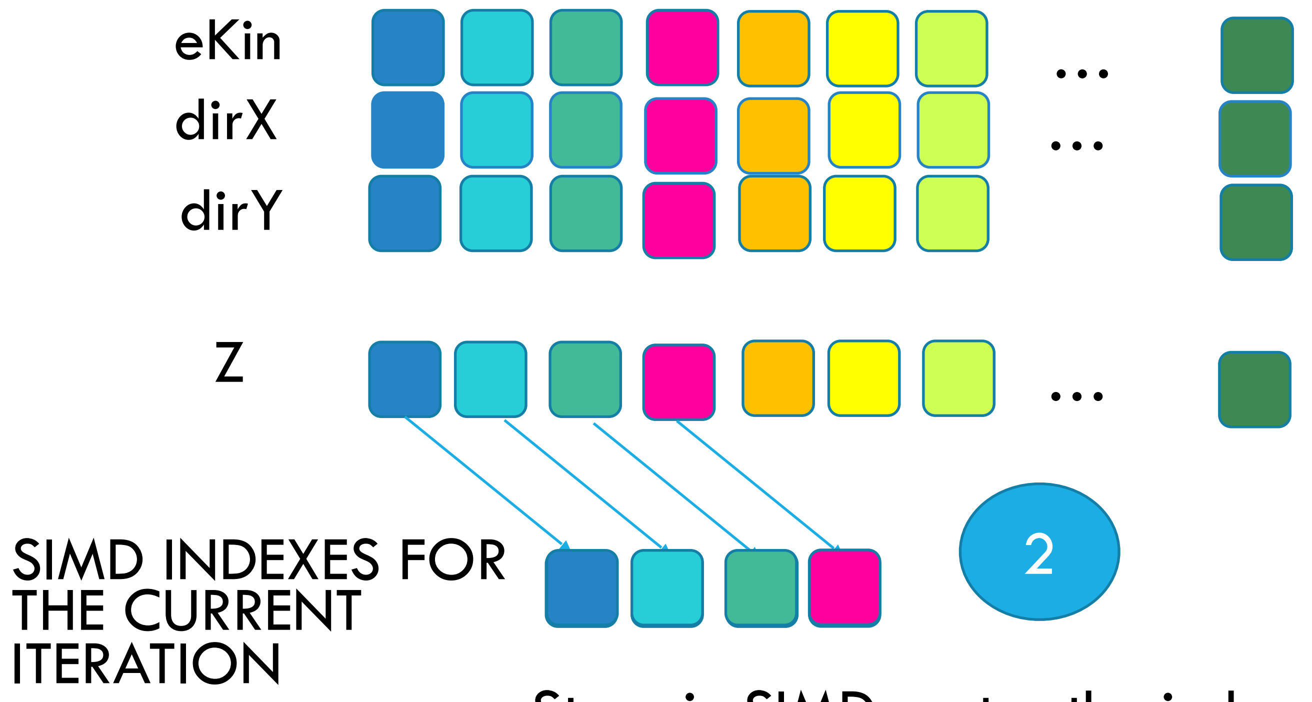
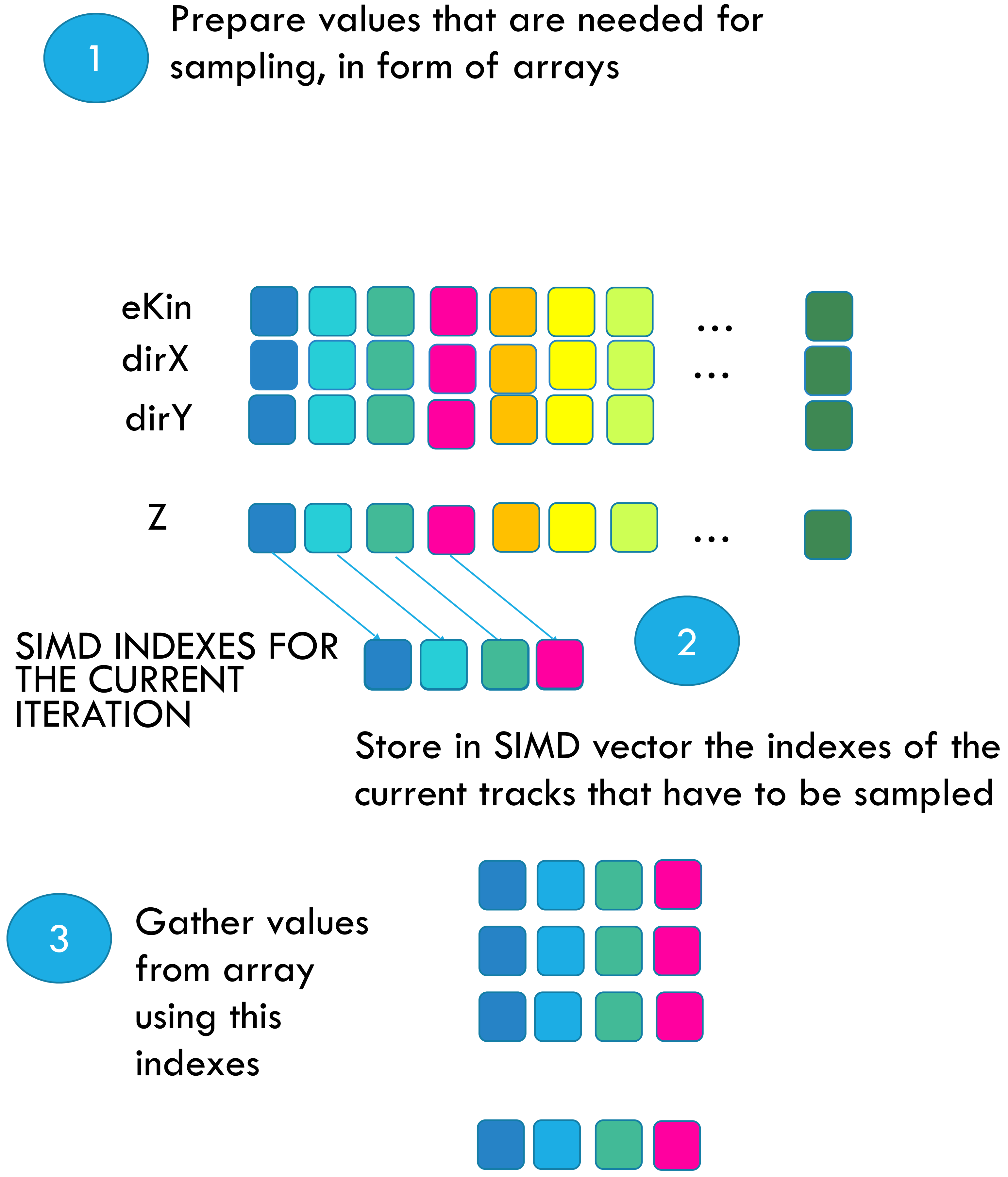


2 Store in SIMD vector the indexes of the current tracks that have to be sampled

3 Gather values from array using this indexes

VECTORIZATION OF REJECTION SAMPLING



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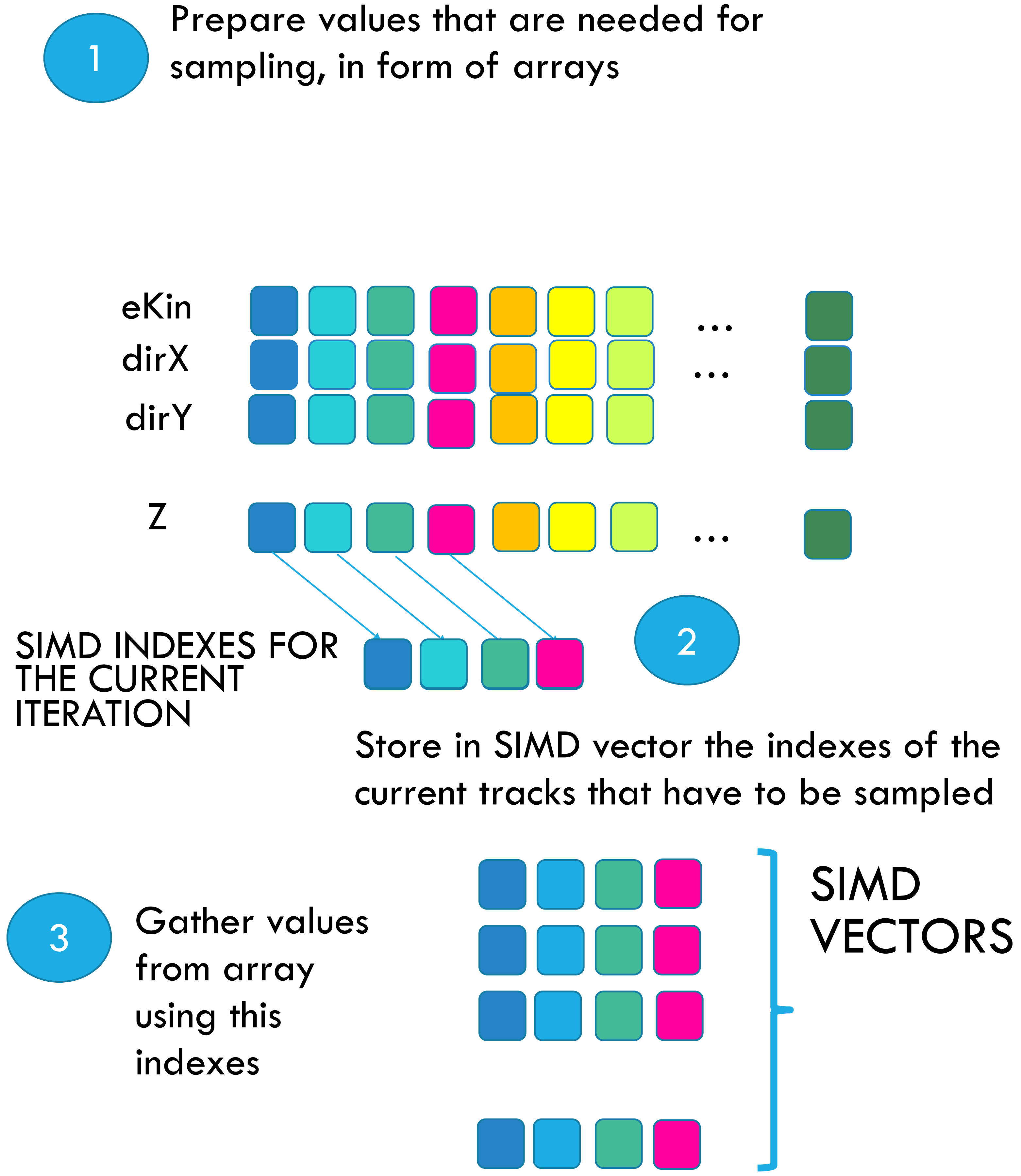

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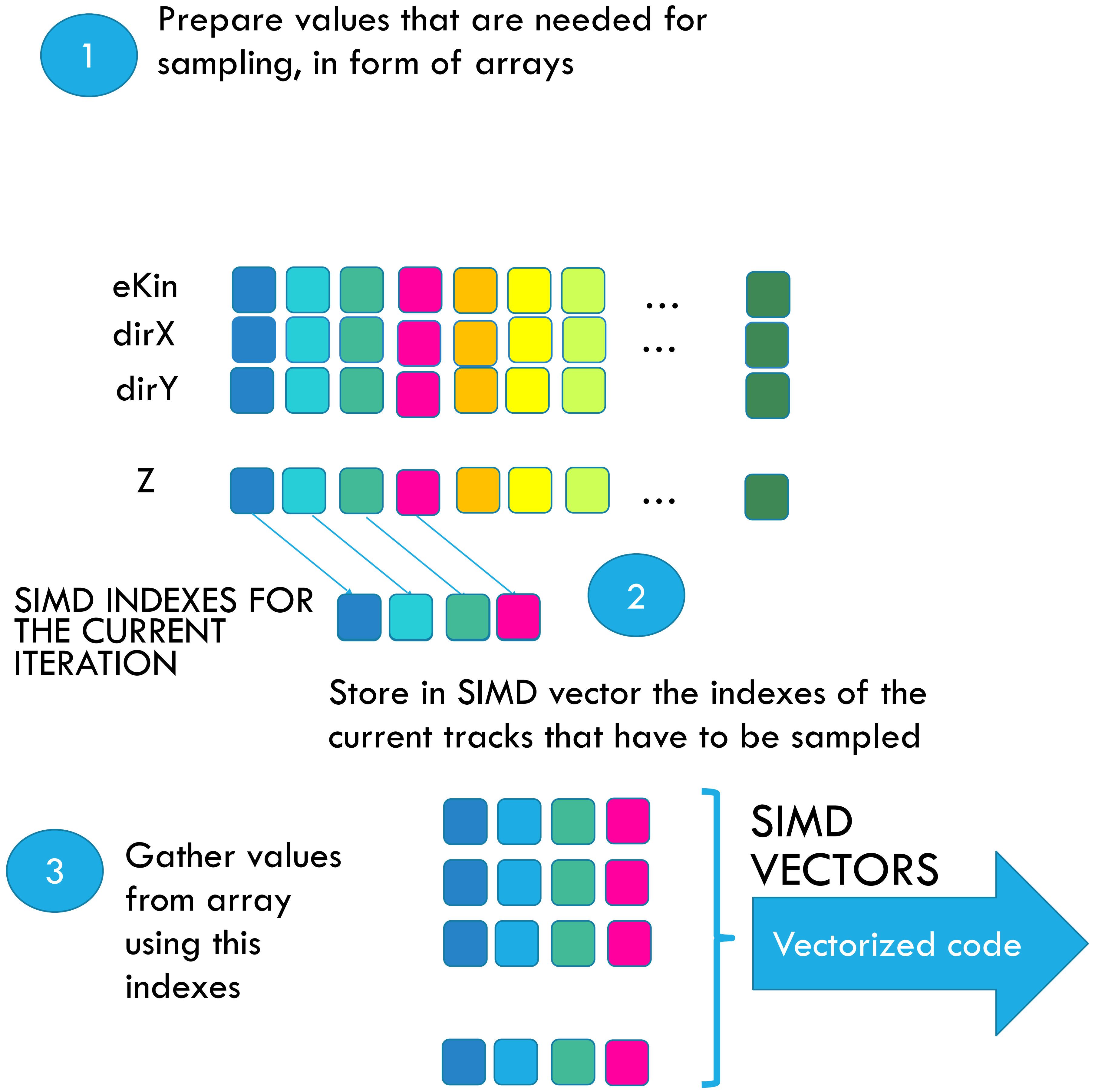

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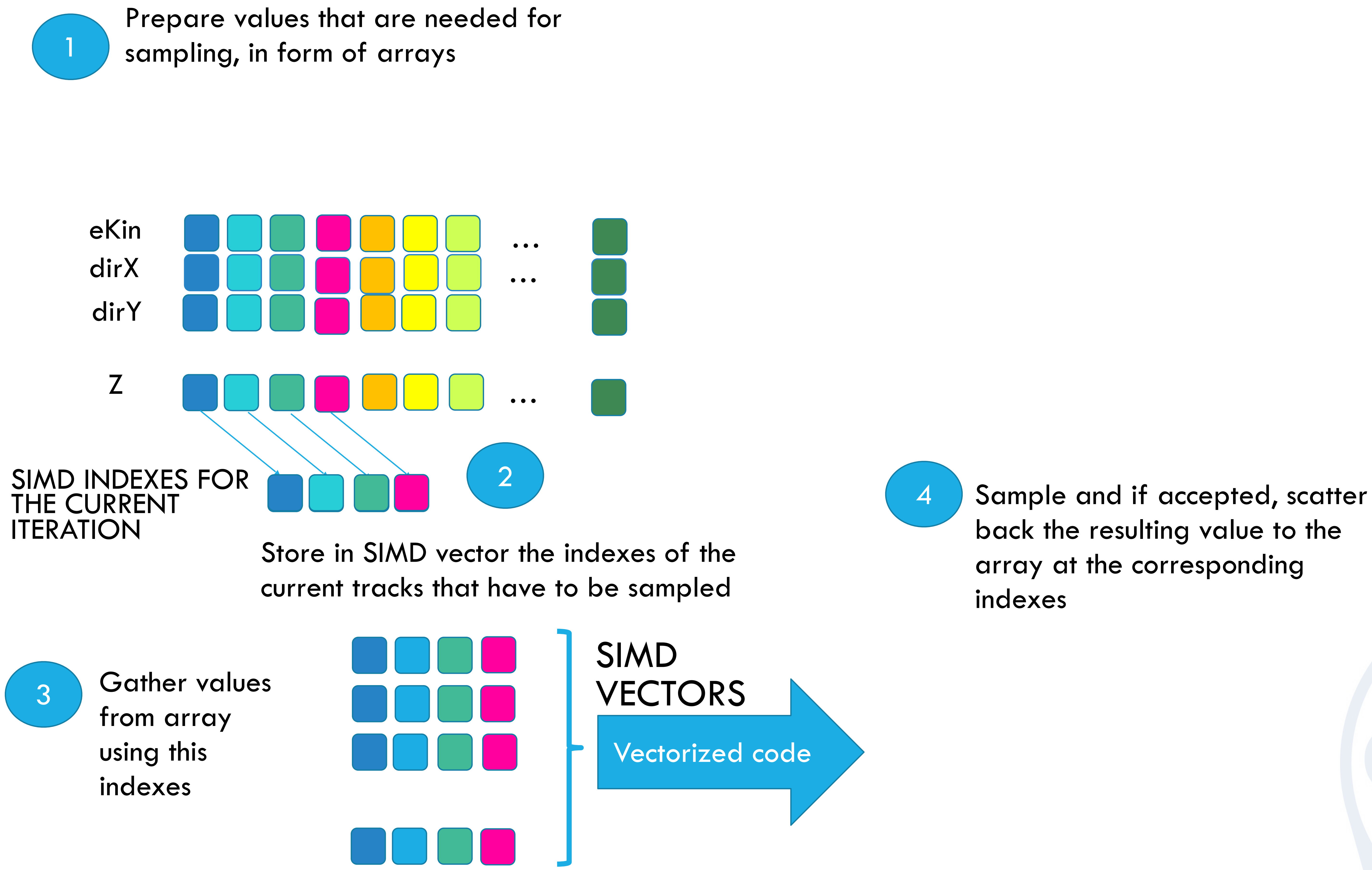

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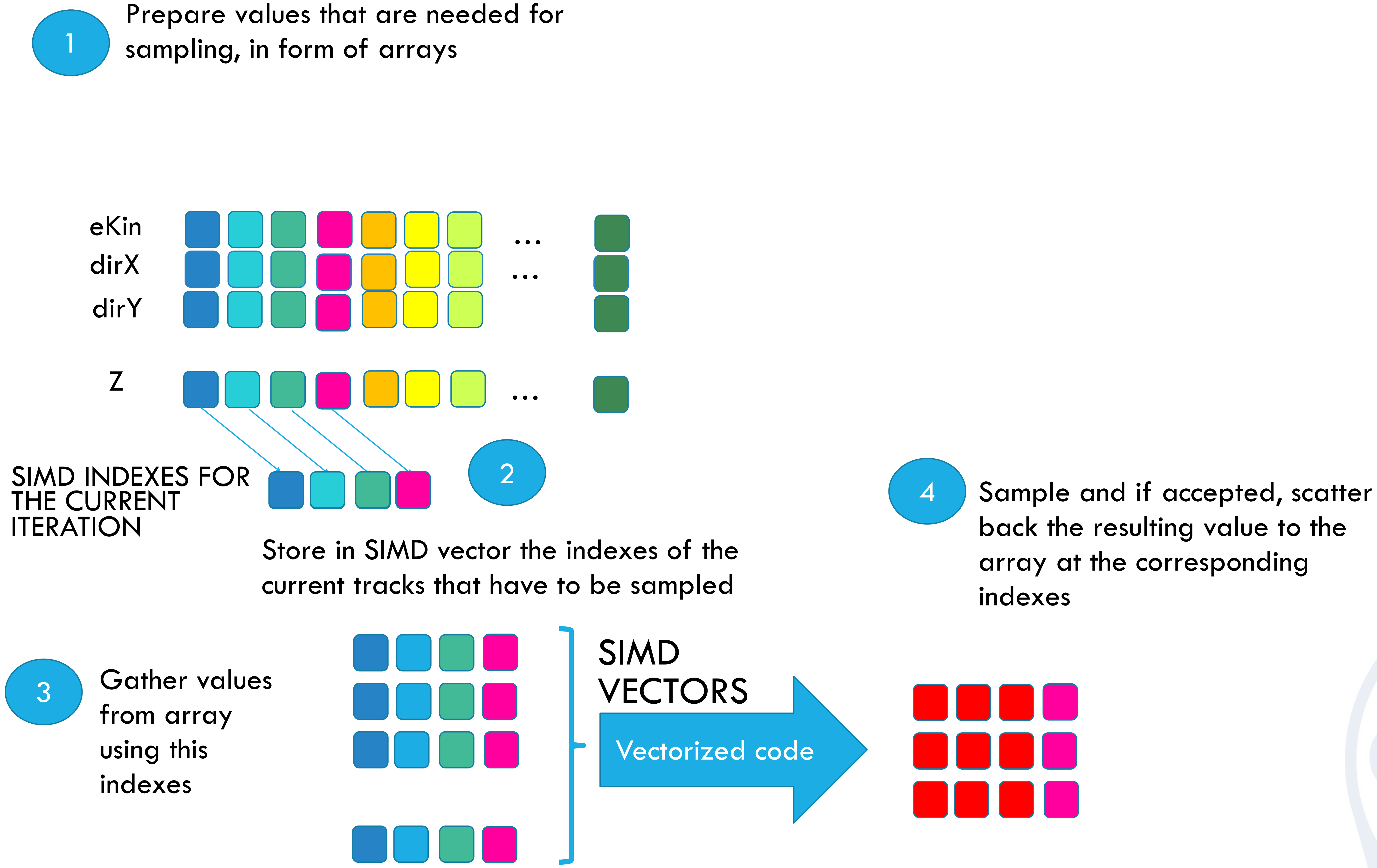

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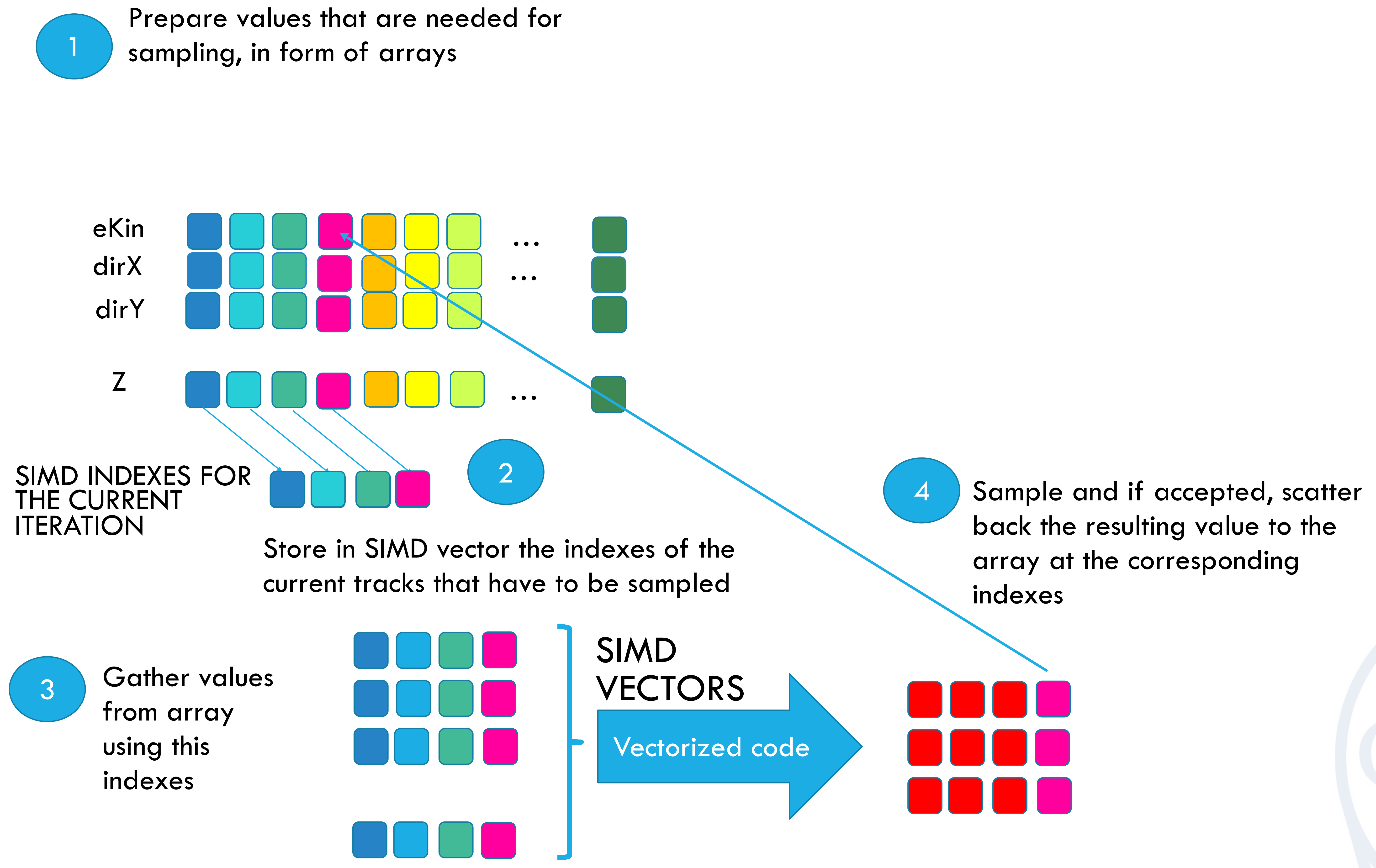

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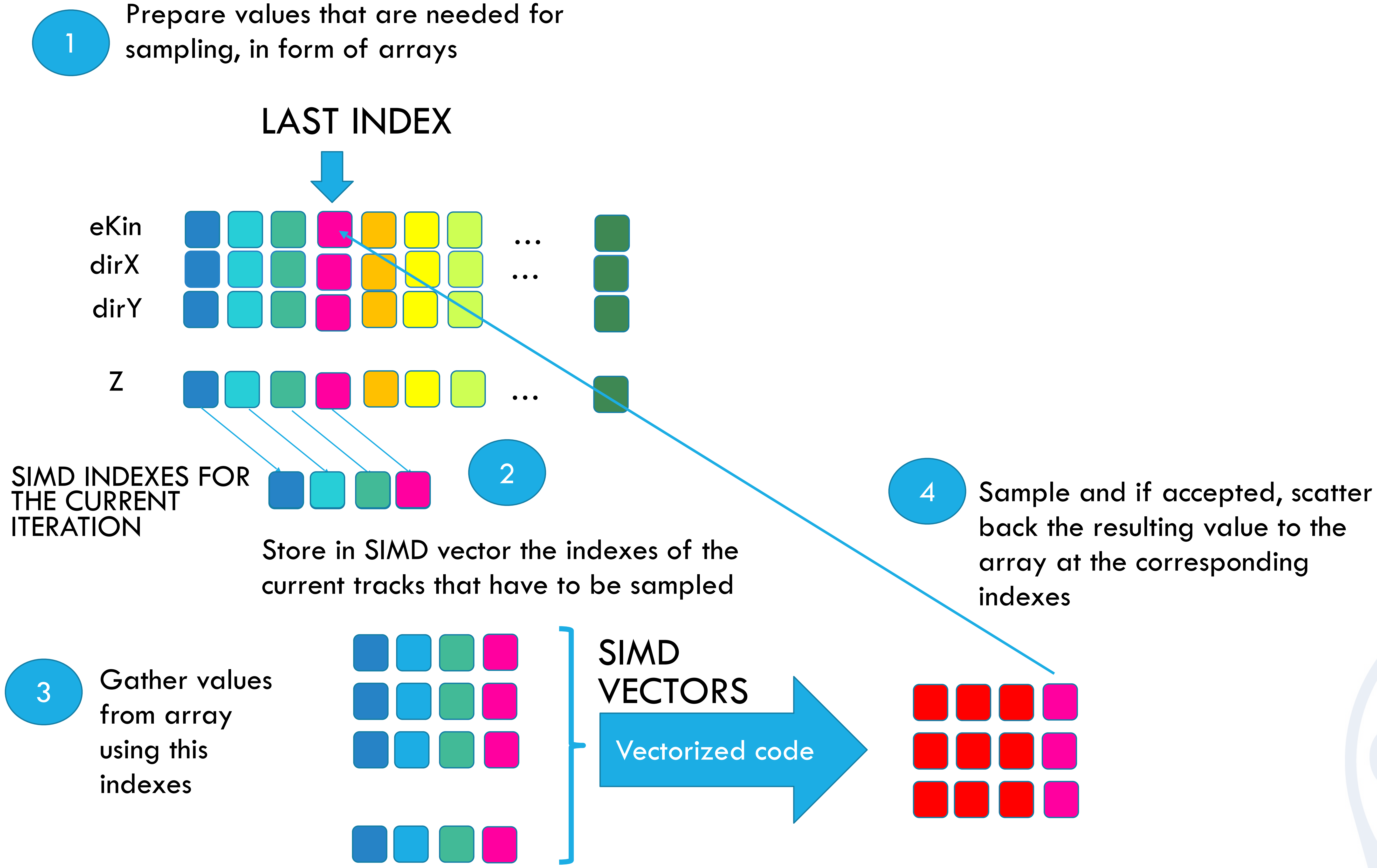

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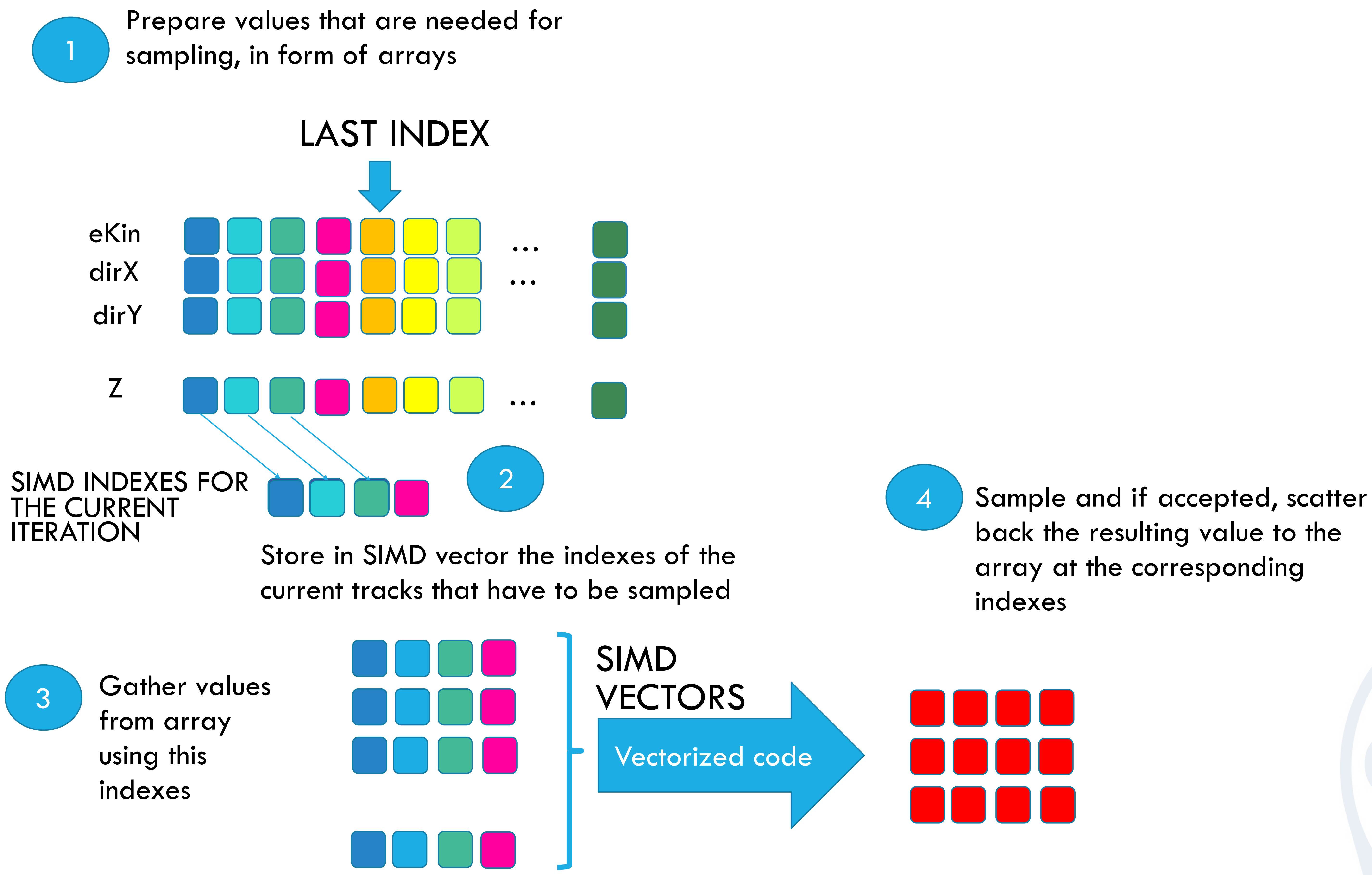

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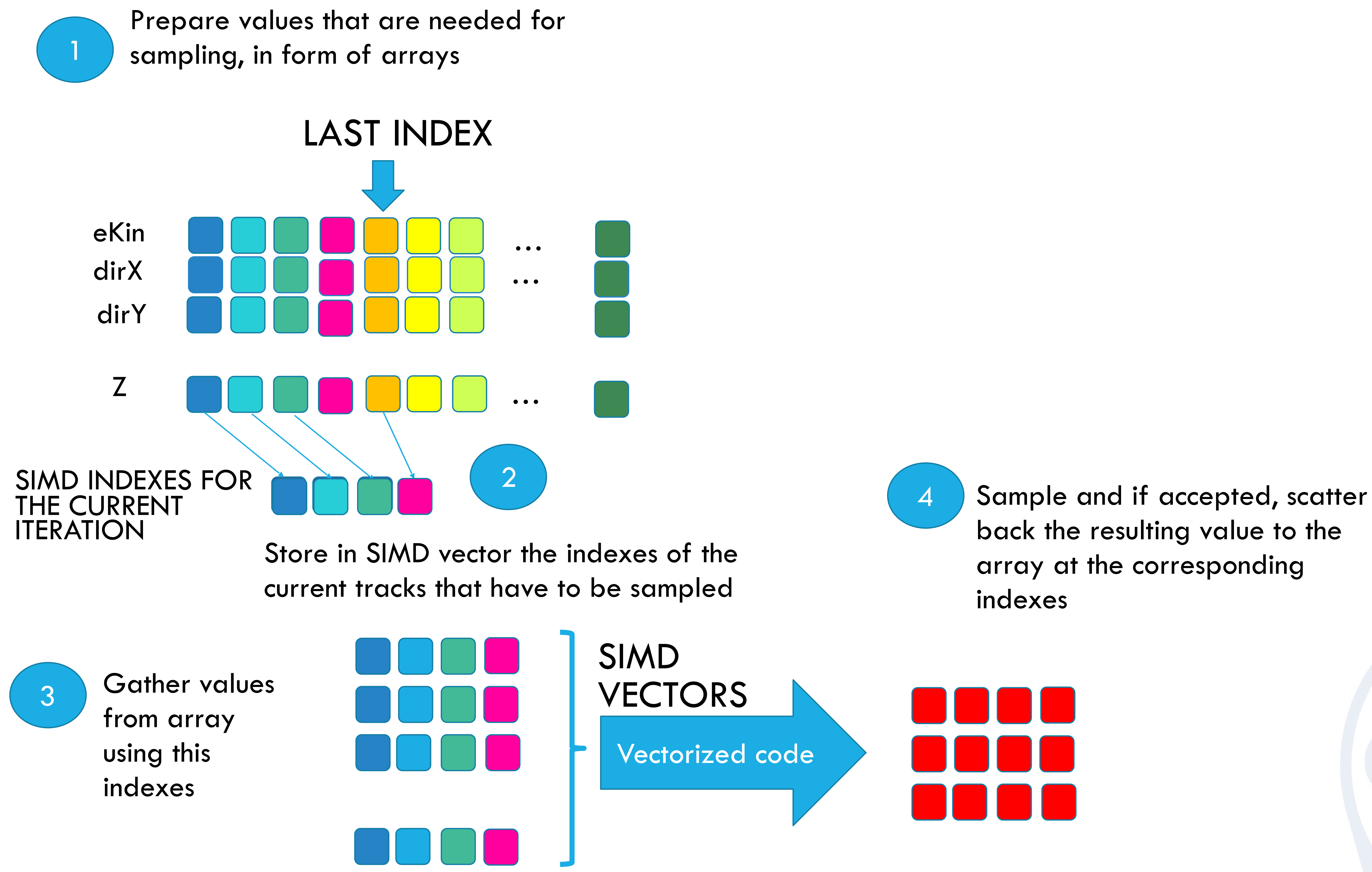

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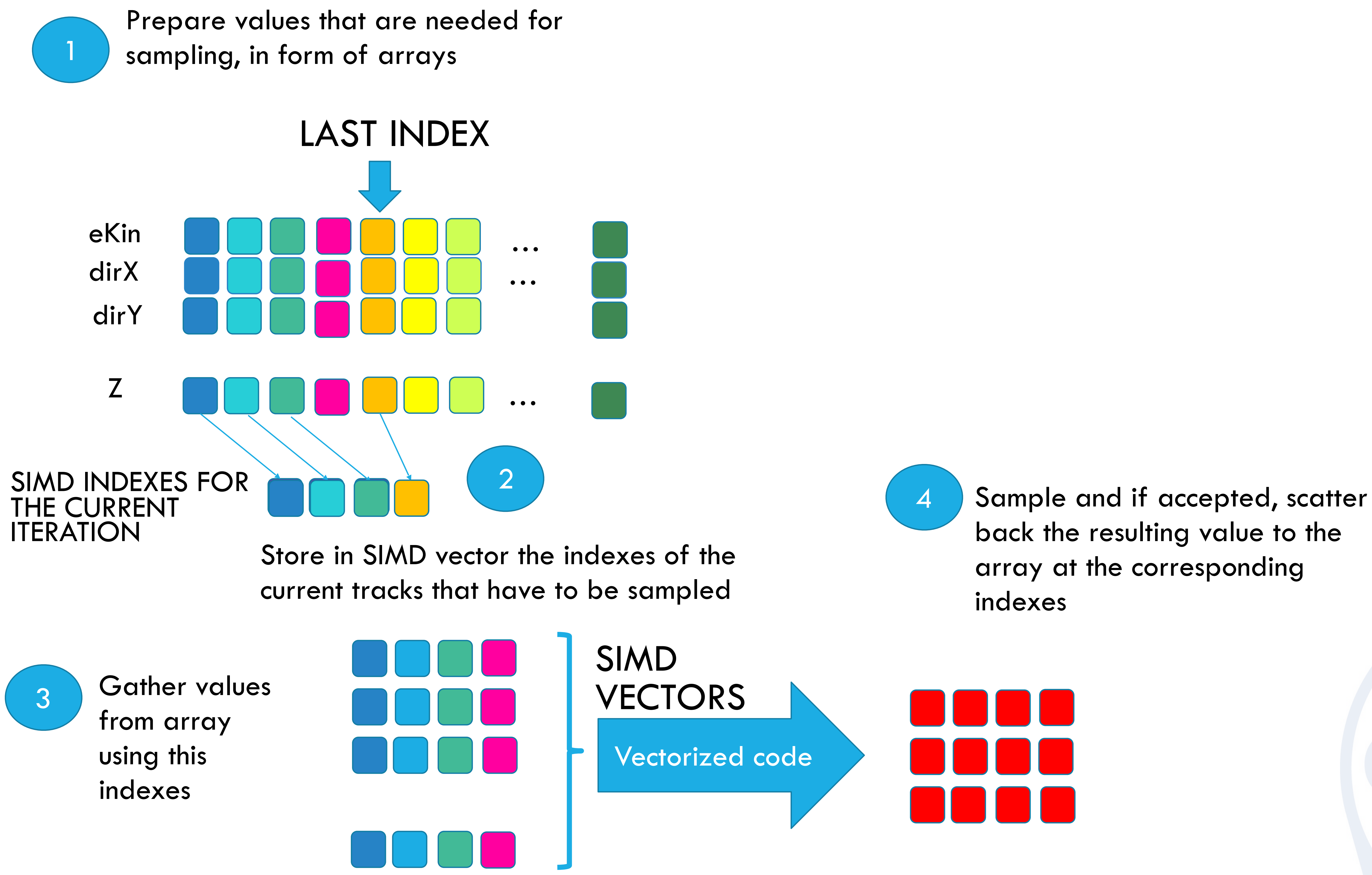

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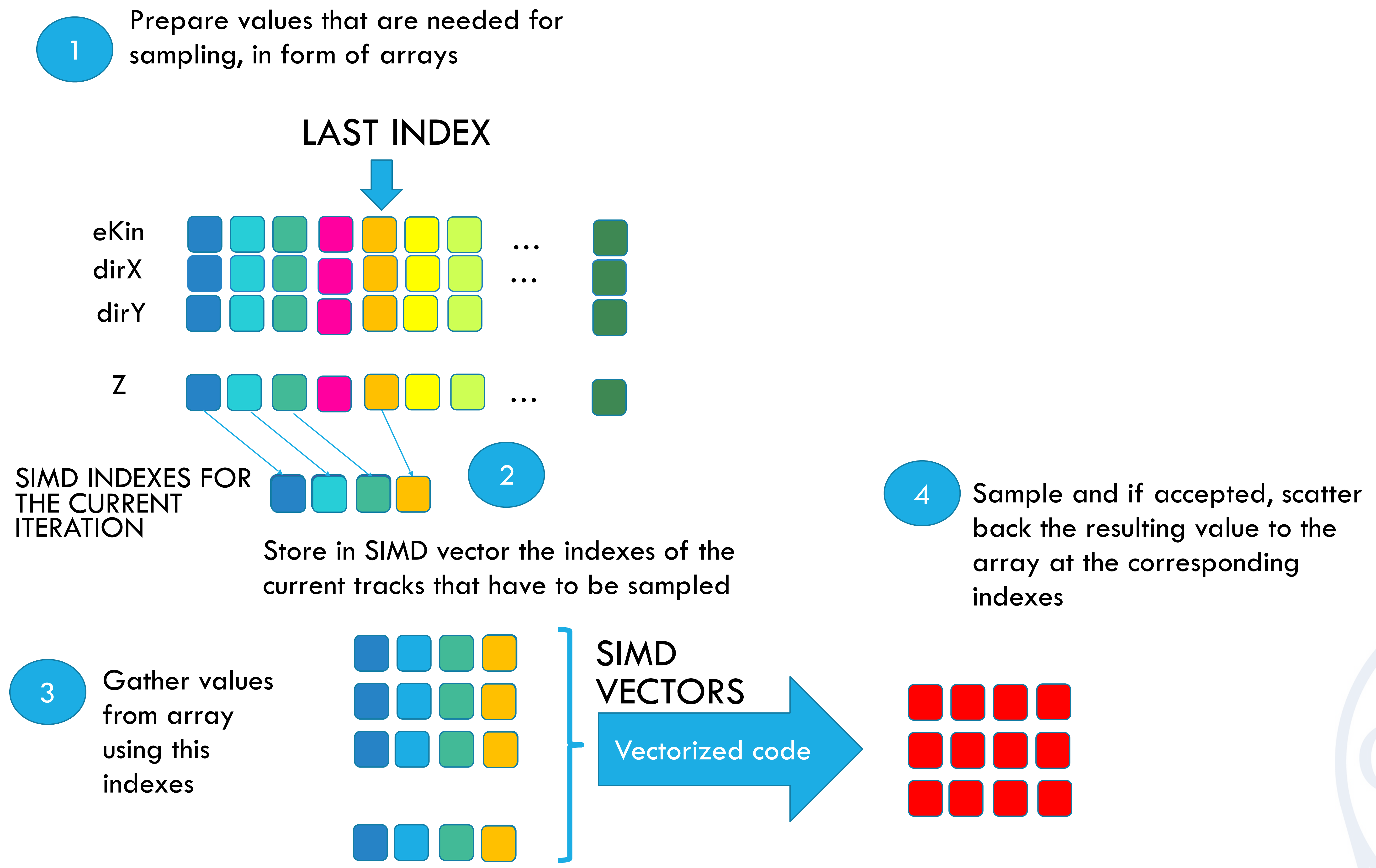

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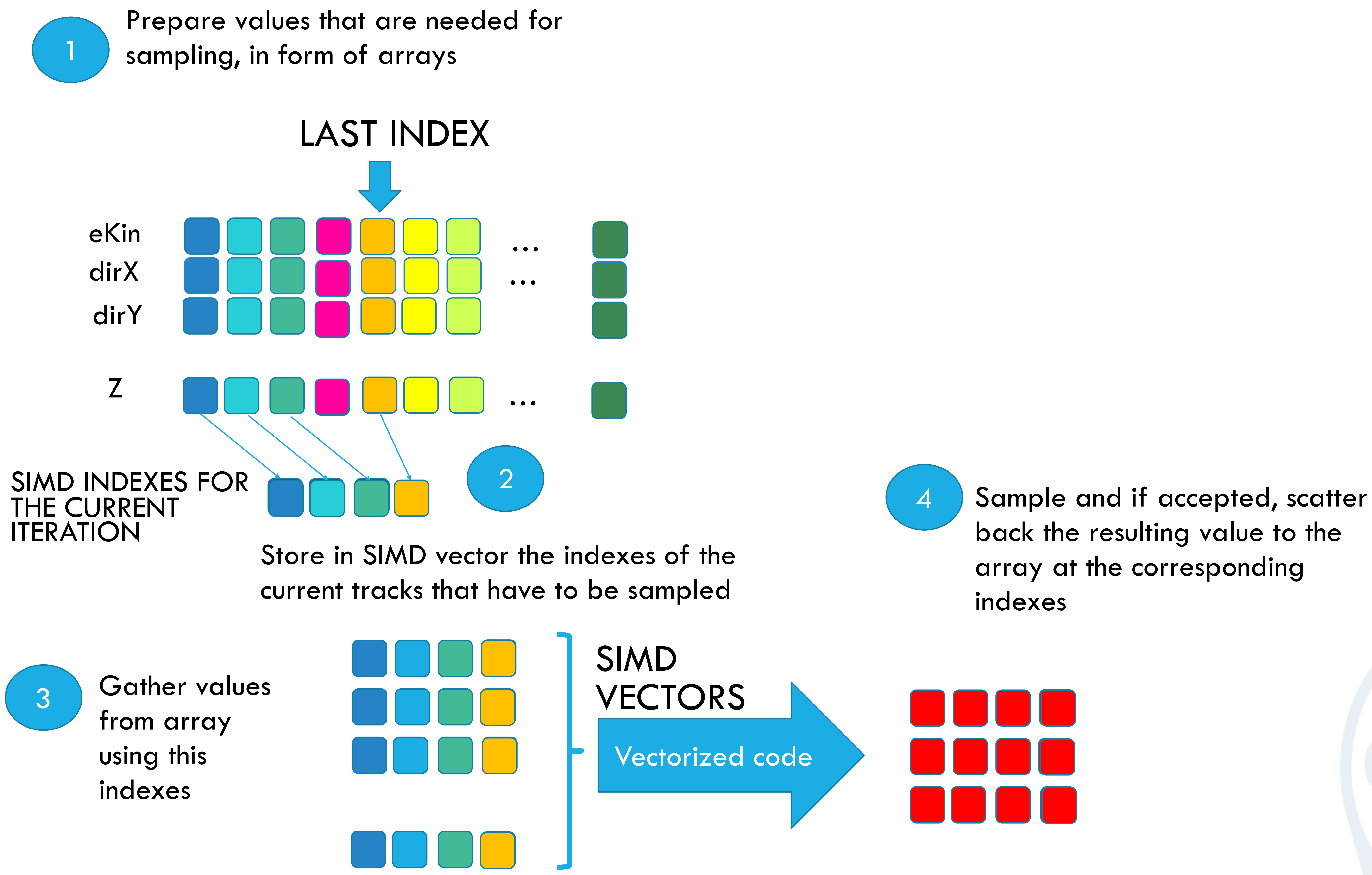

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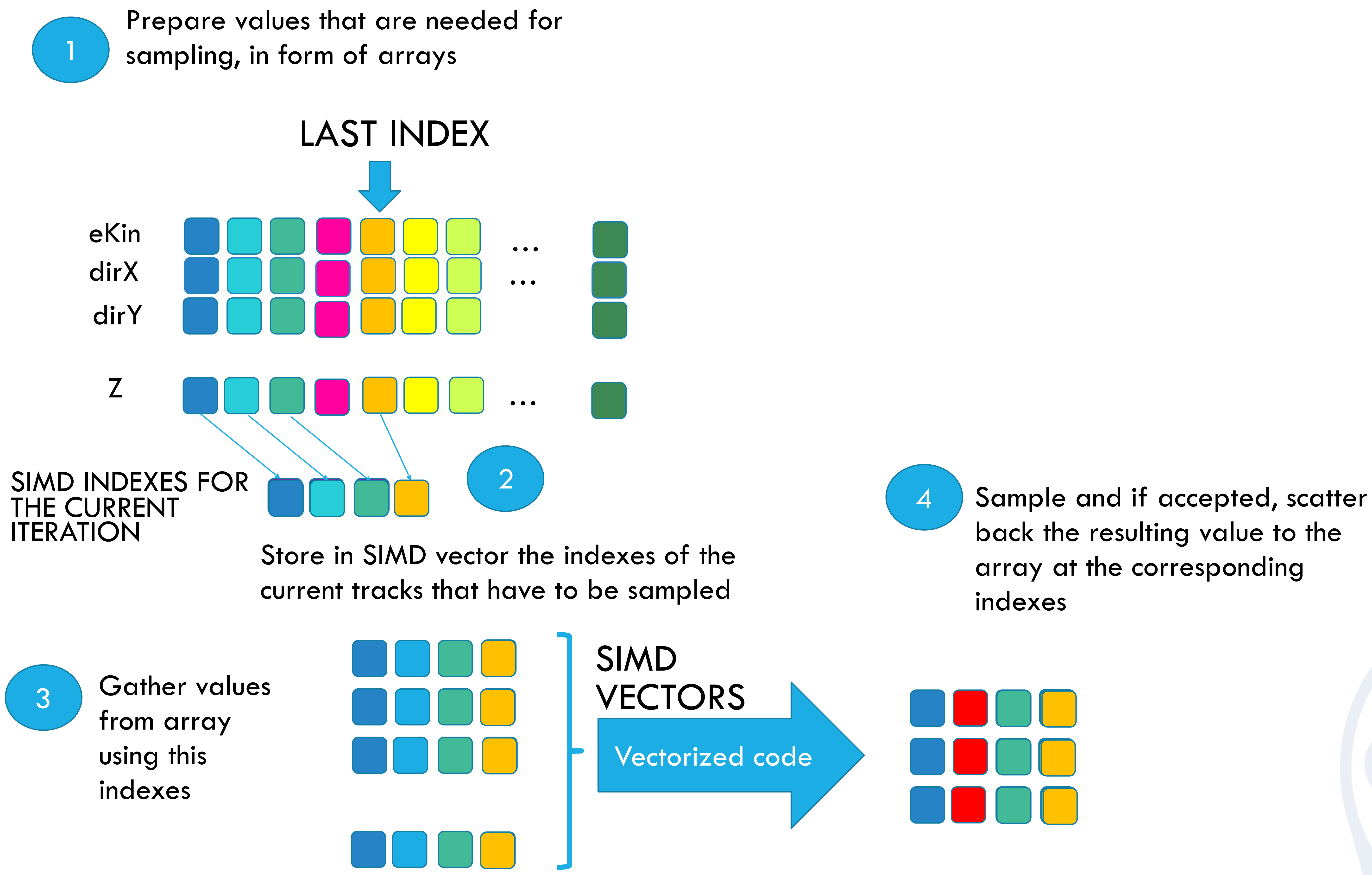

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