A QCD Performance Portability Study using Kokkos

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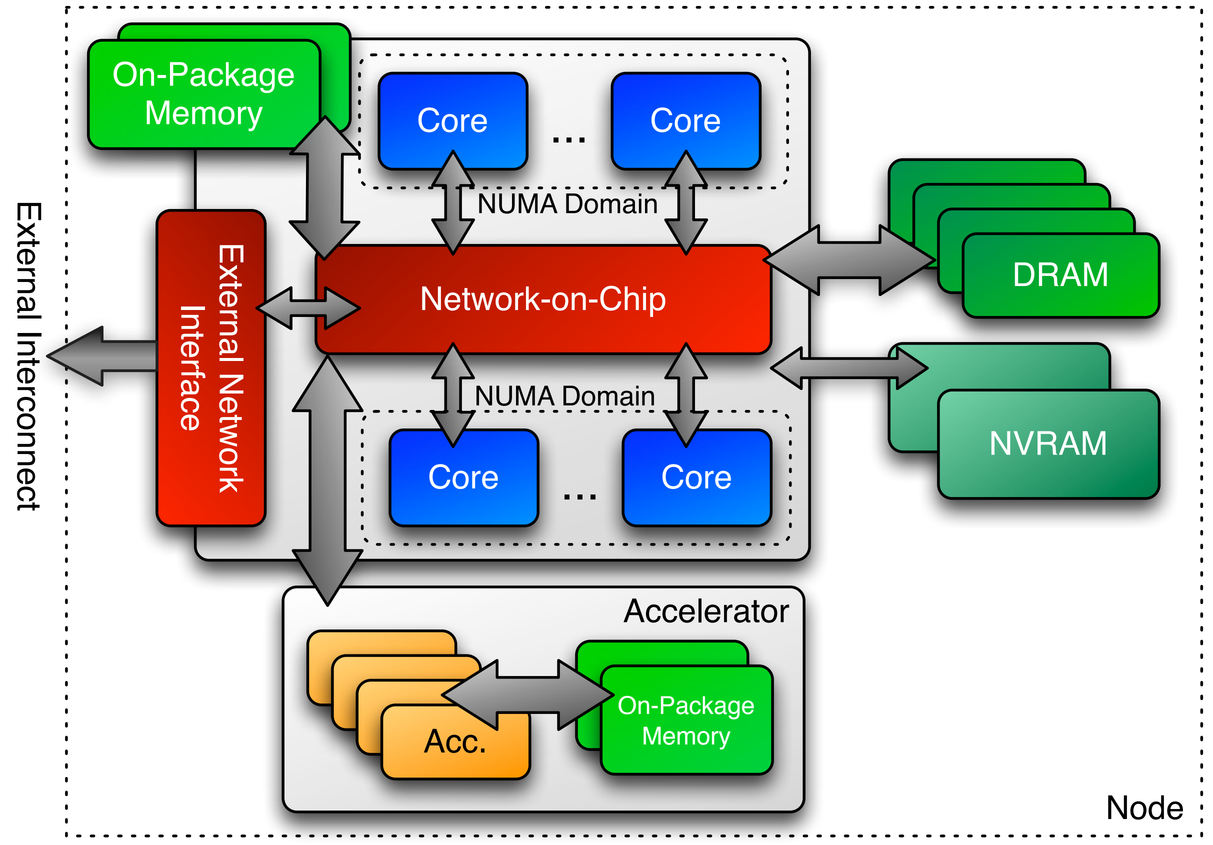
Perf. Portability Study with Kokkos

- With hardware diversity and looking forward to new systems, performance portability is crucial.
- Kokkos is a C++ library providing parallel programming constructs, developed and maintained at Sandia National Lab. (see: github.com:kokkos/kokkos)
  - Node model: multicore CPUs, accelerator devices, several memory spaces
  - Patterns: parallel_for, reduction, scan, DAG/futures
  - Back Ends: OpenMP, CUDA, OpenMP-target, pthreads, …
- As Part of our ECP & NESAP work we investigated porting a Key QCD Kernel (Wilson Dslash) to Kokkos
  - work done mostly during 4 week visit to NERSC
  - and at a GPU Hackathon organized by OLCF & NASA
  - in collaboration with NERSC, NVIDIA and the Kokkos team



A schematic of a typical compute node modeled by Kokkos: Image from Kokkos Tutorial Slide Deck: KokkosTutorialARL2016.pdf

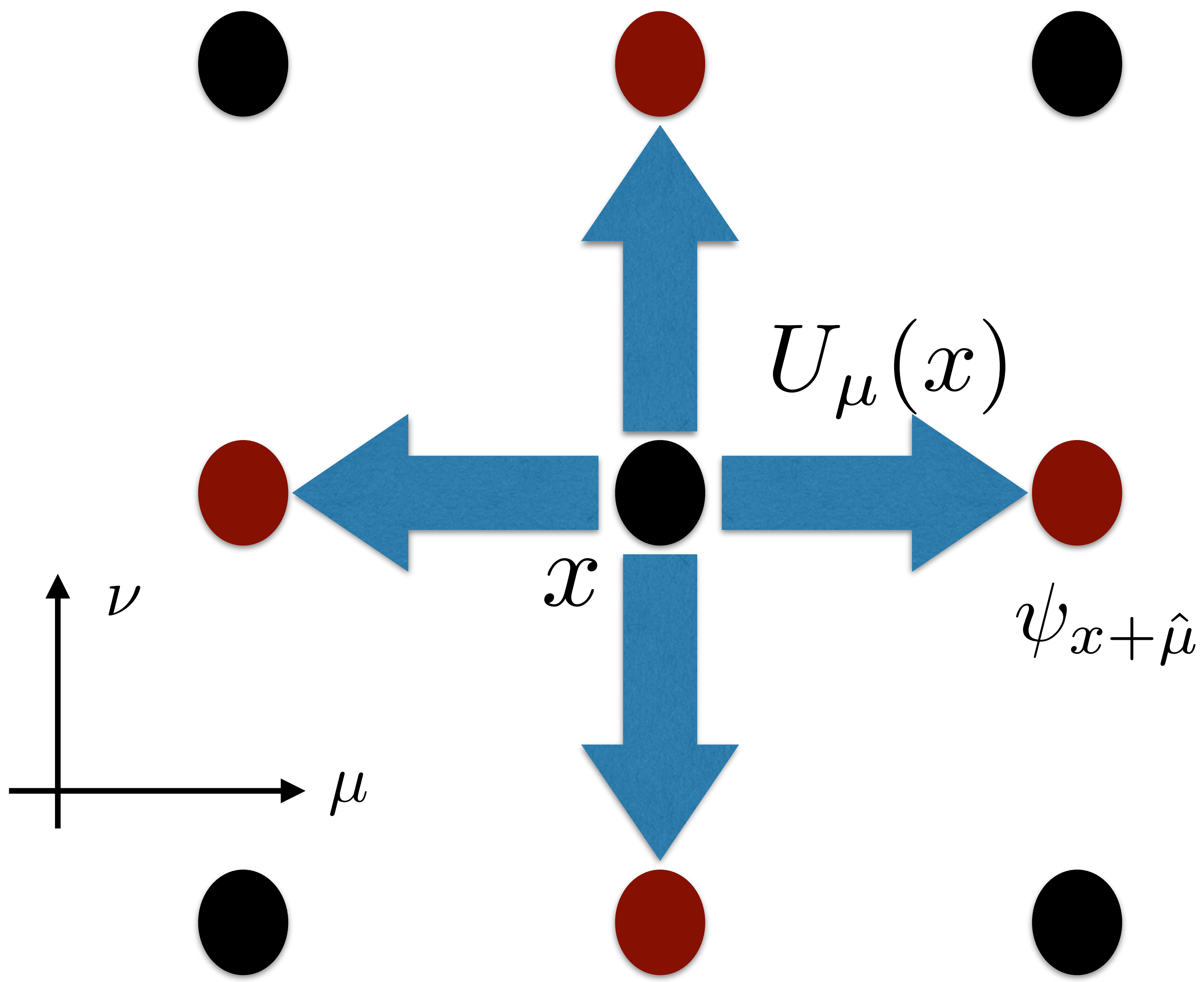
```
int N=…  // Some large number
View<double[N]> x("x");
View<double[N]> y("y");
double  a = 0.5;

parallel_for(N,
     KOKKOS_LAMBDA(const size_t i) {
              y(i) += a*x(i);
          }
);
```

A basic example of a Kokkos Code using Views, parallel_for and C++ 11 lambdas

The Wilson Dslash Operator

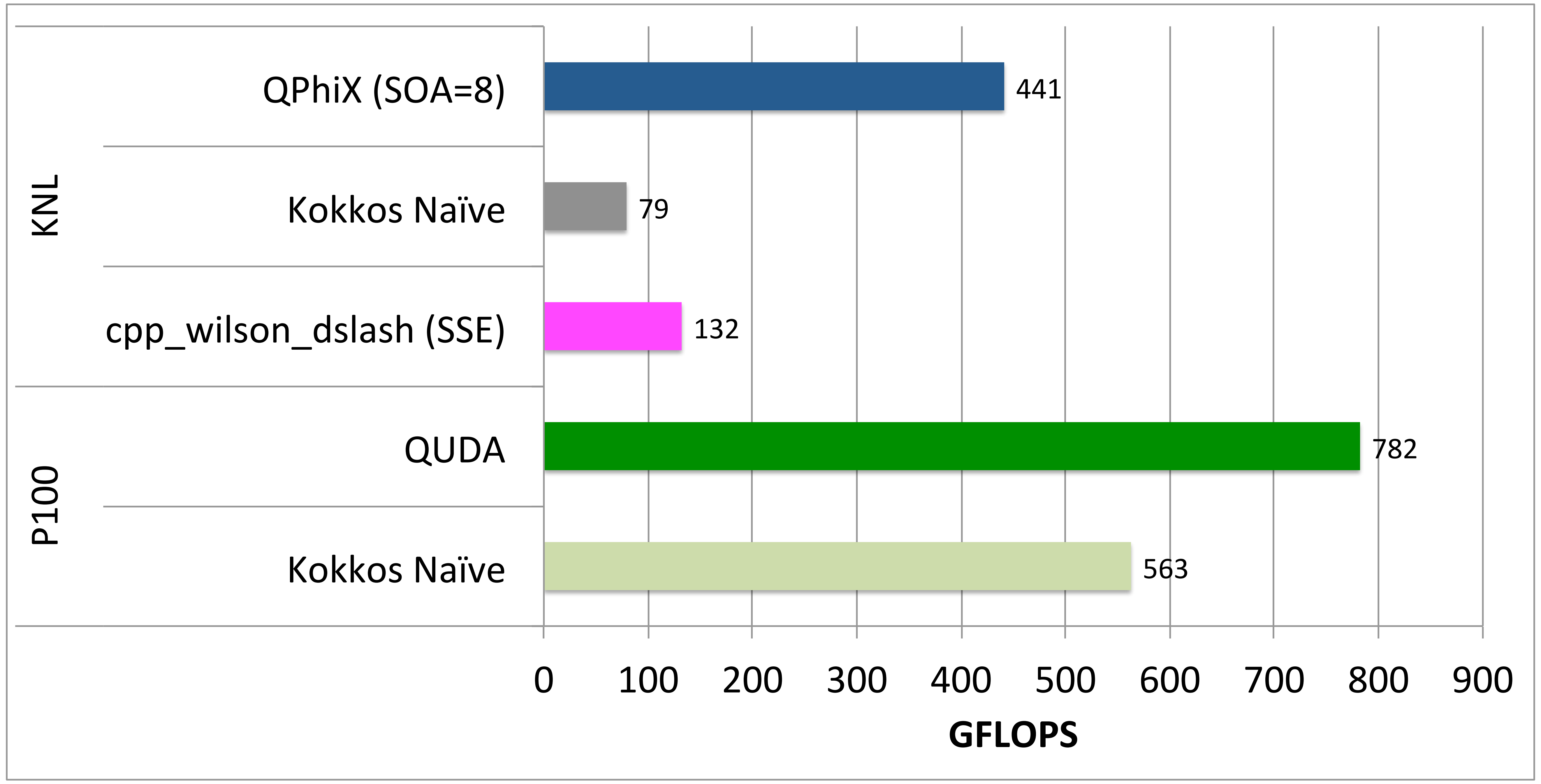
- 4D Sparse Matrix-Vector Operator: $\chi = \not{D}\, \psi$ (SRHS)
- For each neighboring site
  - project 4x3 spinor on the site to 2x3-spinor
  - multiply spinor components by a 3x3 matrix (2 multiplies)
  - reconstruct 4x3-spinor result and accumulate
- Both spinors and 3x3 matrix use complex numbers
- 3x3 matrices and vectors: **tricky to vectorize**
  - Vectorize over lattice sites: BFM, QPhiX, BNL-code…
  - Or over RHS vectors for: $\chi_i = \not{D}\, \psi_i$ i=1,2,…. (MRHS)
- MRHS allows reuse of gauge fields
  - useful even if one vectorizes over the sites (BNL, QUDA)



$$\not{D}_{x,y}\, \psi_y = \sum_\mu (1-\gamma_\mu)\, U_\mu(x)\, \psi_{x+\hat{\mu}} + (1+\gamma_\mu)\, U^\dagger_\mu(x-\hat{\mu})\psi_{x-\hat{\mu}}$$

Initial Kokkos Results (SRHS)

- KNL
  - Performance was very low
  - Even lower than previous legacy codes
  - ***Reason: no (auto) vectorization***
    - 3x3 matrices, 3 vectors
- GPU
  - Initially large amount of register spill to local memory
  - Needed to adjust CUDA launch bounds for kernels (Kokkos::LaunchBounds policy) - Kokkos team has since fixed this default
  - After this performance was pretty good

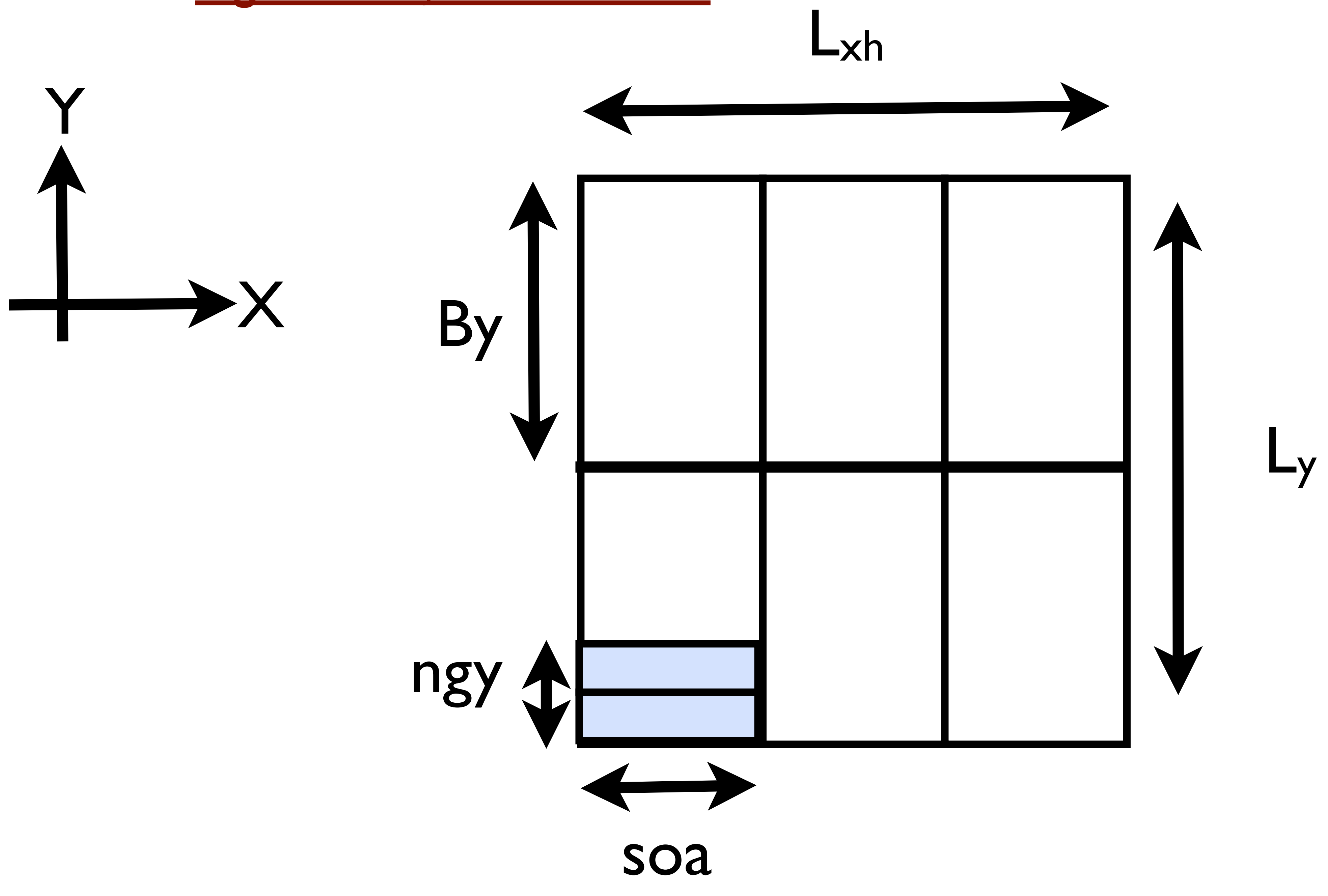


Single RHS Dslash Performances: Vol=32x32x32x32 sites

Site-wise vectorization schemes

X-Y Tiling, e.g. QPhiX (idea by D. Kalamkar)

e.g. B. Joo, et. al. ISC'13

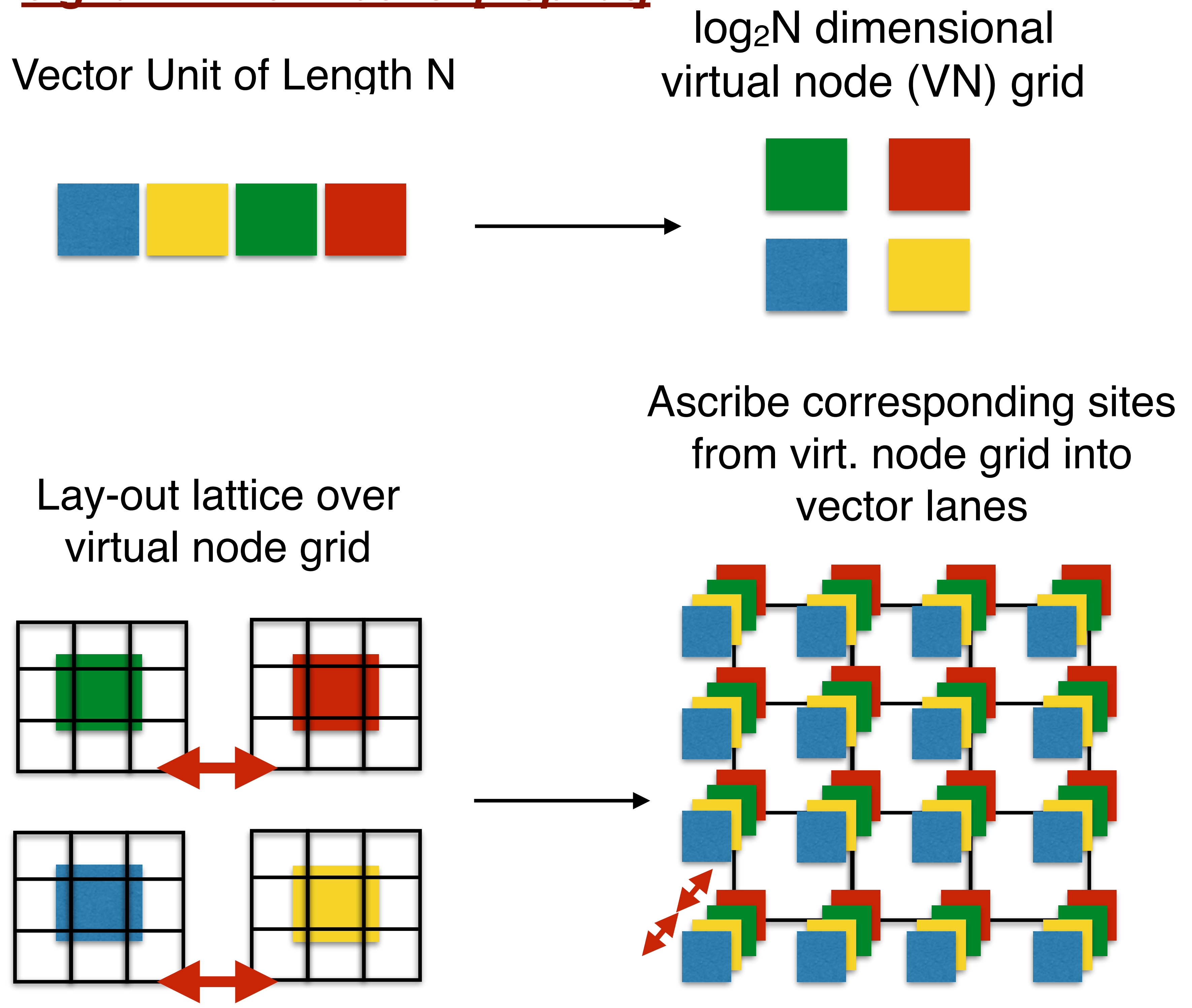


Assemble full Vector from ngy x soa pieces:

- *e.g. ngy=4, soa=4, ngy=2 soa=8, or general gather*
- *unaligned loads for some neighbors in x-y plane*
- *user now has to choose soa to suit problem*

Virtual Node Vectorization (P. Boyle, e.g. in Grid, BFM)

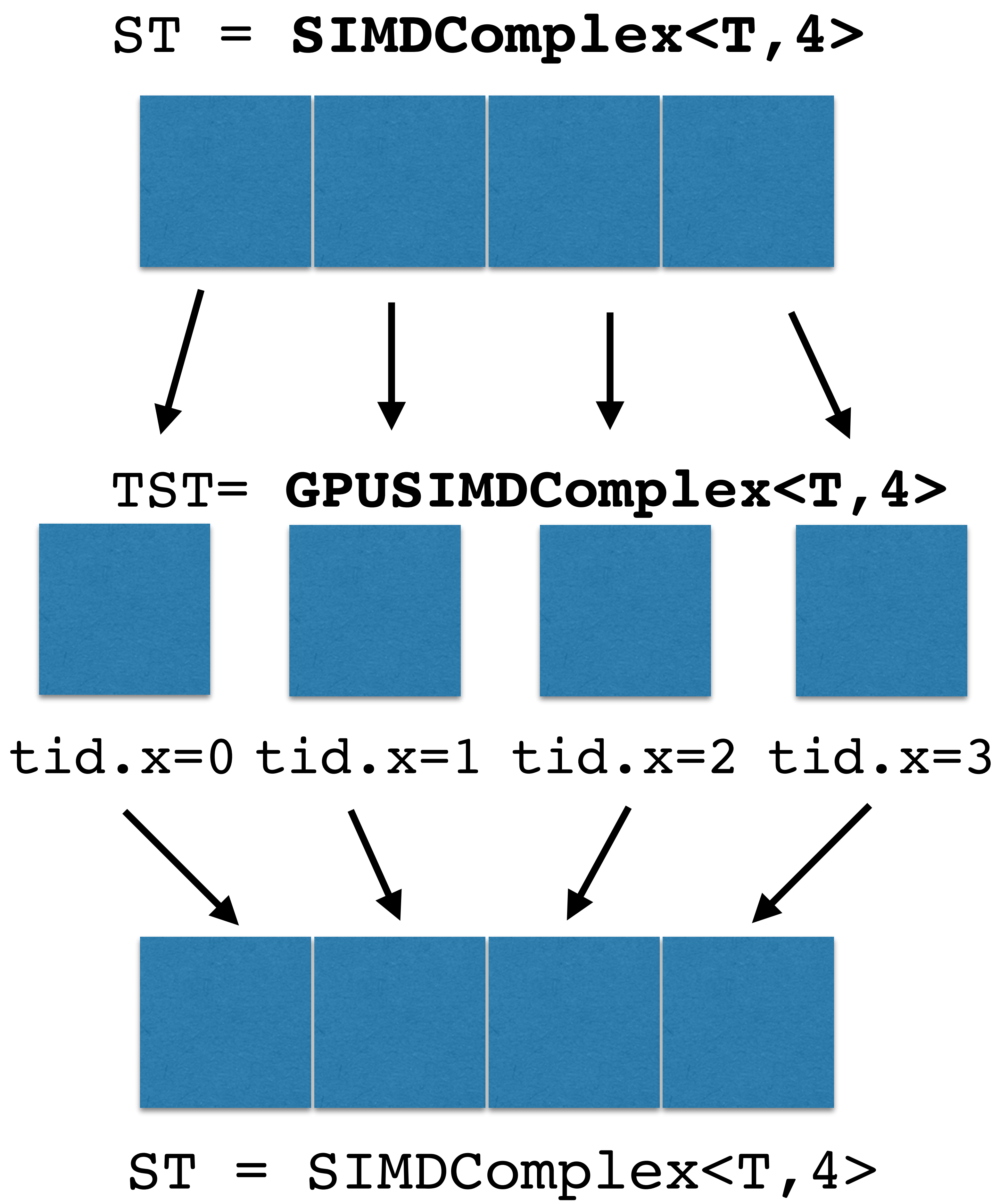
e.g. arXiv:1512.03487[hep-lat]



Nearest neighbor from other VN :
data from other lane => lane permutations

Vectorization And GPUs

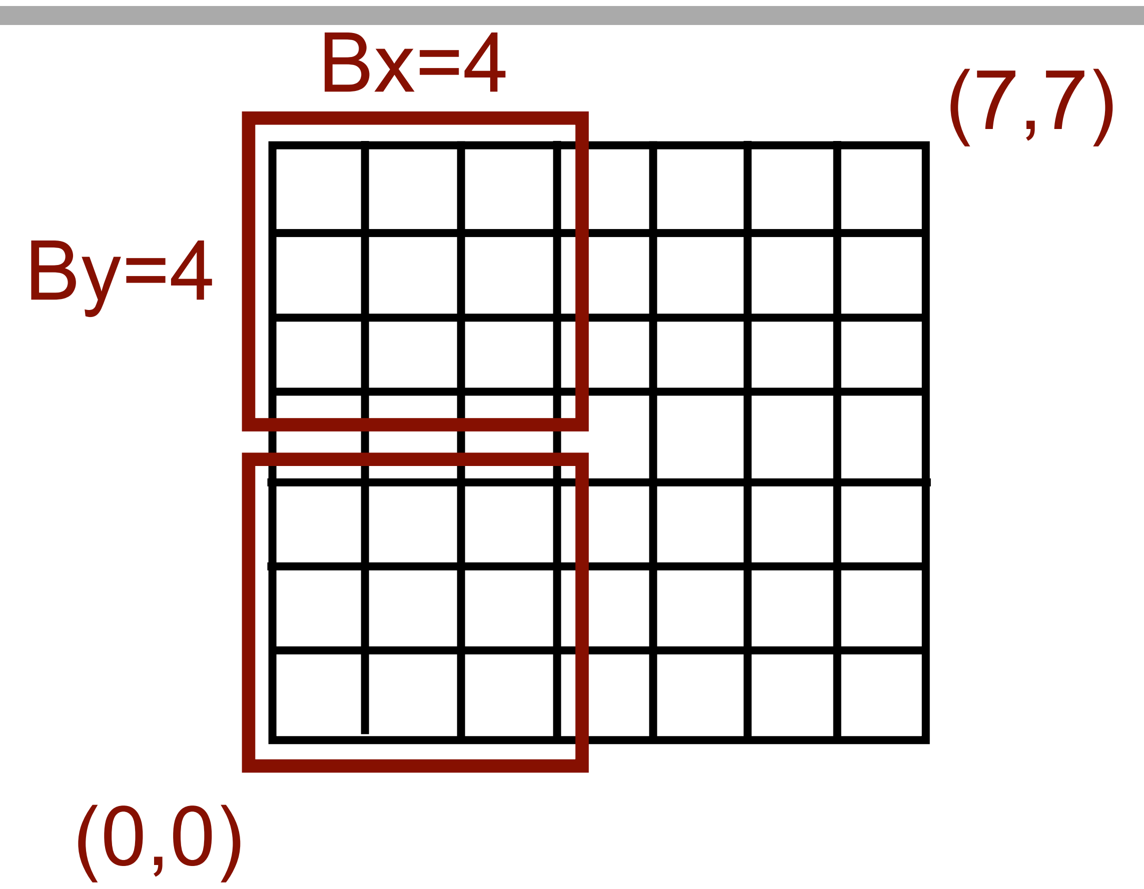
- What does it mean to `vectorize' for GPUs ?
- Approach 1: Use warp threads as vector lanes
  - Kokkos implements with "ThreadVectorRange"
    - x-dimension of thread block for CUDA
    - loop + maybe #pragma ivdep fo OpenMP
- Approach 2: GPU Vector Length is 1
  - Vector code reduces to unvectorized on GPU
  - This is fine, since 'unvectorized' was already good.
- Implemented Approach 1 for MRHS case
- Implemented Approach 2 for SRHS case
  - used 'Grid'-like Virtual Node approach



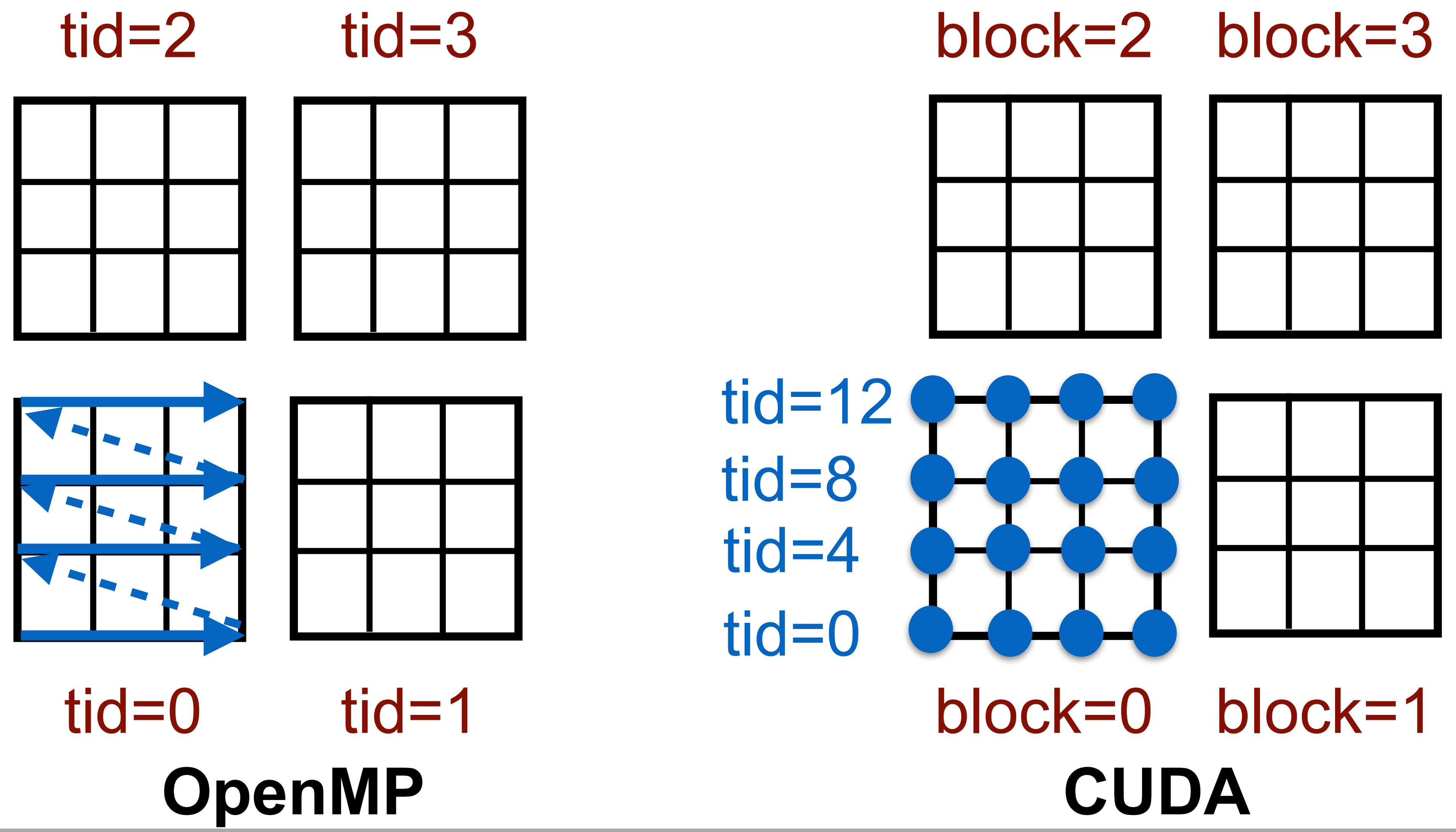
Schematic of Approach 1 on GPU: TST is a type for thread-local objects.

Other Optimizations

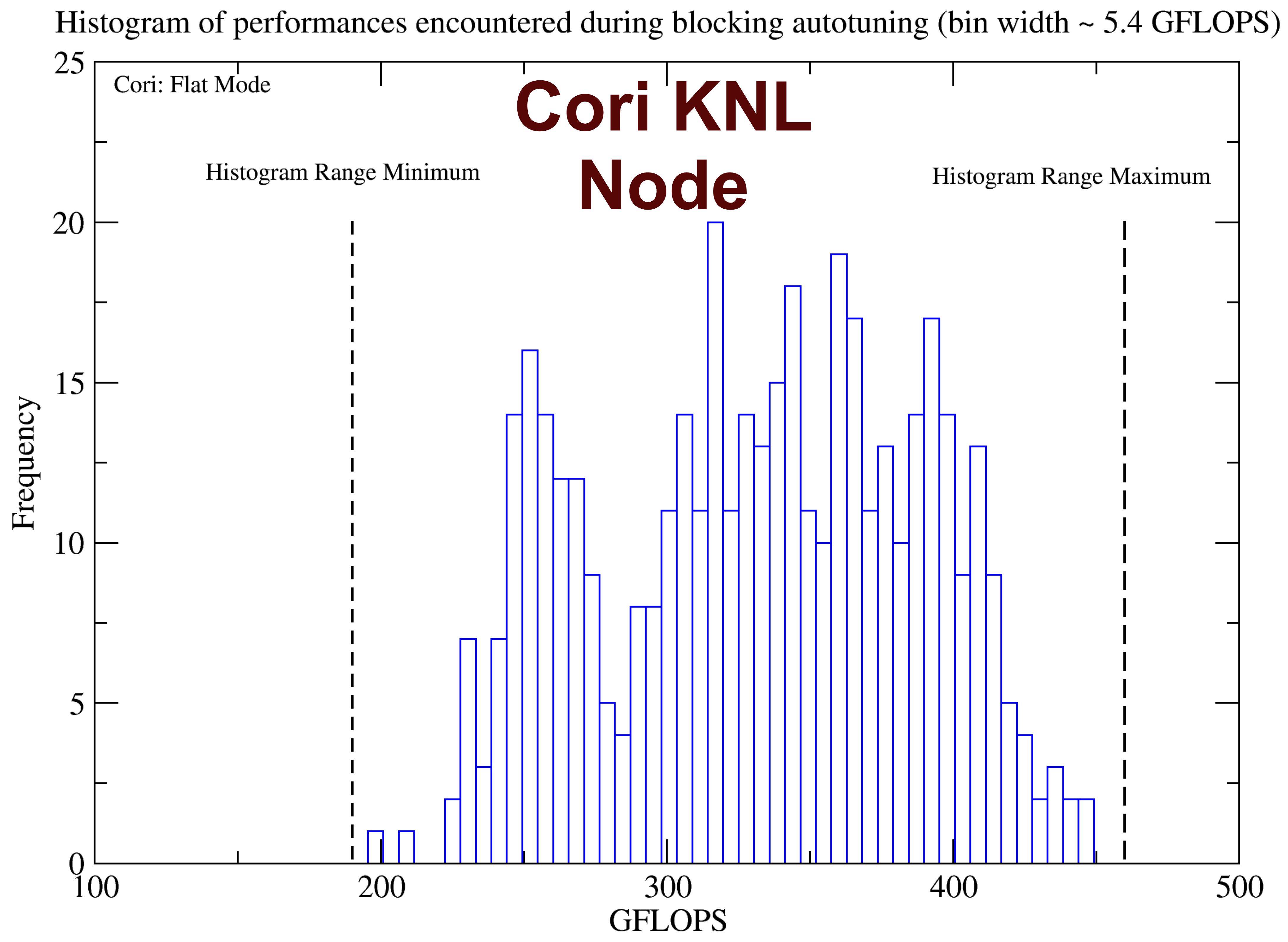
- Vectorize VN permutes using AVX512 intrinsics
  - using `_m512_permutexvar_ps()`
- spin <-> color loop interchange (help L1 locality)
- 4D Blocking using Kokkos::MDRange exec. policy
  - tune block size for performance
- Gauge Field Access:
  - keep copies of back pointing links => unit stride access for gauge fields
  - KNL: pre-permute links from back neighbor: no gauge permute in Dslash
- GPU: derived complex number class from float2

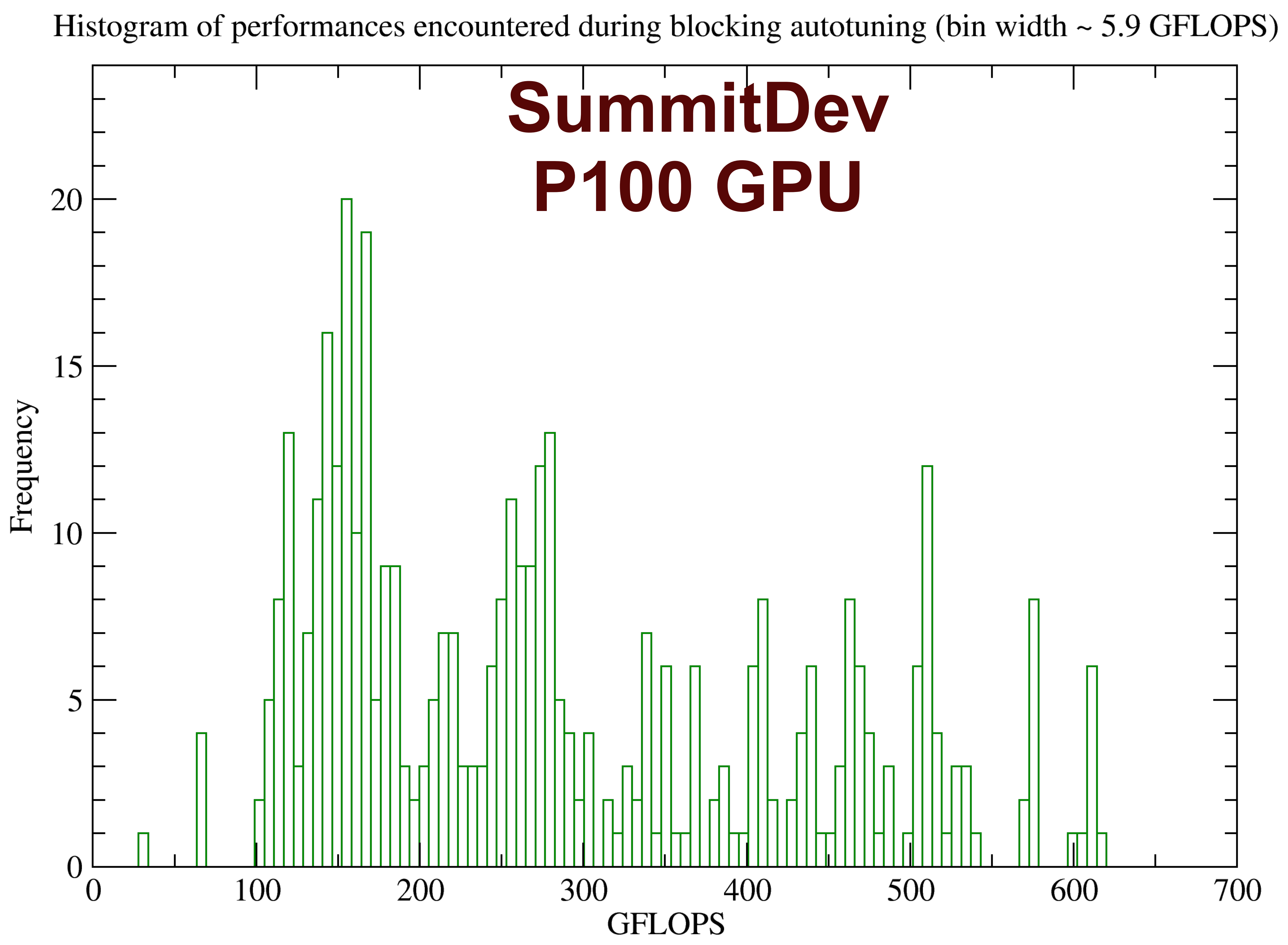



```
MDRangePolicy<2,IterateLeft,IterateLeft>
                    policy({0,0},{8,8},{4,4});
```



Block Tuning for MDRange

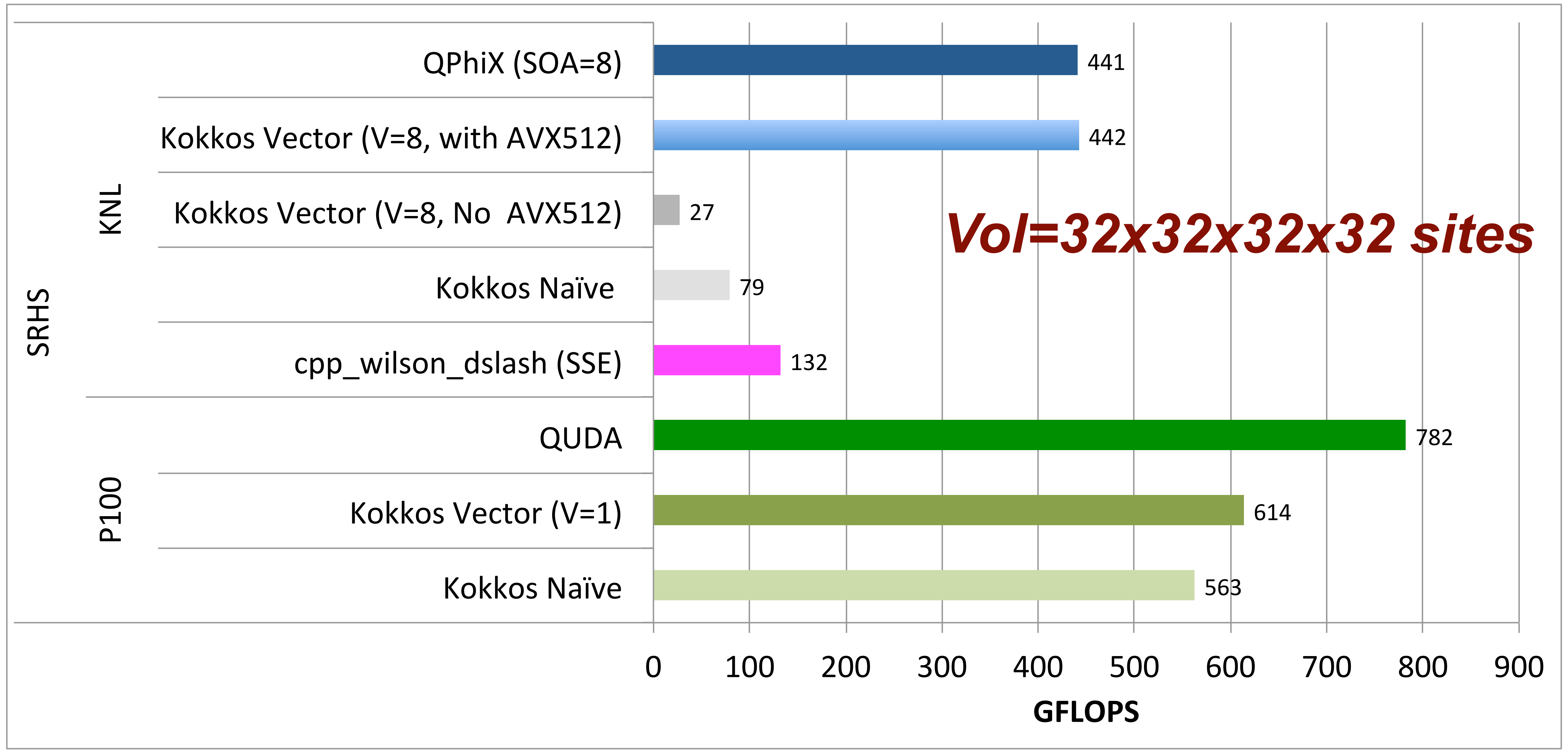


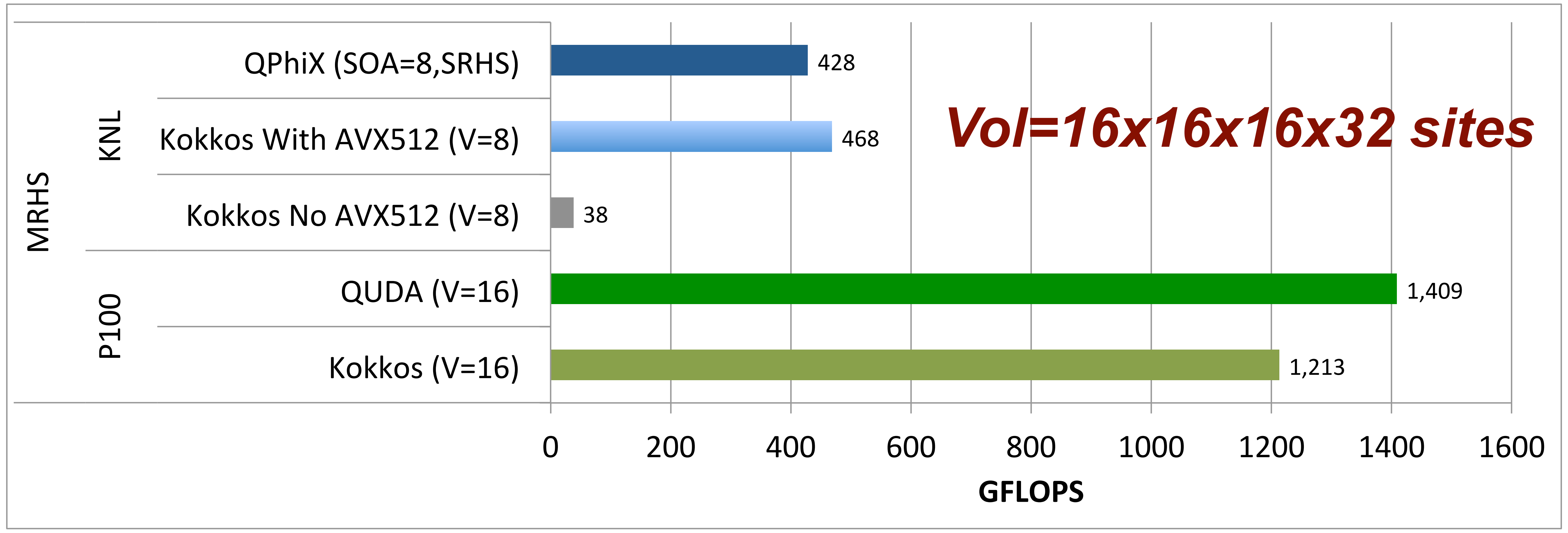


- Block Tuning gave broad performance distributions, with few (<10) tunings giving the highest performance. Autotuning is a must & unfortunately the space is big (4D).

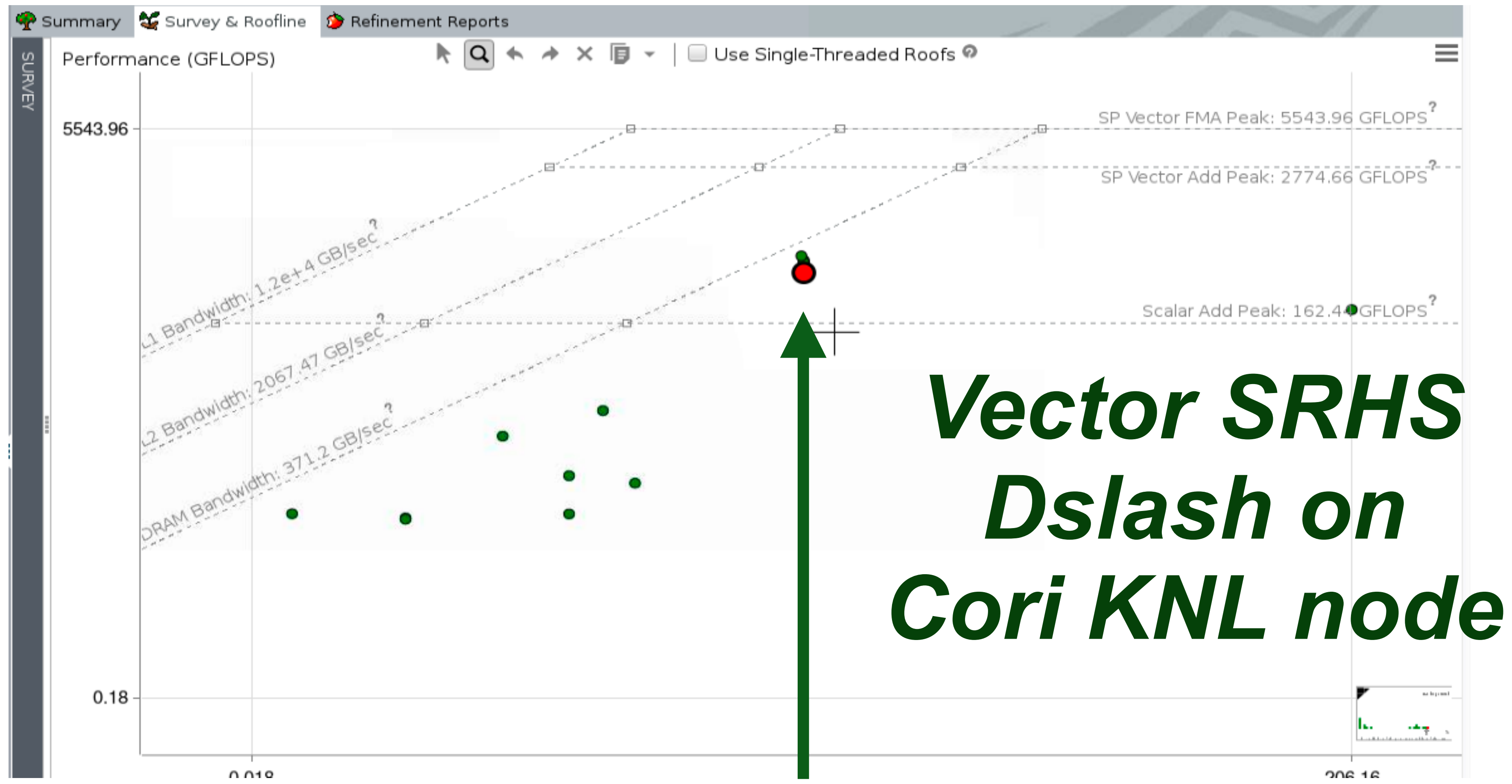
Current Performance Summary

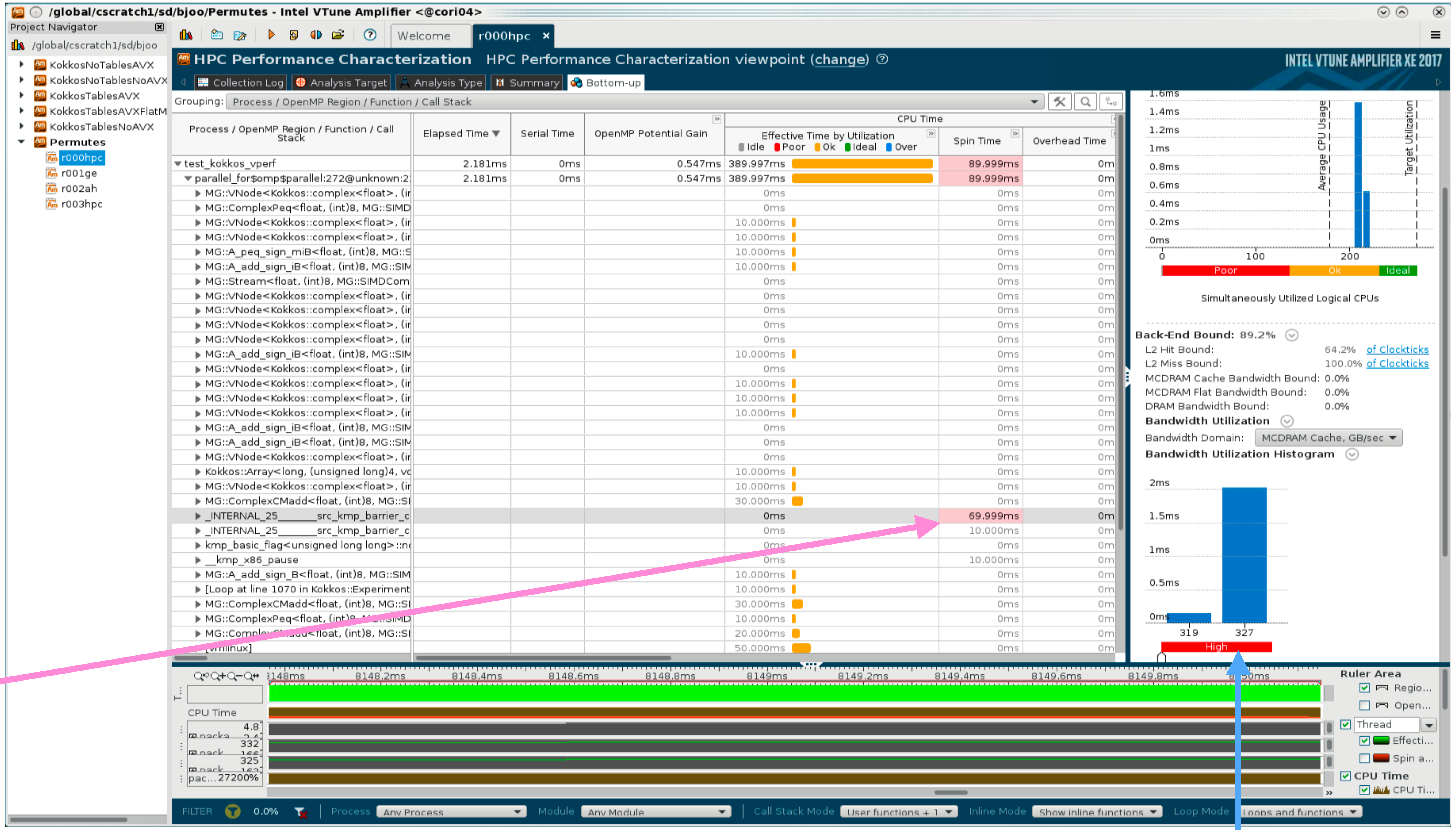
- SRHS Case:
  - ***Kokkos Vectorized Dslash with AVX512 and tuned blocking matches QPhiX on Cori KNL node (68 cores, 272 threads)***
  - Unvectorized & No AVX cases are slow
  - Kokkos Naive CUDA version is 72% of QUDA on P100 (SummitDev)
  - ***Vectorized (but V=1) QUDA version benefits from block tuning, memory & locality optimizations and md_parallel_for: 79% of QUDA on P100 (SummitDev)***
- MRHS Case:
  - ***Kokkos With AVX512 exceeds corresp. QPhiX SRHS performance on Cori KNL node for 8 RHS***
  - Kokkos Without AVX512 is very slow
  - ***Kokkos CUDA version is 86% of QUDA for 16 RHS on SummitDev (P100)***





Absolute Performance is good too

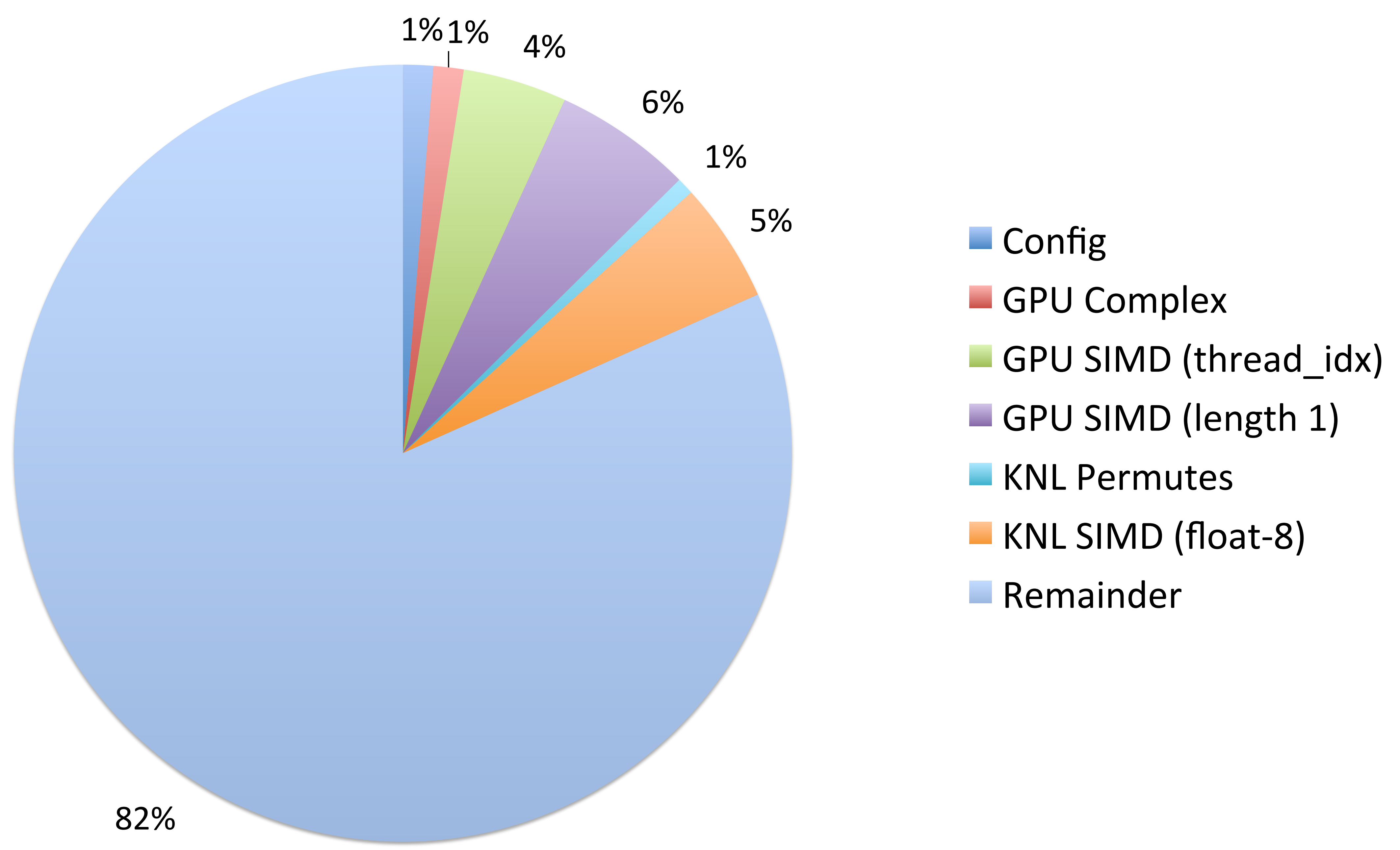




- Little Below Roofline. Reported L1 AI=1.97
- Vtune is concerned with spin wait in barrier
- Good CPU usage and mem BW Usage

How much Non-portable stuff is there?

- Total code is 4545 lines of code
  - excluding unit tests which bring it to 7100
- KNL Specific (AVX512) : 274 lines
  - permutes for Virtual Node 34 lines
  - complex ops for float-8 SIMD: 240 lines
- GPU Specific:
  - Derive complex from float2: 60 lines
  - Warp SIMD type & ops (threadIdx.x): 207 lines
  - Length=1 SIMD ops: 275 lines (repeat of scalar)
- Select GPU/CPU Layout, types etc: 60 lines



Line counts are 'approximate'
Carried out by outlining machine specific parts and using SLOCCount

Summary and Conclusions

- Kokkos freed us from the need to deal directly with OpenMP pragmas, CUDA etc
- It did not save us from having to optimize.
- On KNL we had to vectorize our complex arithmetic and permutations with intrinsics
  - ~274 LOC out of ~4500 and we would need to repeat for double prec, other AVX flavors, etc.
  - Kokkos implementing an optimized complex SIMD type could move this burden to Kokkos
- We needed a performance portable algorithm
  - a vector friendly algorithm, i.e. MRHS or Virtual Node vectorization over sites
  - on GPUs use Warp threads as Vector Lanes or have GPU Vector length = 1.
- Excellent performance on both KNL and GPU after optimzations and block tuning.
- Future work: Parallelize over nodes with MPI, interface with Trilinos, …

Acknowledgments

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