Performance and portability of accelerated lattice Boltzmann applications with OpenACC

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Outline

The D2Q37 Lattice Boltzmann Model

- Lattice Boltzmann method (LBM) is a class of computational fluid dynamics (CFD) methods
- LBM methods simulate a discrete **Boltzmann** equation, which under certain conditions, reduce to the **Navier-Stokes** equation
- **virtual particles** called **populations** arranged at edges of a discrete and regular grid are used to simulate a synthetic and simplified dynamics
- the interaction is implemented by two main functions applied to the virtual particles: **propagation** and **collision**
- D2Q37 is a D2 model with 37 components of velocity (populations)
- suitable to study behaviour of **compressible** gas and fluids optionally in presence of **combustion** [1] effects
- correct treatment of *Navier-Stokes*, heat transport and perfect-gas ($P = \rho T$) equations

[1] chemical reactions turning cold-mixture of reactants into hot-mixture of burnt product.

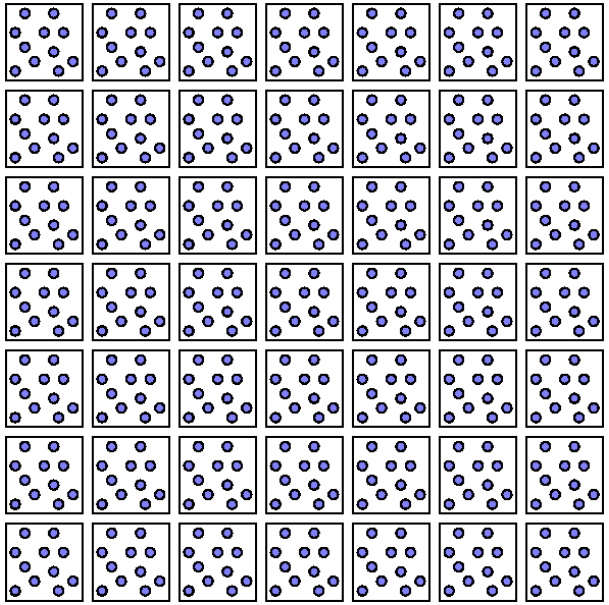
Computational Scheme of LBM

```
foreach time-step

  foreach lattice-point
    propagate();

  foreach boundary-point
    bc();

  foreach lattice-point
    collide();
```



Embarassing parallelism

Sites can be processed in parallel applying in sequence propagate and collide

Challenge

Design an efficient implementation to exploit a large fraction of available peak performance on different heterogeneous architectures

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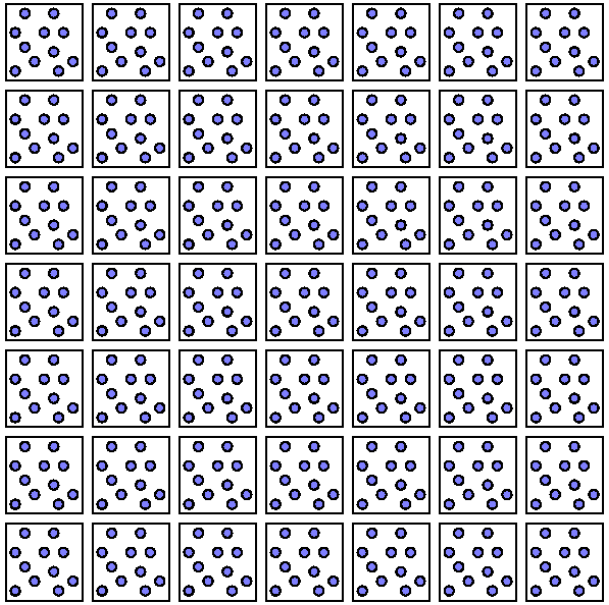

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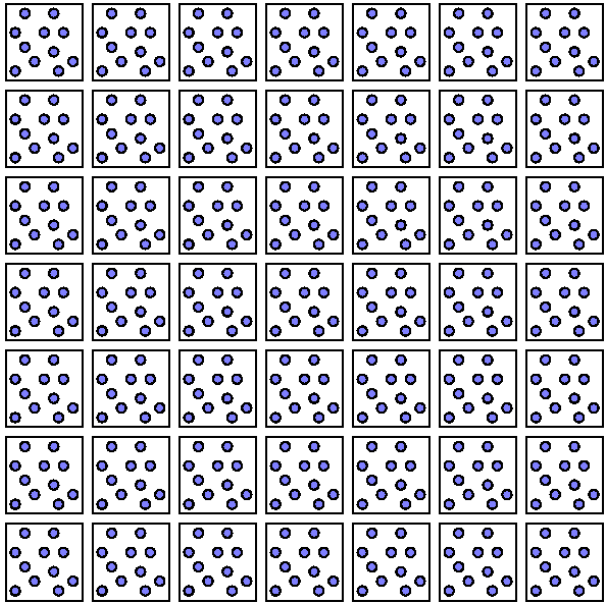

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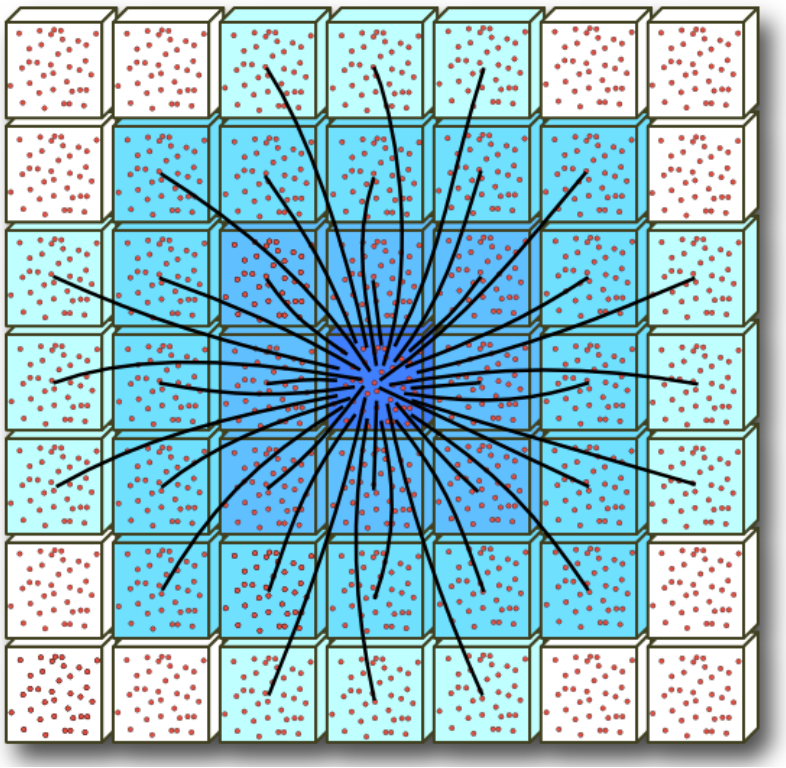
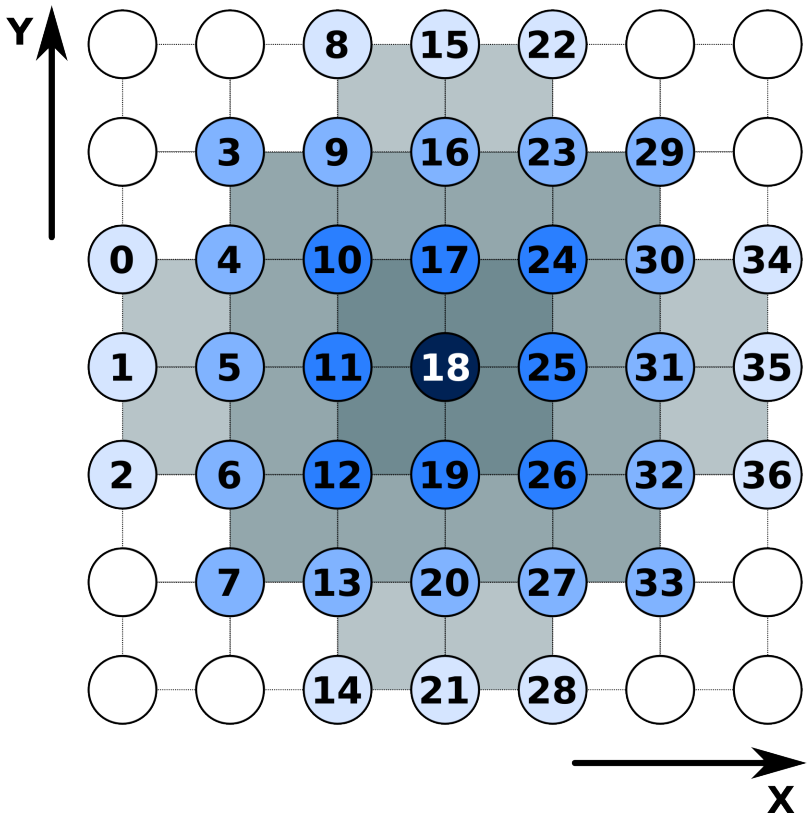
D2Q37: propagation scheme

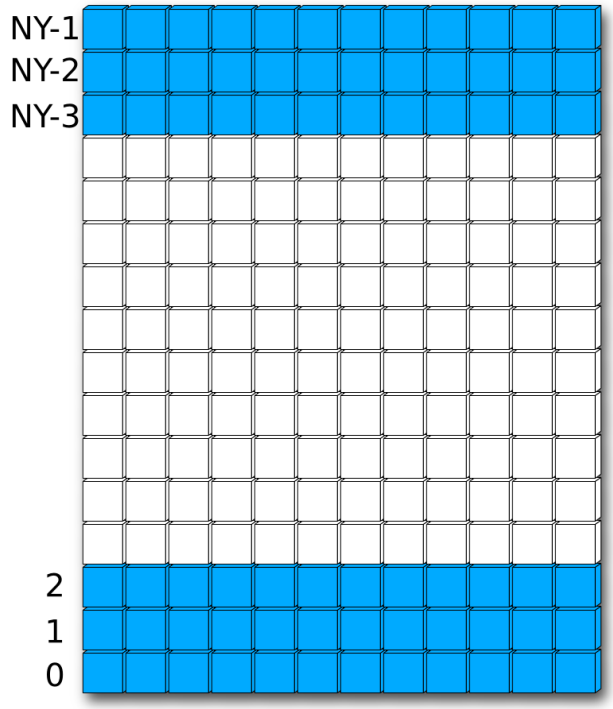




- require to access neighbours cells at distance 1,2, and 3,
- generate memory-accesses with **sparse** addressing patterns.

D2Q37: boundary-conditions

- we simulate a 2D lattice with period-boundaries along x-direction
- at the top and the bottom boundary conditions are enforced:
  - to adjust some values at sites $y = 0 \ldots 2$ and $y = N_y - 3 \ldots N_y - 1$
  - e.g. set vertical velocity to zero

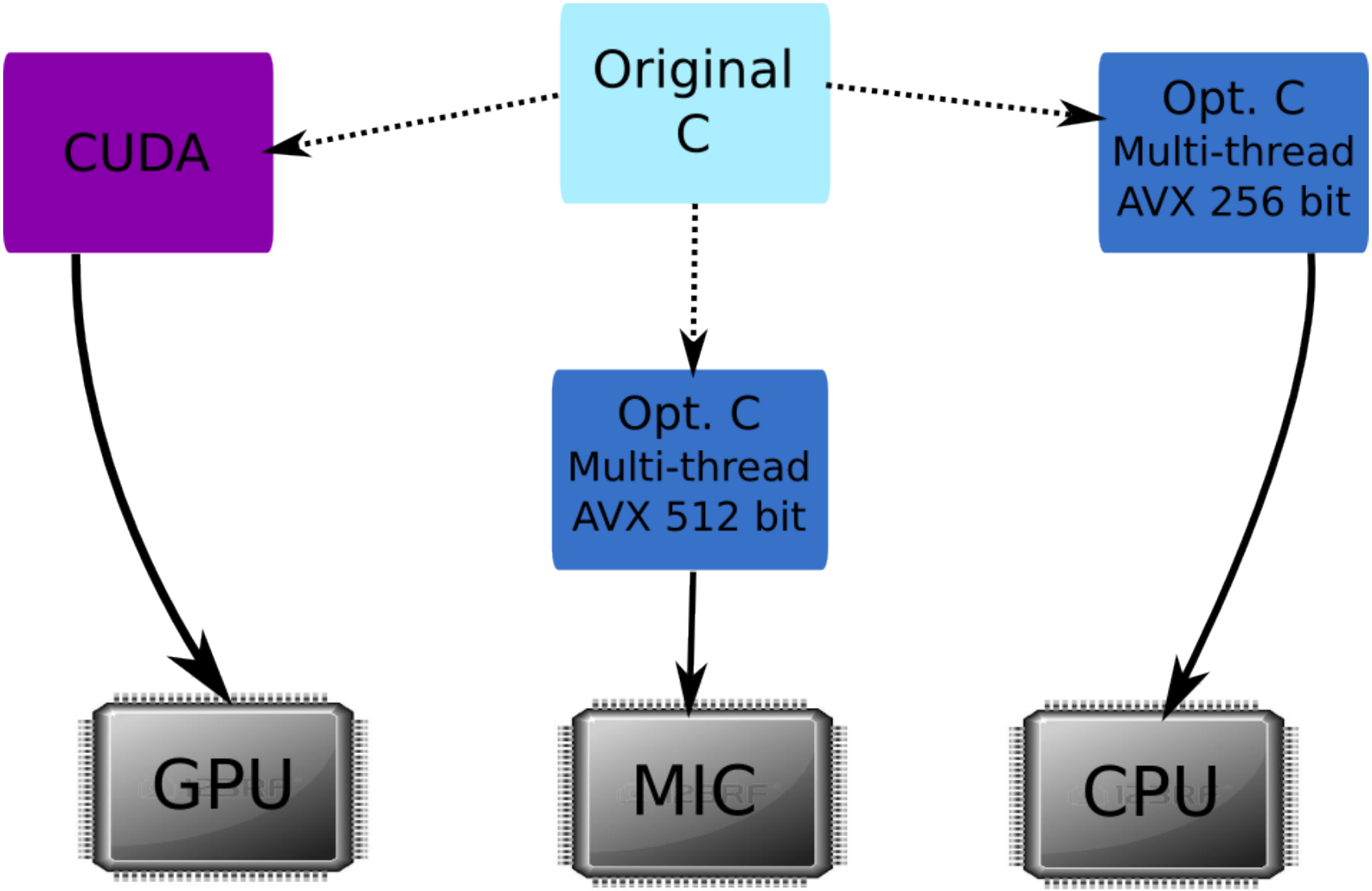


This step (bc) is computed before the collision step.

D2Q37 collision

- collision is computed at each lattice-cell
- computational intensive: for the D2Q37 model requires $\approx$ 7600 DP operations
- completely local: arithmetic operations require only the populations associate to the site

Code implementations



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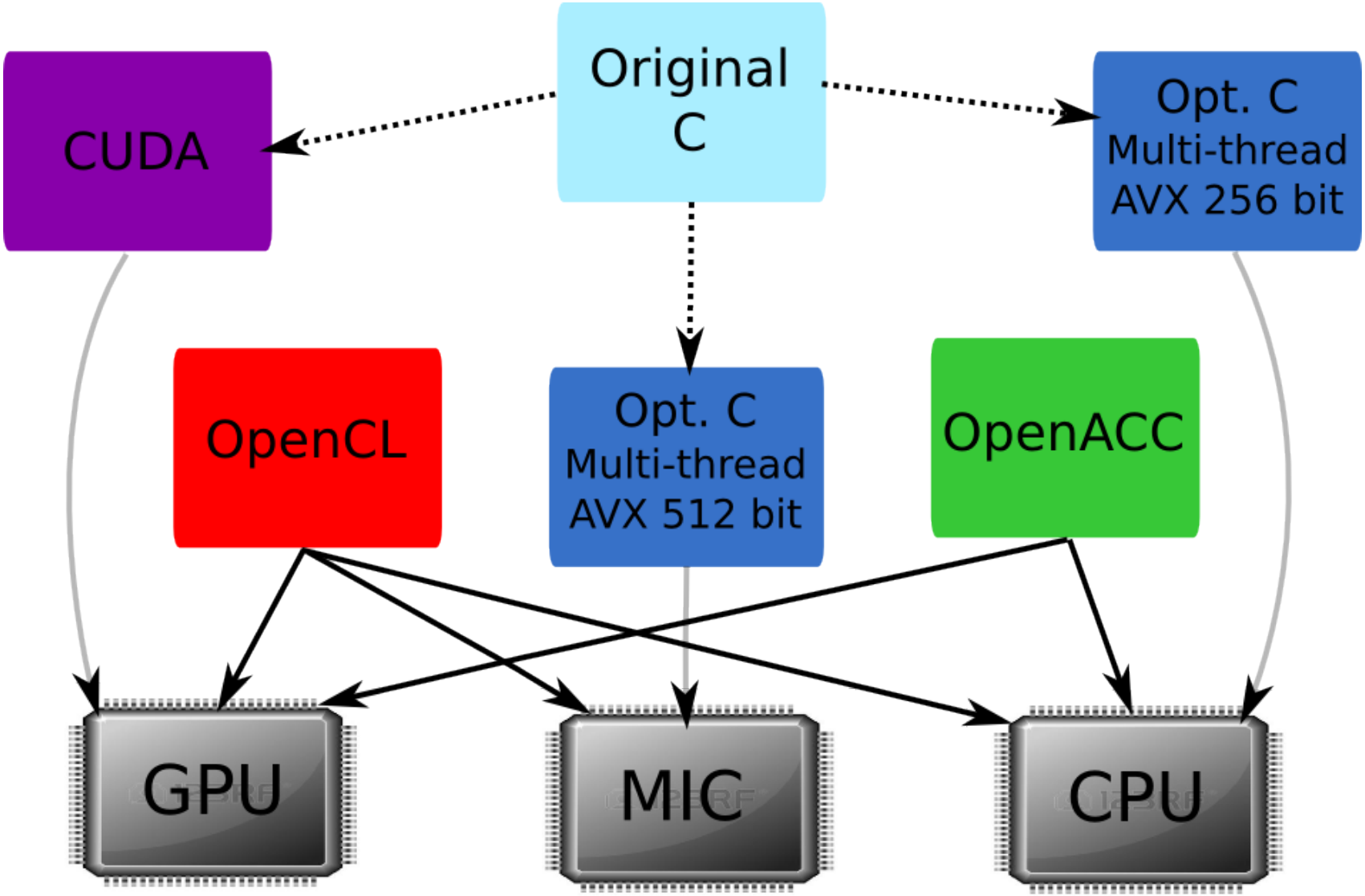


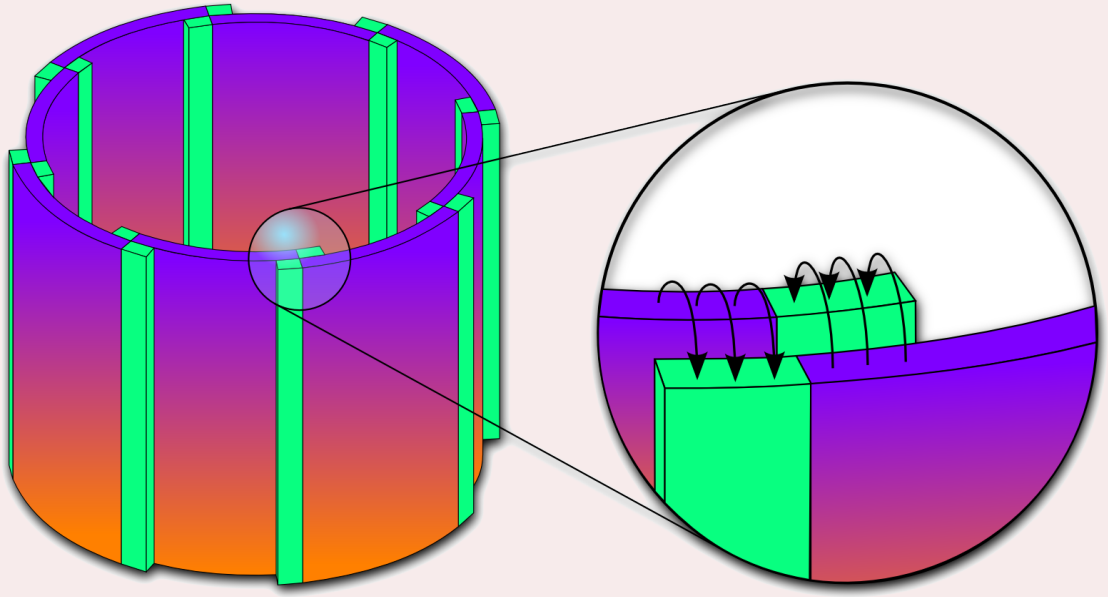
OpenACC example

Propagate function:

```
inline void propagate(const data_t* restrict prv, data_t* restrict nxt ) {

  int ix, iy, site_i;

  #pragma acc kernels present(prv) present(nxt)
  #pragma acc loop gang independent
  for ( ix=HX; ix < (HX+SIZEX); ix++) {
    #pragma acc loop vector independent
    for ( iy=HY; iy<(HY+SIZEY); iy++) {

      site_i = (ix*NY) + iy;

      nxt[           site_i] = prv[           site_i - 3*NY + 1];
      nxt[   NX*NY + site_i] = prv[   NX*NY + site_i - 3*NY    ];
      nxt[ 2*NX*NY + site_i] = prv[ 2*NX*NY + site_i - 3*NY - 1];
      nxt[ 3*NX*NY + site_i] = prv[ 3*NX*NY + site_i - 2*NY + 2];
      nxt[ 4*NX*NY + site_i] = prv[ 4*NX*NY + site_i - 2*NY + 1];
      nxt[ 5*NX*NY + site_i] = prv[ 5*NX*NY + site_i - 2*NY    ];
      nxt[ 6*NX*NY + site_i] = prv[ 6*NX*NY + site_i - 2*NY - 1];

 ...
```

Multi-GPU implementation using MPI

Before each iteration, processes swap halos with neighbours



Propagate can not start before halo exchange is completed...

...on sites which are near to the halos!

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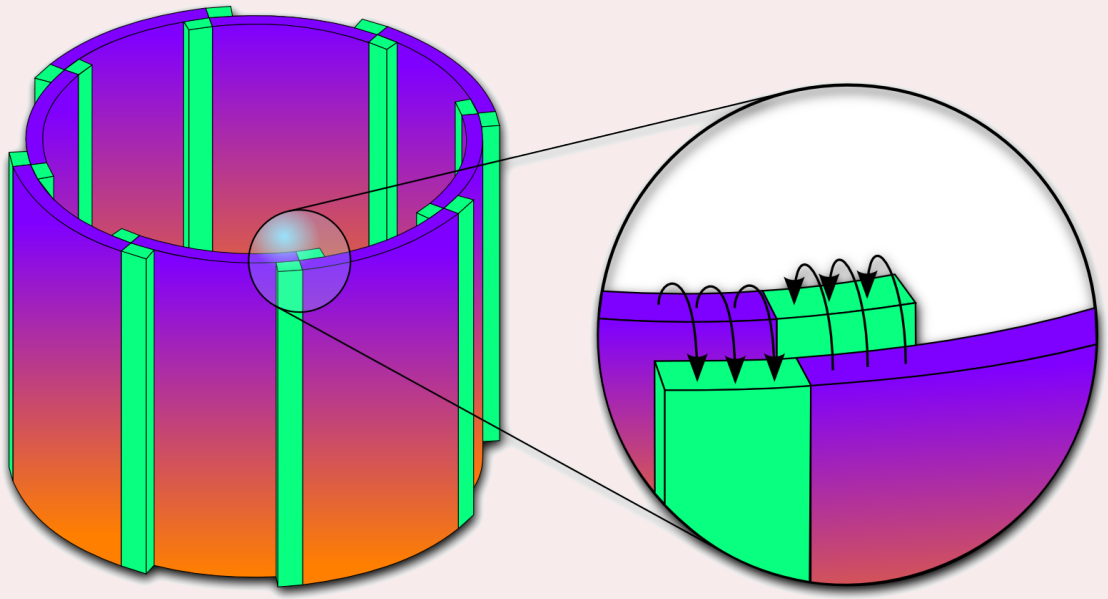

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Overlapping communications with Bulk processing

```
// processing of bulk
propagateBulk( f2, f1 ); // async execution on queue (1)
bcBulk( f2, f1 );        // async execution on queue (1)
collideInBulk( f2, f1 ); // async execution on queue (1)

#pragma acc host_data use_device(f2) {
  for ( pp = 0; pp < 37; pp++ ) {
    MPI_Sendrecv ( &(f2[...]), 3*NY, ... );
    MPI_Sendrecv ( &(f2[...]), 3*NY, ... );
  } }

// processing of the three leftmost columns
propagateL( f2, f1 );    // async execution on queue (2)
bcL( f2, f1 );           // async execution on queue (2)
collideL( f1, f2 );      // async execution on queue (2)

// processing of the three rightmost columns
propagateR( f2, f1 );    // async execution on queue (3)
bcR( f2, f1  );          // async execution on queue (3)
collideR( f1, f2  );     // async execution on queue (3)
```

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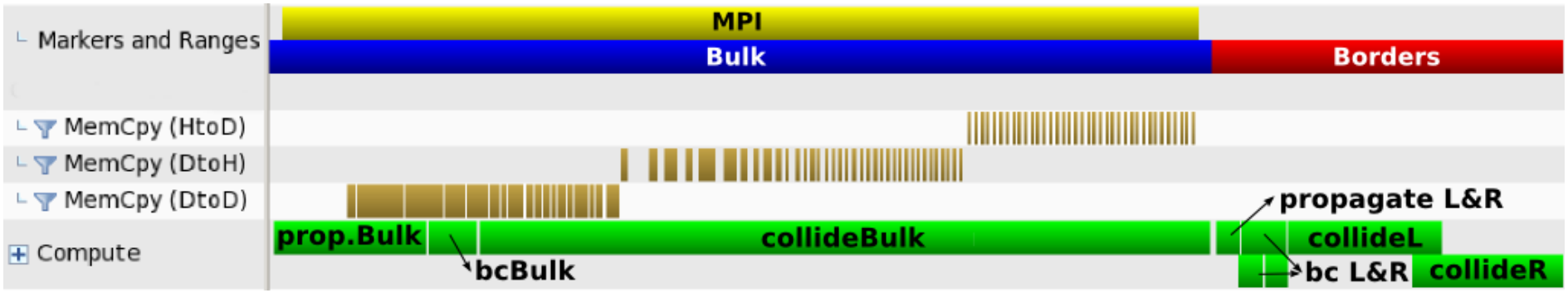

Scalability Model

We model the execution time of the whole program as $T \approx \max\{T_a, T_b\}$

$$T_a = T_{\text{bulk}} + T_{\text{borderL}} + T_{\text{borderR}} \ , \qquad T_b = T_{\text{MPI}} + T_{\text{borderL}} + T_{\text{borderR}}$$

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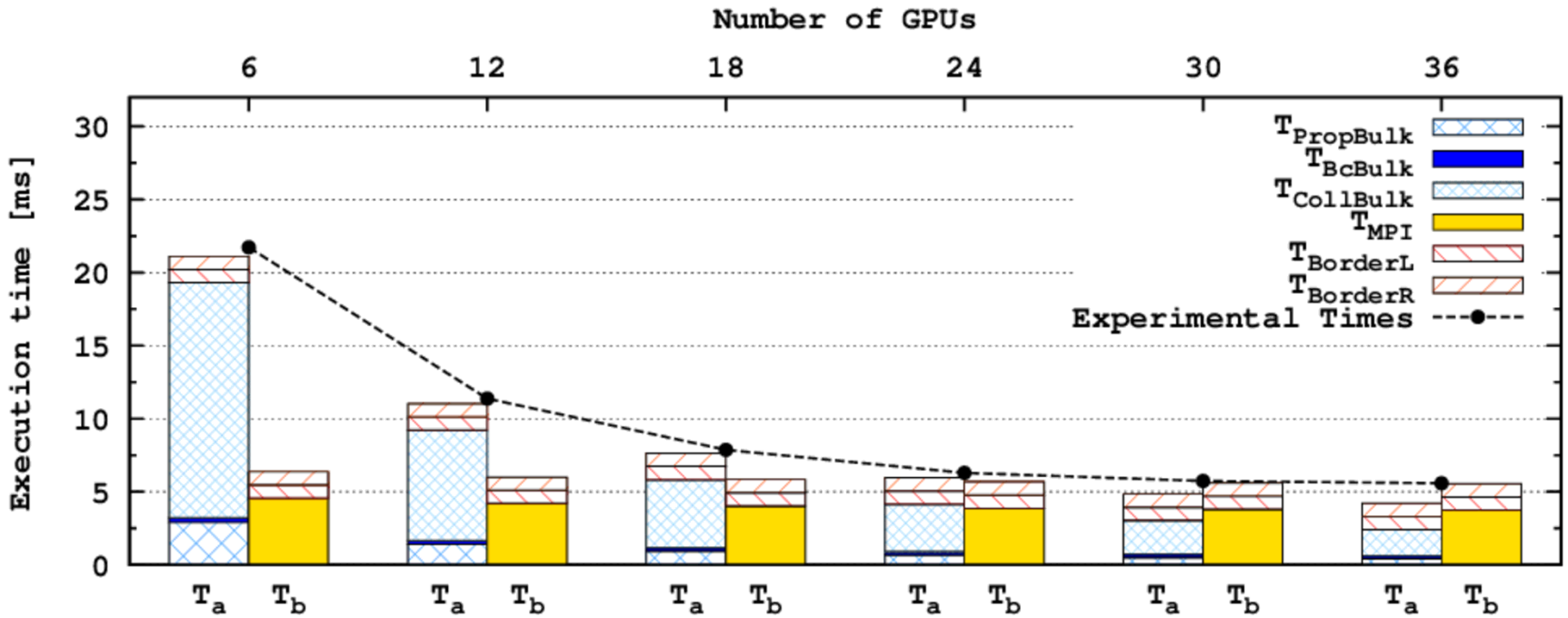
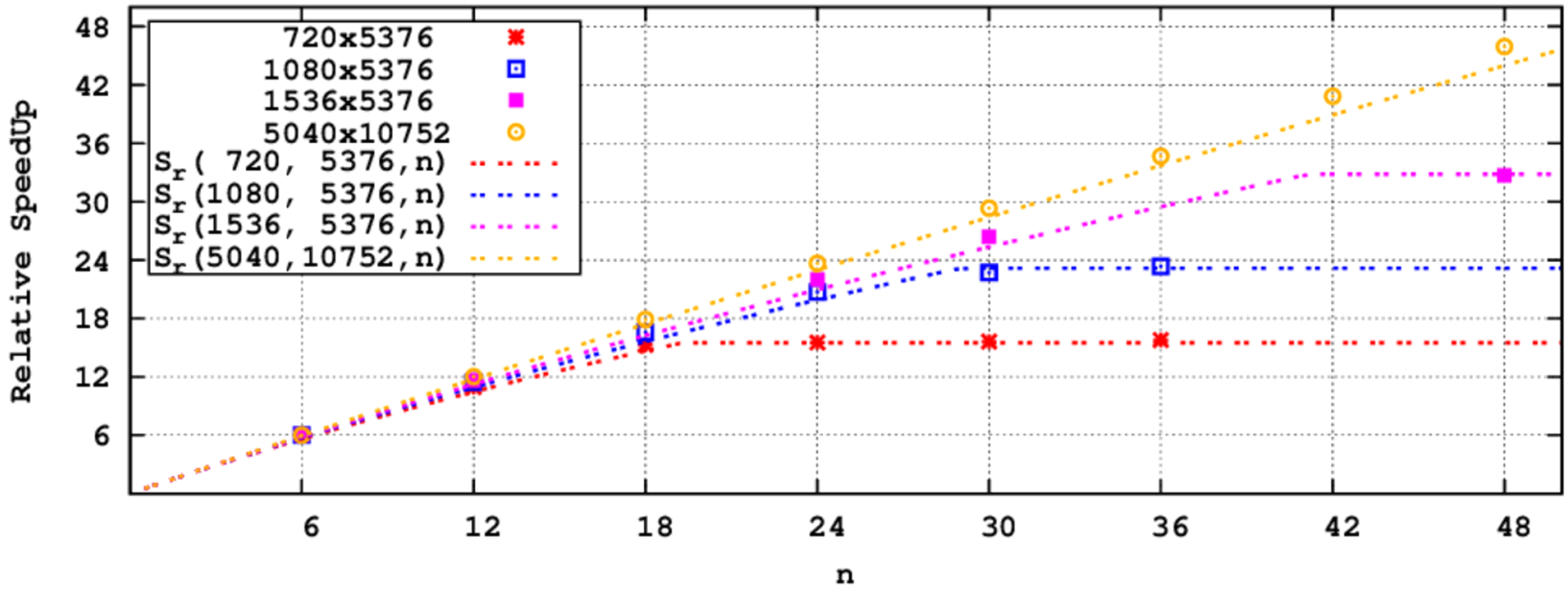


A General Model to predict Strong Scaling

Given that: bulk processing is proportional to $(L_x \times L_y)$; boundary conditions scale as L_x; communication and borders processing scales as L_y;

$$T(L_x, L_y, n) = \max\left\{\alpha\frac{L_x}{n}L_y + \beta\frac{L_x}{n}, \quad \gamma L_y\right\} + \delta L_y$$

$$S_r(L_x, L_y, n) = \frac{T(L_x, L_y, 1)}{T(L_x, L_y, n)}$$



Straightforward portability

Target architecture for the compilation is specified by appropriate options to the PGI compiler:

- `-ta=nvidia` for NVIDIA GPUs
- `-ta=radeon` for AMD GPUs
- `-ta=multicore` for *x*86 multicore CPUs (since PGI 15.9)

But, what about performances?

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Architectures specs and results

	Intel Xeon	NVIDIA K80	AMD S9150
processor codename	E5-2630 v3	GK210	Hawaii XT
#physical-cores	8	13 x2	44
#logical-cores	16	2496 x2	2816
nominal clock Freq. (GHz)	2.1	0.562	0.900
Max Boosted clock Freq. (GHz)	2.6	0.875	–
Nominal GFLOPS (DP)	269	935 x2	2530
Boosted GFLOPS (DP)	331.56	1455 x2	–
Mem Bandwidth (GB/s)	59	240 x2	320

	E5-2630 v3	GK210	Hawaii XT
propagate [GB/s]	10	155	216
collide [MLUPS]	8	55	53

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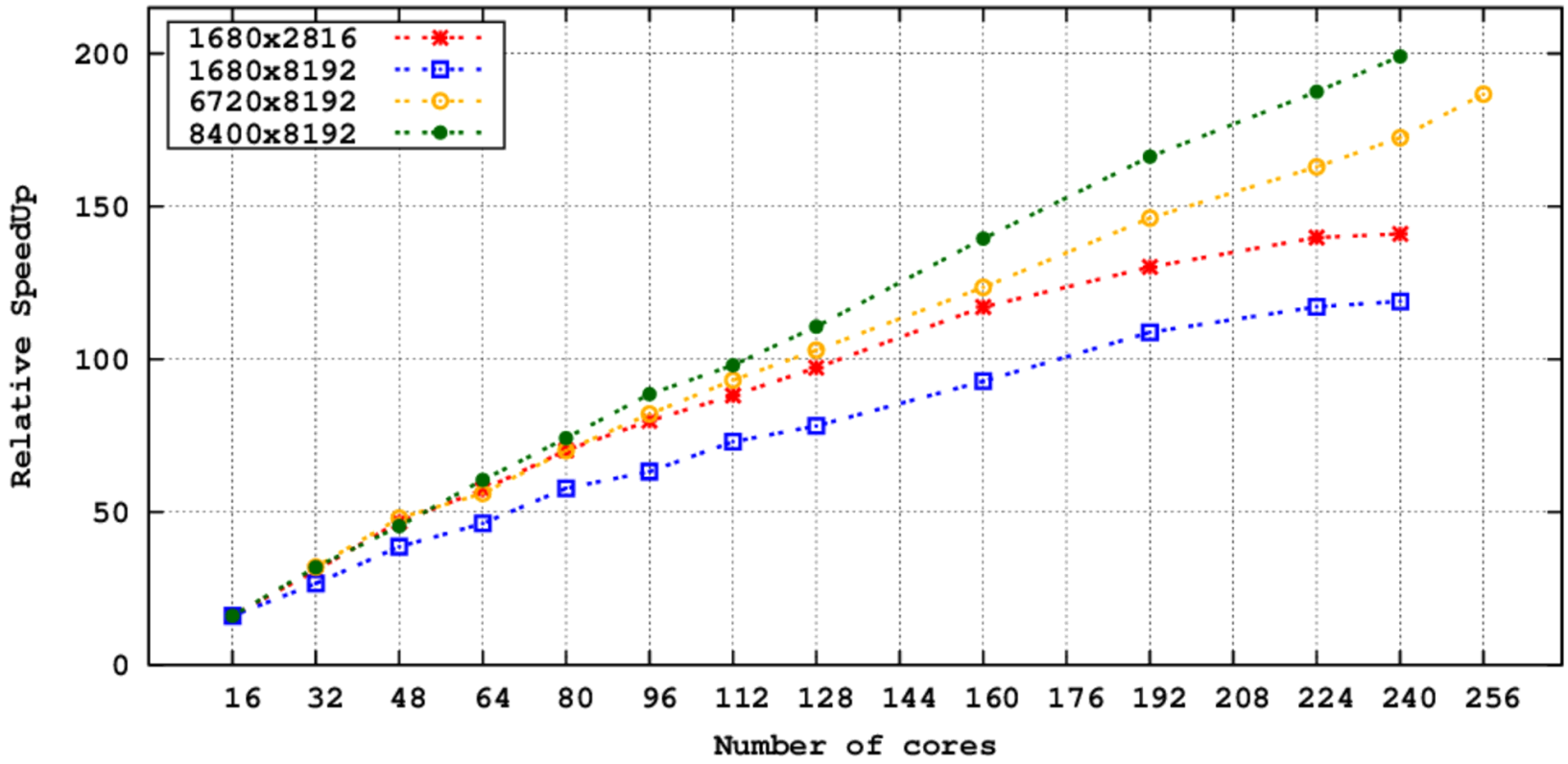
Using a bit of architecture specific optimizations

```
#pragma acc kernels present(prv) present(nxt)
#pragma acc loop gang independent
for ( ix=HX; ix < (HX+SIZEX); ix++) {
  site_i = (ix*NY);

  #pragma acc loop seq independent
  for ( ipop=0; ipop<37; ipop++ ) {

    #pragma acc loop vector independent
    for ( iy=HY; iy < (HY+SIZEY); iy++) {
      nxt[ipop*NX*NY+site_i+iy] = prv[ipop*NX*NY+site_i+iy+OFFSET[ipop]];
    }

  }
}
```

	E5-2630 v3	GK210	Hawaii XT
propagate v1 [GB/s]	10	155	216
propagate v2 [GB/s]	32	145	223
collide v1 [MLUPS]	8	55	53
collide v2 [MLUPS]	12	6	5

Scalability on a CPU cluster



Performance comparison of various programming frameworks on various processors.

	E5-2630 v3			GK210		Hawaii XT	
compiler model	ICC 15 Intrinsics	ICC 15 OMP	PGI 15.10 OACC	NVCC 7.5 CUDA	PGI 15.10 OACC	GCC OCL	PGI 15.10 OACC
`propagate` [GB/s]	38	32	32	154	155	232	216
$\mathcal{E}_p$	65%	54%	54%	64%	65%	73%	70%
`collide` [MLUPS]	14	11	12	117	55	76	54
`collide` [GFLOPs]	92	71	78	760	356	494	351
$\mathcal{E}_c$	28%	22%	24%	52%	24%	19%	14%
Tot perf. [MLUPS]	11.5	9.2	9.8	80.7	45.6	63.7	47.0

Conclusion

- we have successfully ported, tested and benchmarked a complete LBM code using OpenACC
- we obtained a good code maintainability, thanks to minimal code modification w.r.t. plain C version
- code is portable across different accelerators
- performances are portable with some limitations

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Thanks for Your attention

	Tesla K40			Xeon-Phi 7120	E5-2699-v3	
Code Version	CUDA	OCL	OACC	OCL	1CPU C	2CPU C
$T_{\text{Pbc+Prop}}$ [msec]	13.78	15.80	13.91	30.46	120.71	61.40
MLUPS	285.32	248.86	282.72	129.10	32.98	64.84
GB/s	168.91	147.33	167.37	76.42	19.53	19.19
$\mathcal{E}_p$	59%	51%	58%	22%	29%	28%
T_{Bc} [msec]	4.42	6.41	2.76	3.20	1.62	0.80
T_{Collide} [msec]	39.86	136.93	78.65	72.79	136.24	67.95
FLOP/site	6472	6613	6504	7600	7600	7600
MLUPS	99	29	50	54	29	29
$\mathcal{E}_c$	45%	13%	23%	34%	34%	34%
T_{WC}/iter [msec]	58.07	159.14	96.57	106.45	259.79	131.88
MLUPS	68	25	41	37	15	30

Table: Performance comparison between NVIDIA K40 GPU, Intel Xeon-Phi 7120, single and dual Intel multi-core CPUs (Haswell-v3 micro architecture); the lattice size is 1920×2048 points.

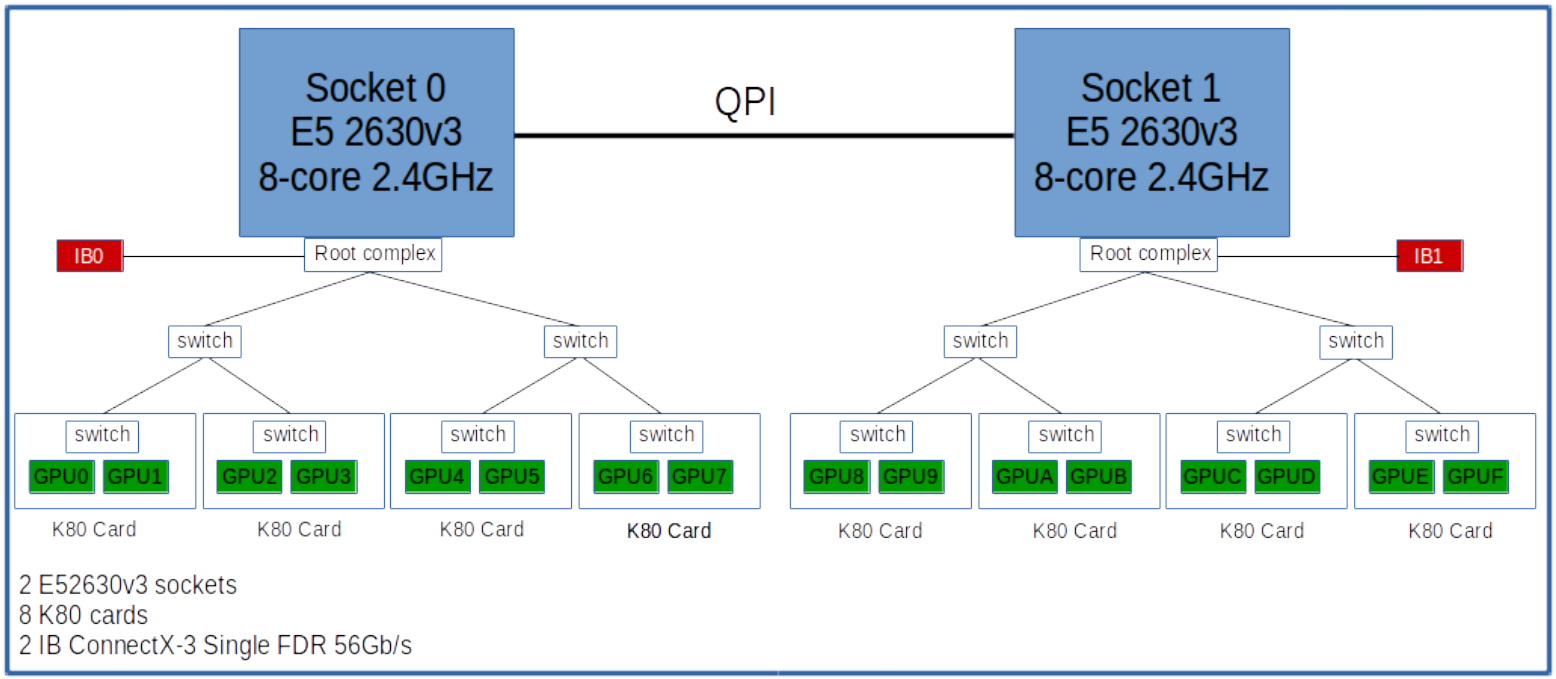
Cluster Overview

Compute nodes:

Supermicro SYS-4028GR-TR

- 2 x Intel Xeon E5-2630v3
- 8 x NVIDIA K80 (2xGPU)
- 2 x Mellanox ConnectX-3 Single FDR 56Gb/s Infiniband cards

Nodes Overview



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