Multipart SU(N) mode in QCDGPU package for Monte Carlo lattice simulations

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Outline

Lattice approach

Lattice QCD – one of non-perturbative approaches to QCD

Continuous space-time $\rightarrow$ Discrete lattice

Discretized operators

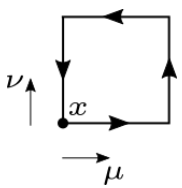
Gluonic fields – SU(N) matrices on the lattice links

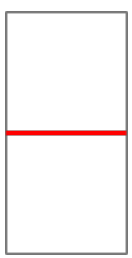
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \, \mathcal{O}[U] e^{-S[U]} \quad \rightarrow \quad \langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_{U_n} \mathcal{O}[U_n]$$

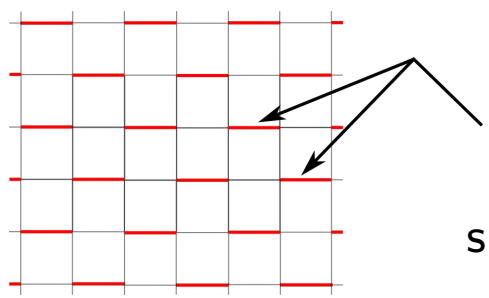
$$\mathcal{Z} = \int \mathcal{D}U \, e^{-S[U]}, \quad \int \mathcal{D}U = \prod_{x,\mu} \int dU_\mu(x), \quad U_n \propto e^{-S}$$

Lattice Wilson action:

$$S_W = \beta \sum_{\square} \left[1 - \frac{1}{N} \mathrm{Re}\,\mathrm{Tr} U_{\square} \right],$$







may be updated simultaneously

QCDGPU in general

QCDGPU is a multi-GPU open-source package for lattice Monte Carlo simulations of SU(N) gluodynamics at finite temperature and O(N) models.

It is implemented in C/C++/OpenCL and OpenMP (in multipart mode), tested on AMD and NVIDIA GPUs, AMD and Intel CPUs and may run on other OpenCL-compatible devices.OS independent.

It allows investigation of phenomena in external chromomagnetic field (implemented through the "twisted boundary conditions").

`https://github.com/vadimdi/QCDGPU`

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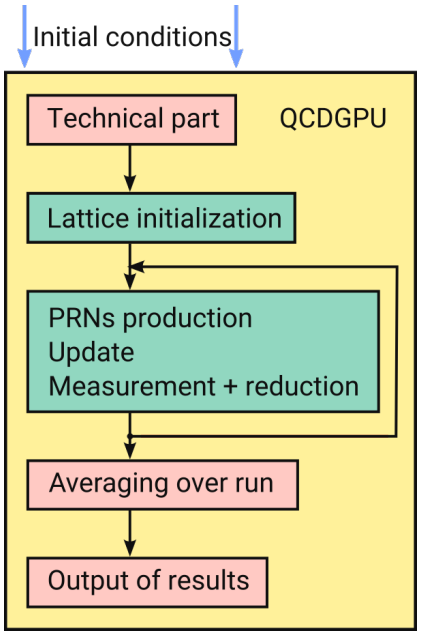
Objectives for the lattice decomposition:

- overcome limited GPU memory
- decrease of computational time

  execution on several devices simultaneously

Package structure

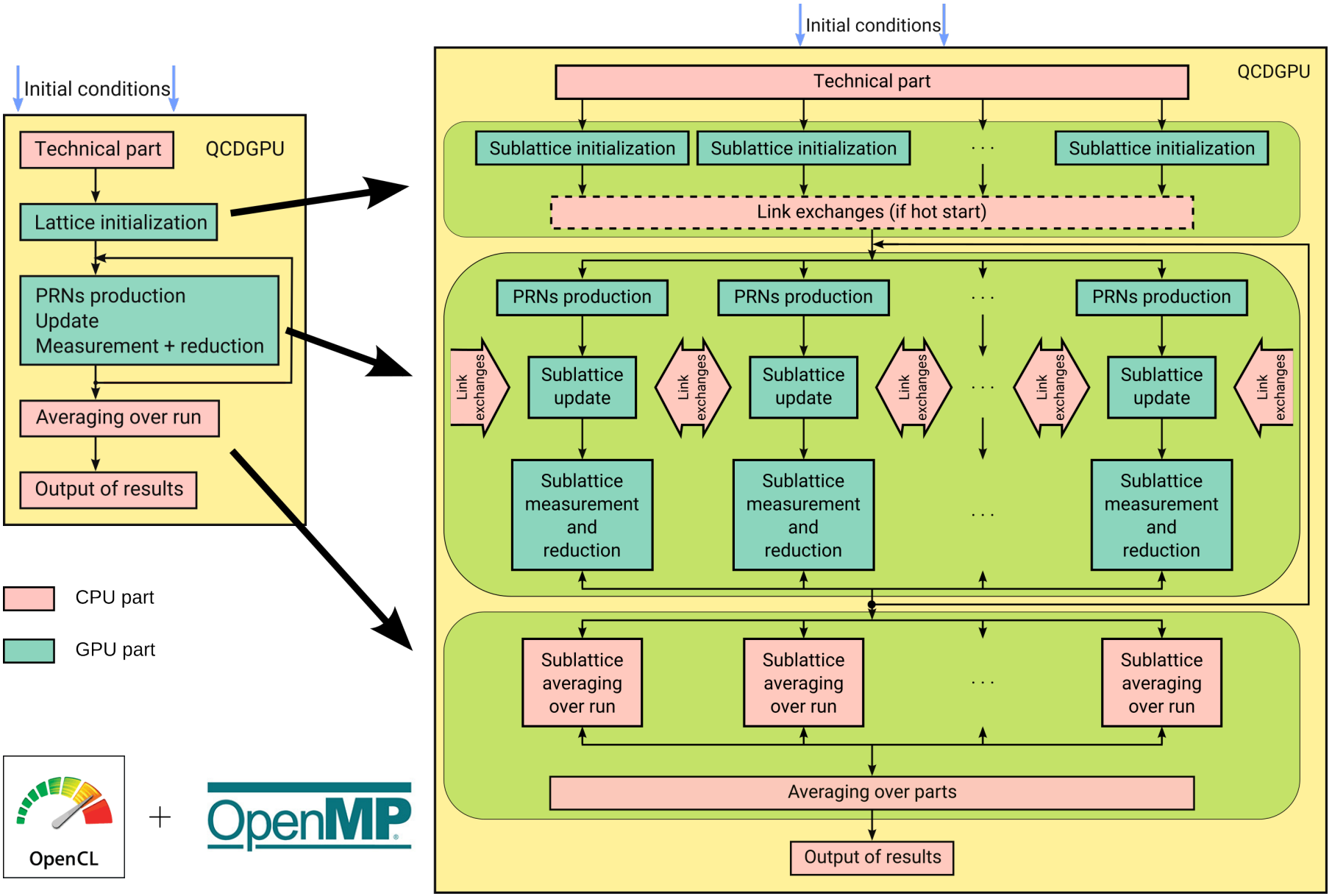


CPU part

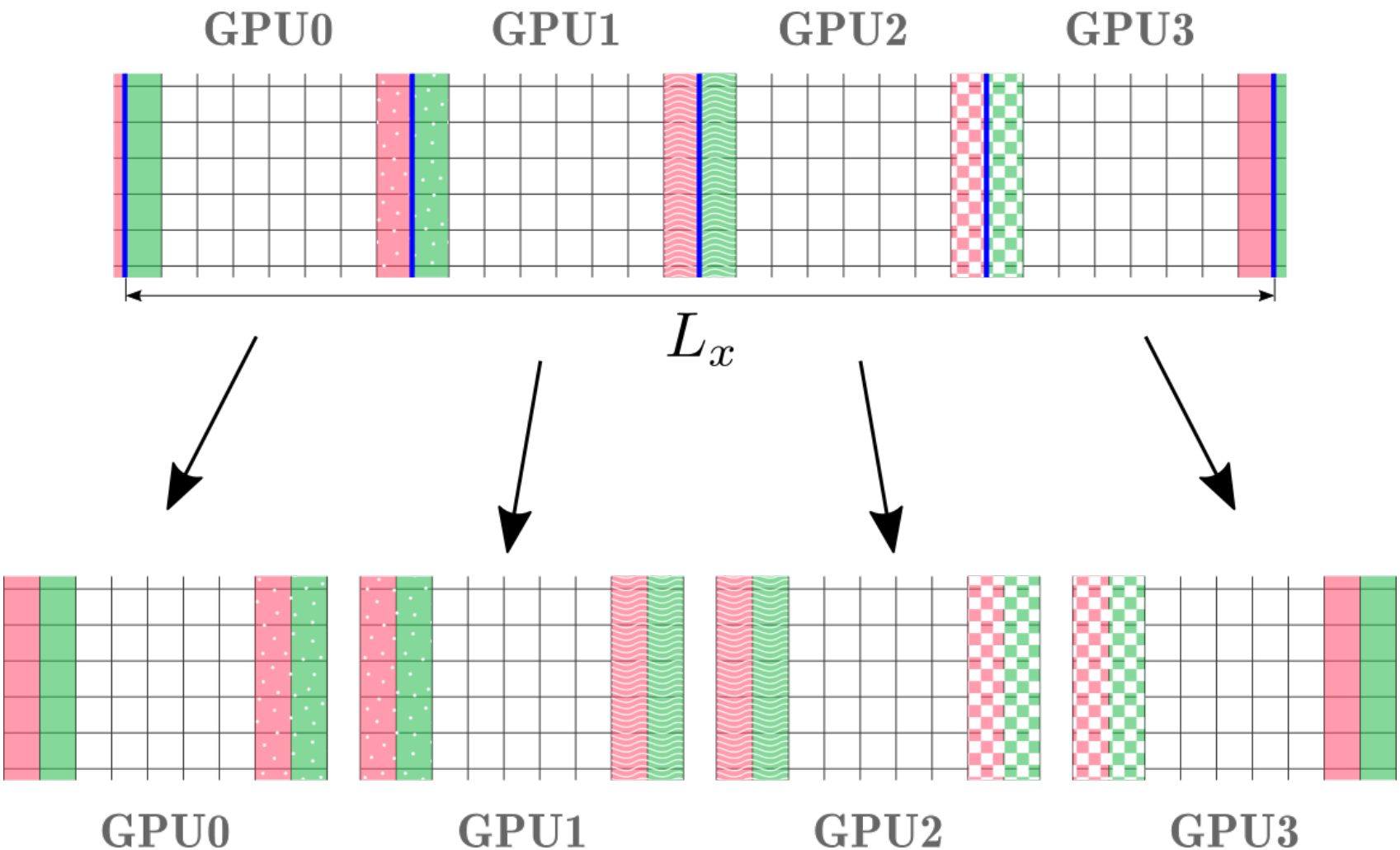
GPU part

OpenCL

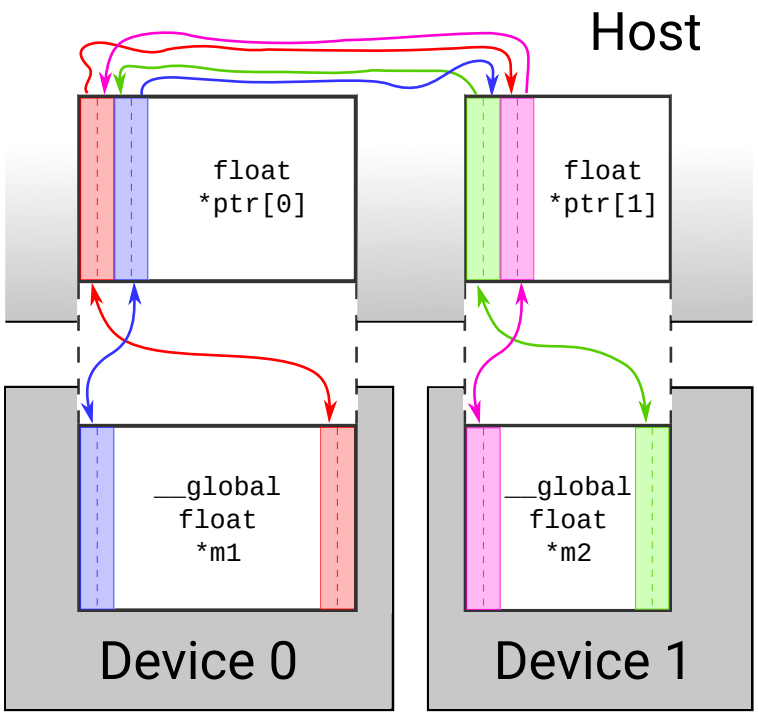
Package structure



Lattice decomposition

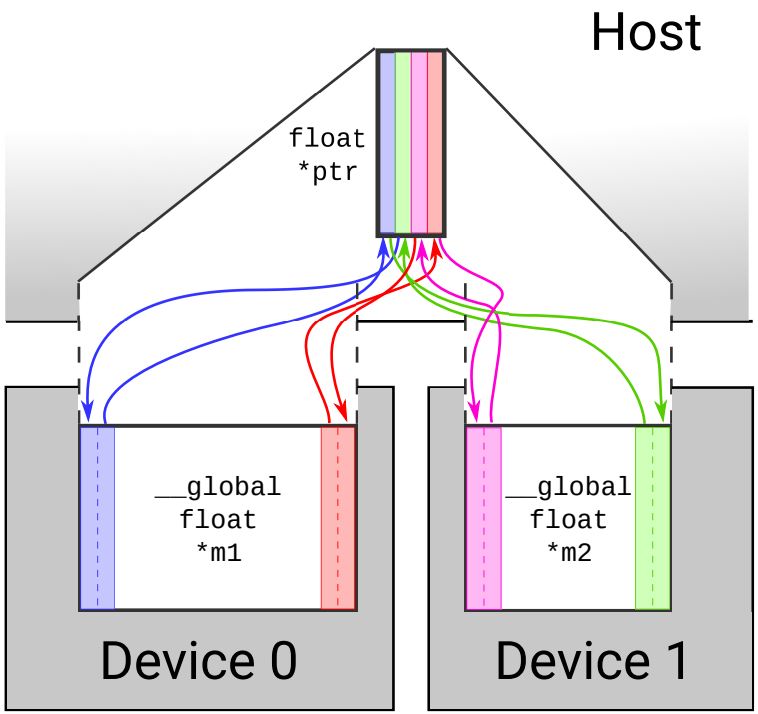


Edges exchange



map / unmap

/* currently fails on AMD GPUs
because of driver bug */



read / write

Pseudorandom numbers

Module for PRNs production is based on PRNGCL library.
Generators available:

1. RANLUX (with several luxury levels)
2. RANMAR
3. RANECU
4. XOR7, XOR128
5. PM
6. MRG32k3a

Random seeding for initialization – various PRNG threads are initialized with different seed tables.

PRNG is initialized with with one integer number – `RANDSERIES`.

At each lattice part, PRNG is initialized with own `RANDSERIES`.

Single/double precision PRNGs are implemented.

`https://github.com/vadimdi/PRNGCL`

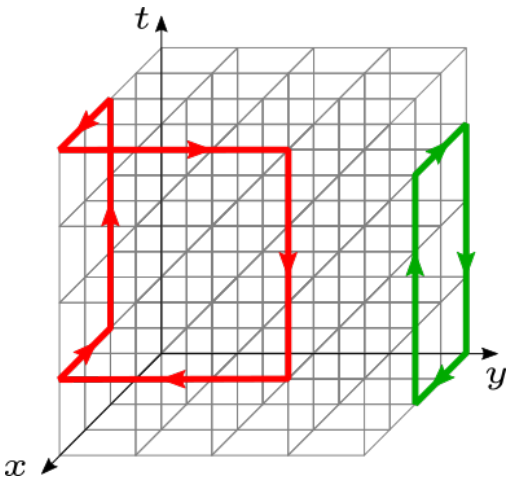
Measured quantities

- plaquette
- Wilson action (also coordinatewise)
- components of tensor of SU(N) electromagnetic field $F^a_{\mu\nu}$

[arXiv:1212.6185v1[hep-lat]]

- Polyakov loop L (also coordinatewise), L^2, L^4
- Wilson loop

The Wilson loop



Continuous theory:

$$W_{\mathcal{L}} = \mathrm{Tr}\left[\mathcal{P}\exp\left(i\oint_{\mathcal{L}} A_\mu dx^\mu\right)\right]$$

Lattice theory:

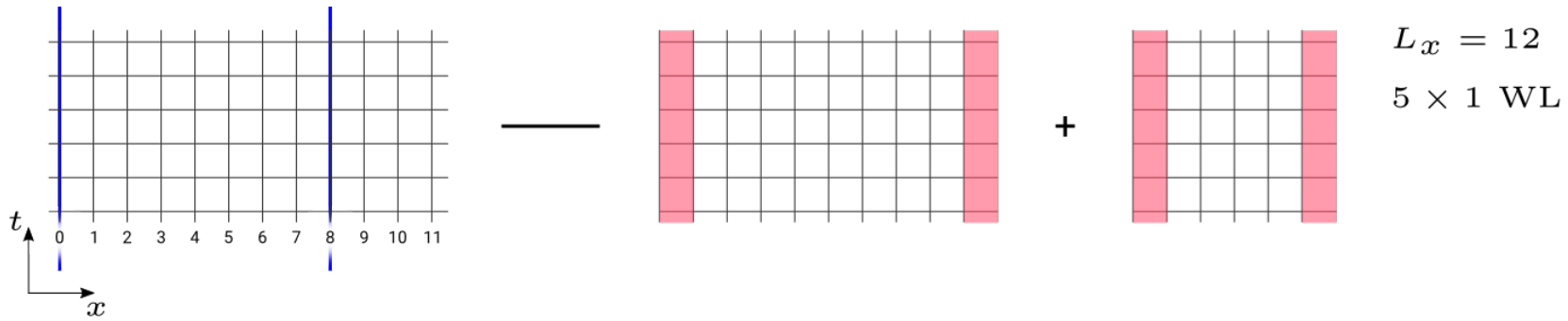
$$W_{\mathcal{L}} = \mathrm{Tr}\left[\prod_{(x,\mu)\in\mathcal{L}} U_\mu(x)\right]$$

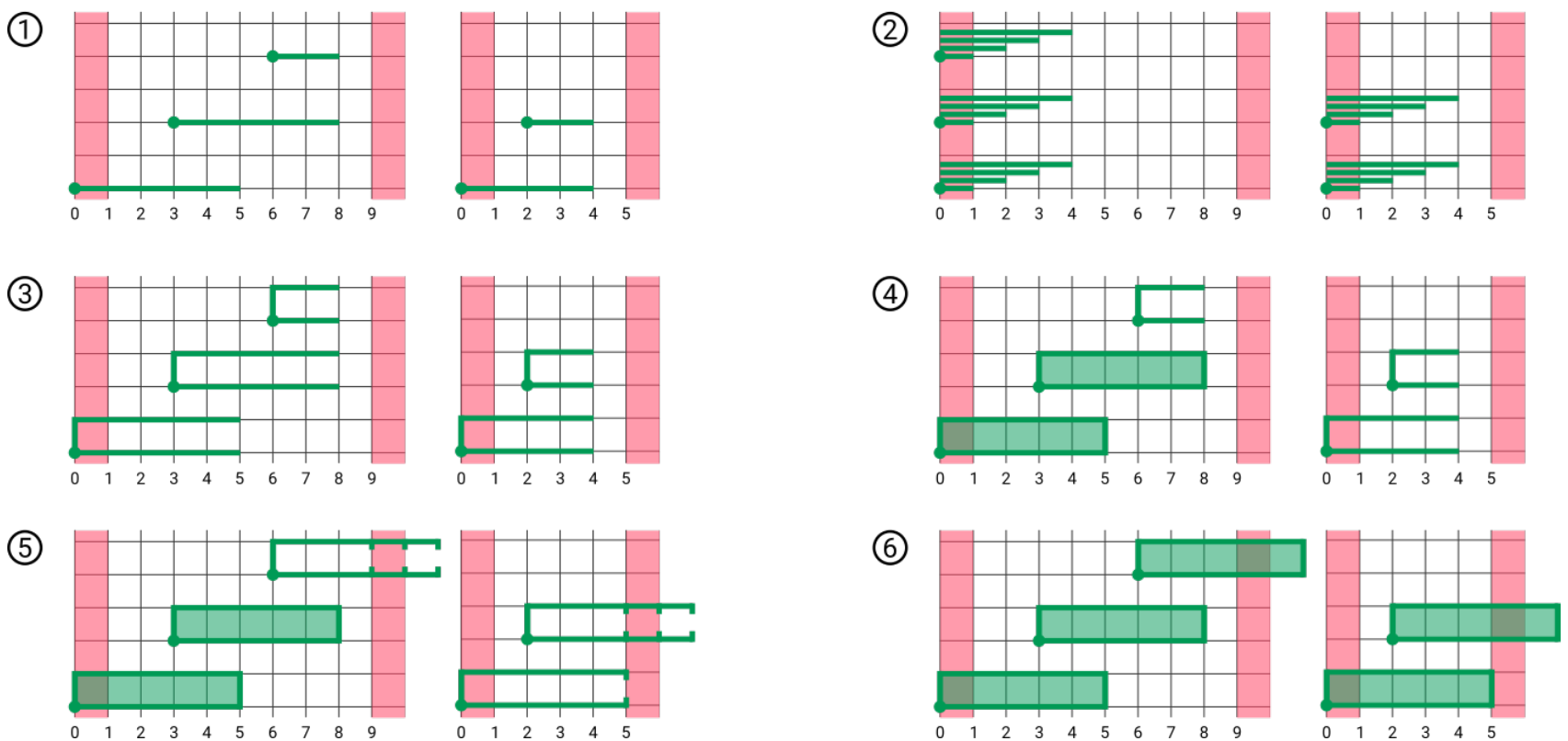
Wilson loops: planar, non-planar

Usage of the Wilson loop:

- indicates the confinement/deconfinement phases
- string tension
- lattice spacing

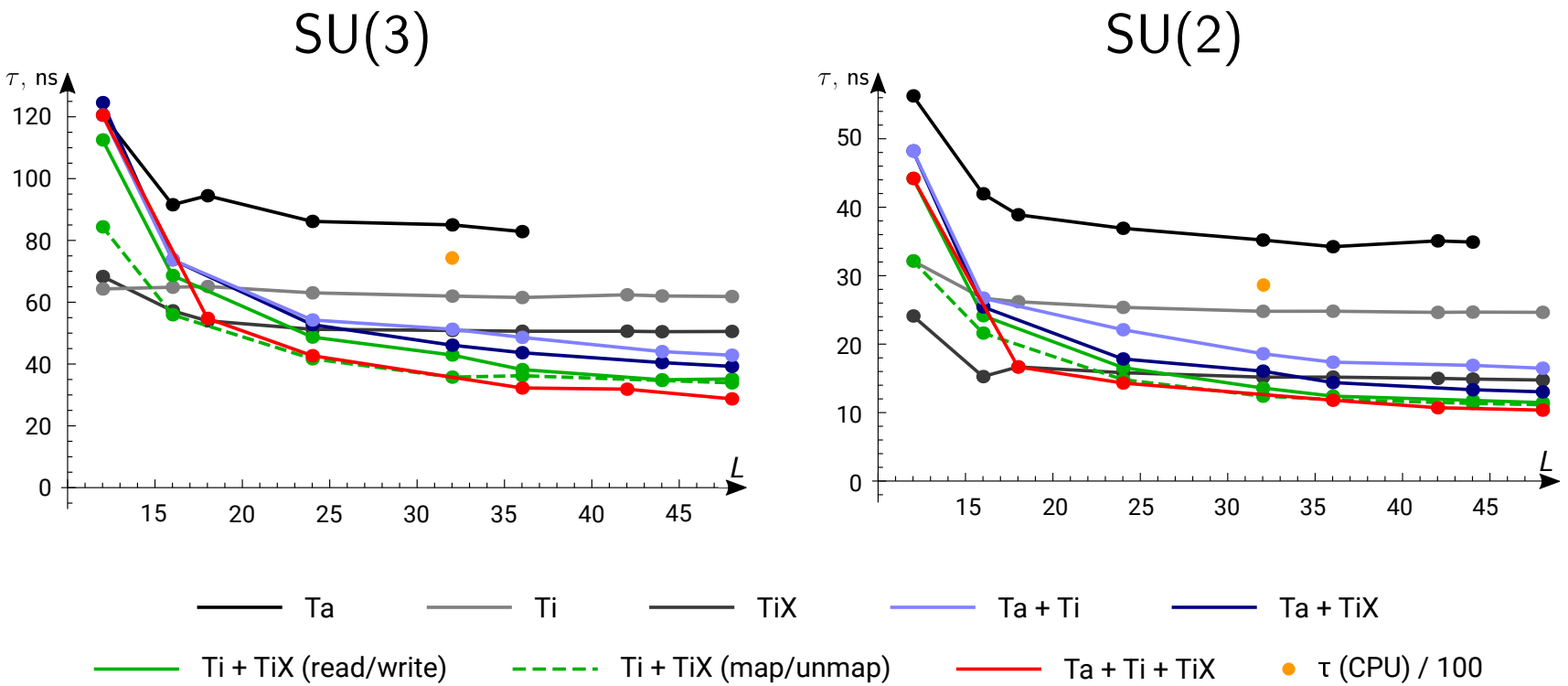
Implementation of the Wilson loop





Performance results

L^4 lattice
τ = (time for 1 lattice update + 1 measurement of S_W)/($N_d \cdot L^4$)



"Cold" start, RANLUX PRNG (luxury level 3, single precision). NHIT = 10, reunitarization is used, double precision.
1 lattice part / device; sizes of the parts are chosen to provide better performance.

Ta – AMD Radeon HD7990 (Tahiti)
Ti – NVIDIA GeForce GTX TITAN
TiX – NVIDIA GeForce GTX TITAN X

[HPC Village] http://openwall.info/wiki/HPC/Village

Conclusions

Multipart mode in SU(N) part of QCDGPU package is implemented using OpenMP:

1. several parts may be processed in parallel on several devices as well as sequentially on a single device
2. two multithread variants of exchange of the edge links are implemented:
   - through map/unmap: is faster but currently isn't supported by AMD
   - through read/write: is some slower but is supported by all GPU manufacturers
3. measurement of usual and particular (like components of $F_{\mu\nu}$ tensor) quantities is implemented in multipart mode. In particular, measurement of the Wilson loop is implemented
4. the $\sim 28.5 - 33\%$ acceleration is obtained in parallel run on two GPUs and $\sim 36 - 43\%$ acceleration on three GPUs for SU(3) model; for SU(2) model these numbers are $19.5 - 24.5\%$ and $22.3 - 29.8\%$, correspondingly.

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Plans for future:

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Thank you for your attention!