QCDGPU: open-source package for Monte Carlo lattice simulations on OpenCL-compatible multi-GPU systems

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QCDGPU is a multi-GPU open-source package for lattice Monte Carlo simulations of pure SU(N) gluodynamics in external magnetic field at finite temperature and O(N) model.

The code is implemented in OpenCL, tested on AMD and NVIDIA GPUs, AMD and Intel CPUs and may run on other OpenCL-compatible devices.

The package contains minimal external library dependencies and is OS platform-independent.

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Motivation

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Requirements for QCDGPU development:

1. scientific importance for high-energy physics
   (spontaneous vacuum magnetization at high temperature, phase transitions behavior in external fields, dependence of phase transition order in O(N) models on coupling constant value, etc.)
2. requirements of huge statistics
3. compatibility with modern computer systems
   (single-, multi-GPU, GPU clusters)
4. software portability
   (heterogeneous systems, Linux and Windows, etc.)
5. adjustable precision
6. stability of the computing environment to fail and the ability to suspend the simulations

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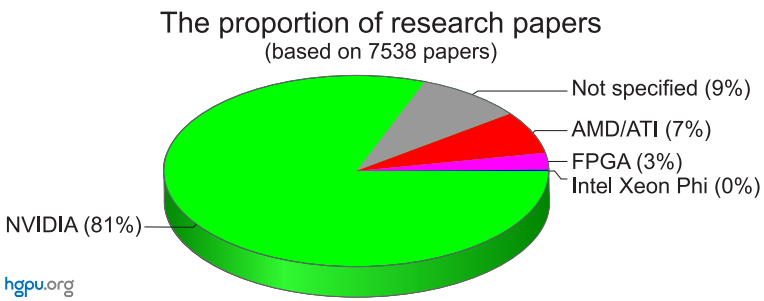
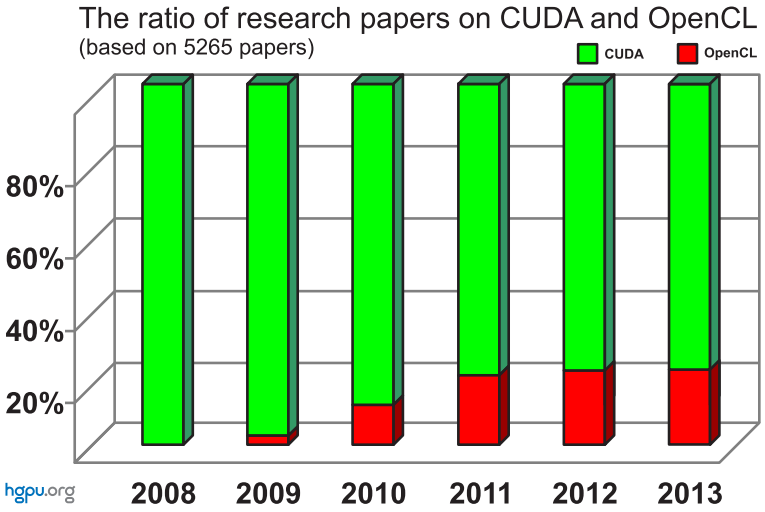
Why OpenCL?

main reason - portability





Currently $\sim$ 20% of all scientific researches using GPU accelerators are performed with OpenCL

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Methods

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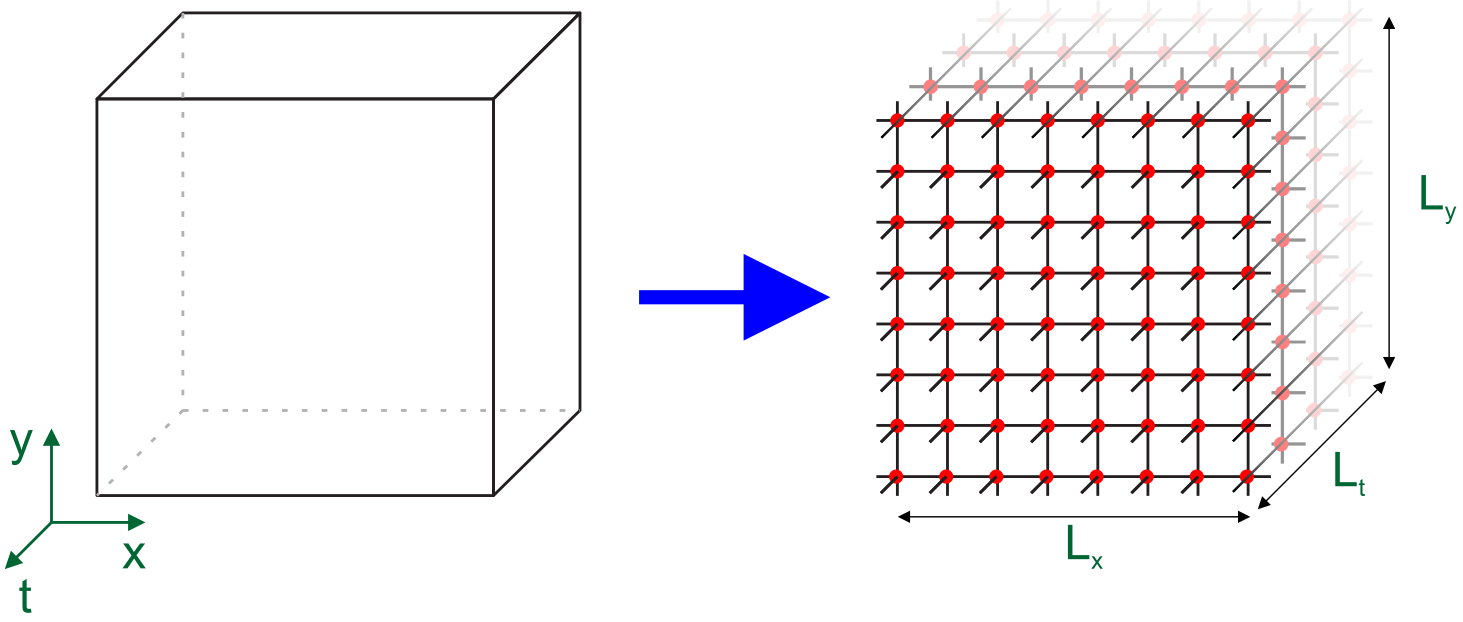
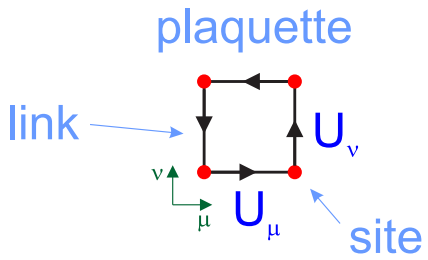
Space-time discretization

Monte Carlo lattice simulation is one of the most powerful numerical methods to study quantum field theory



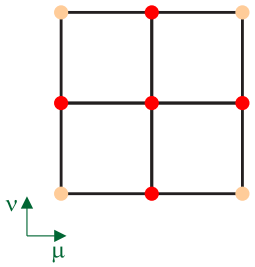
SU(N)



$$S=\sum_{x,\mu,\nu} U_\mu U_\nu U_\mu^+ U_\nu^+$$

action

O(N)



$$S=\sum_{x,\mu} f(\varphi_x,\varphi_{x-\hat{\mu}})$$

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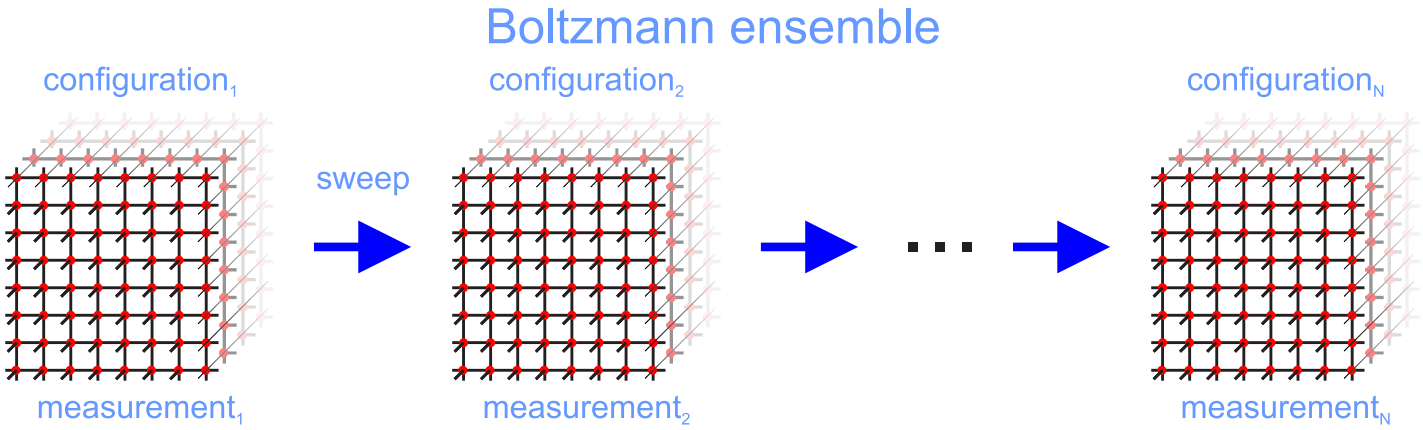
Monte Carlo lattice simulations

Monte Carlo lattice method is suitable for computer implementation and actually is a computer experiment

The aim of the method is to calculate some desired quantities via Boltzmann ensemble of lattice states (configurations)

Update is the modification of site or link according to the distribution function

Sweep is the update of whole lattice to produce new configuration



$$\text{value} = \frac{1}{N}\sum_i \text{measurement}_i$$

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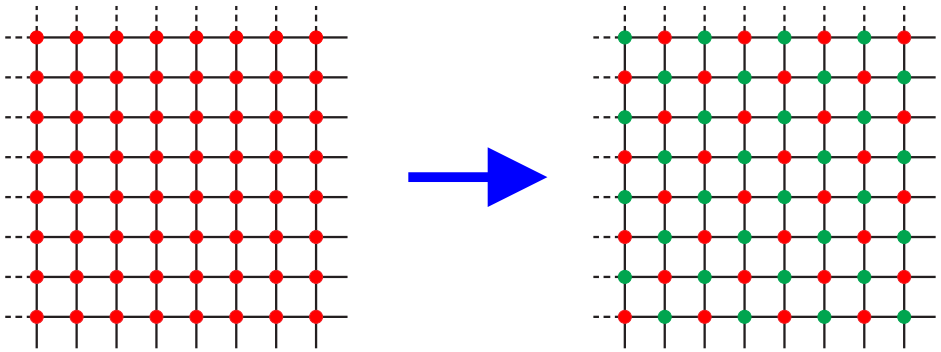
Checkerboard scheme

To parallelize the update process the checkerboard scheme is used



if sum of site's coordinates (**X**+**Y**+**Z**+**T**) is odd
then site is **odd** otherwise site is **even**

Now odd/even sites (links) may be updated simultaneously

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Implementation

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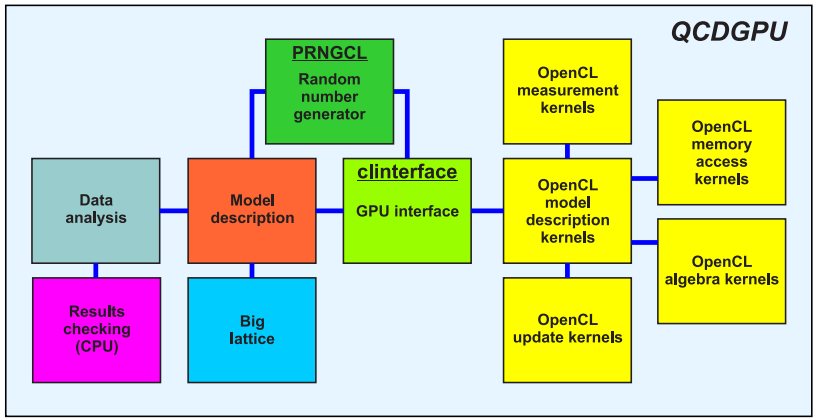
QCDGPU program structure



1. clinterface module
2. Model description module
3. PRNGCL module
4. Big lattice module
5. CPU results checking module

QCDGPU performs all the necessary calculations on computing devices and provides the final simulation results to the host

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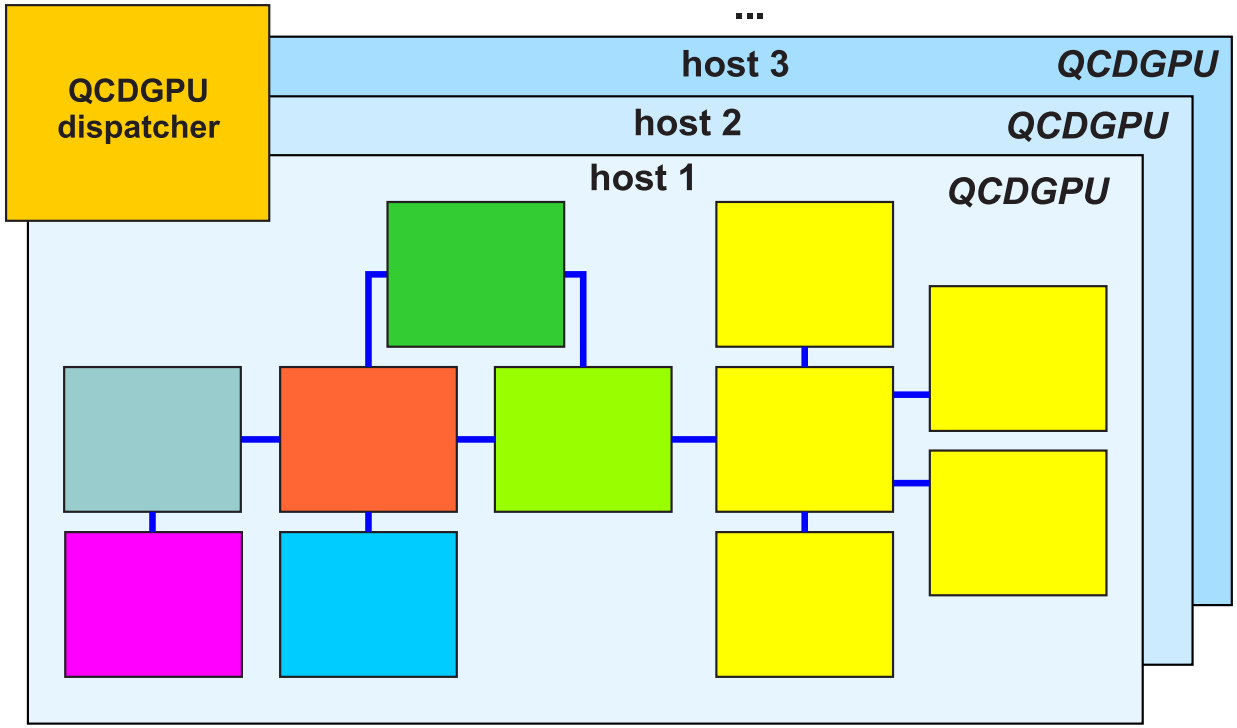
QCDGPU multi-host execution

QCDGPU may be run on several hosts

The interaction of several copies of QCDGPU on different hosts is provided with QCDGPU-dispatcher. It realizes task scheduling for the available copies of QCDGPU according to the parameter space of the problem under investigation



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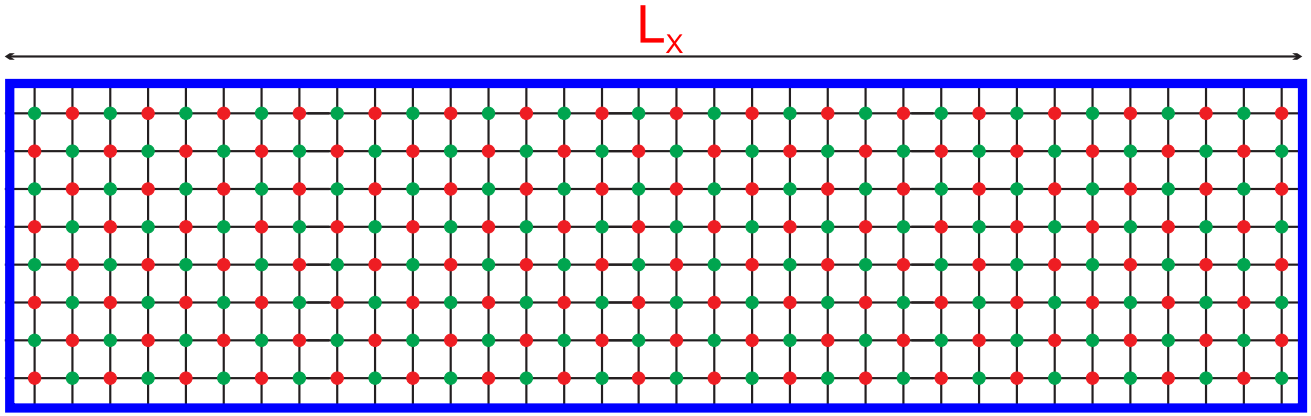
Second level checkerboard scheme



4D lattice $L_X \times L_Y \times L_Z \times L_T$

In most “finite-temperature” cases: $L_X = L_Y = L_Z = L_S > L_T$

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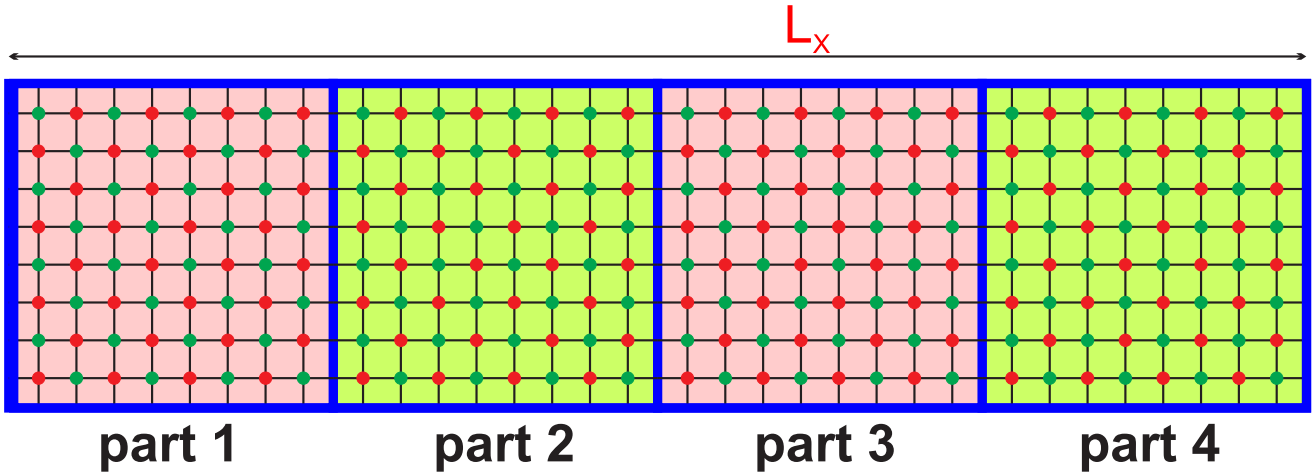
Second level checkerboard scheme



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We divide lattice in X direction

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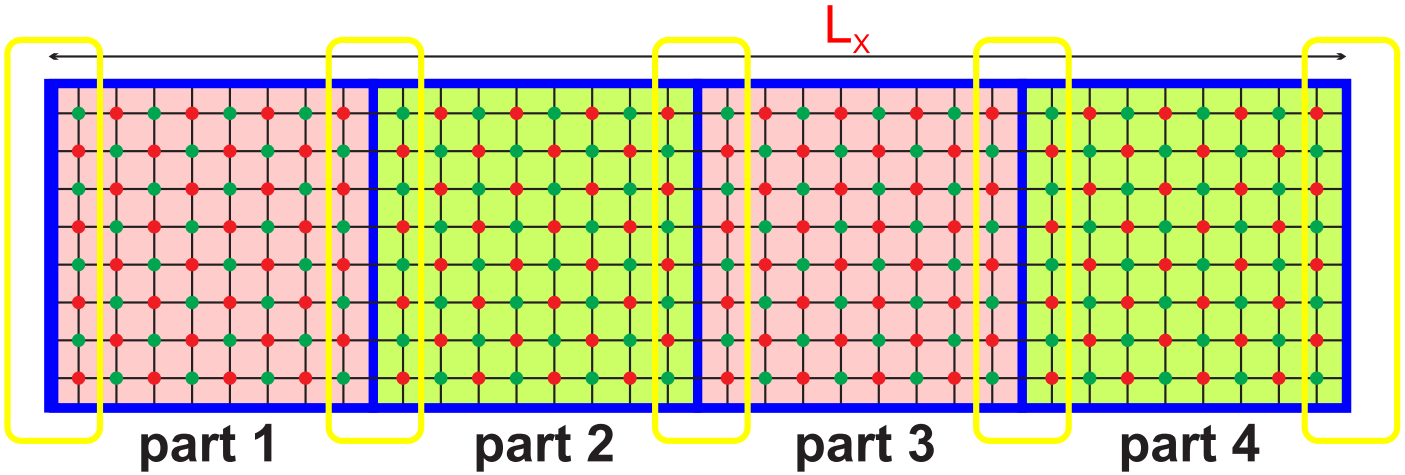

4D lattice $L_X \times L_Y \times L_Z \times L_T$

In most “finite-temperature” cases: $L_X=L_Y=L_Z=L_S>L_T$

We divide lattice in X direction

For updating parts the boundary elements should be accounted

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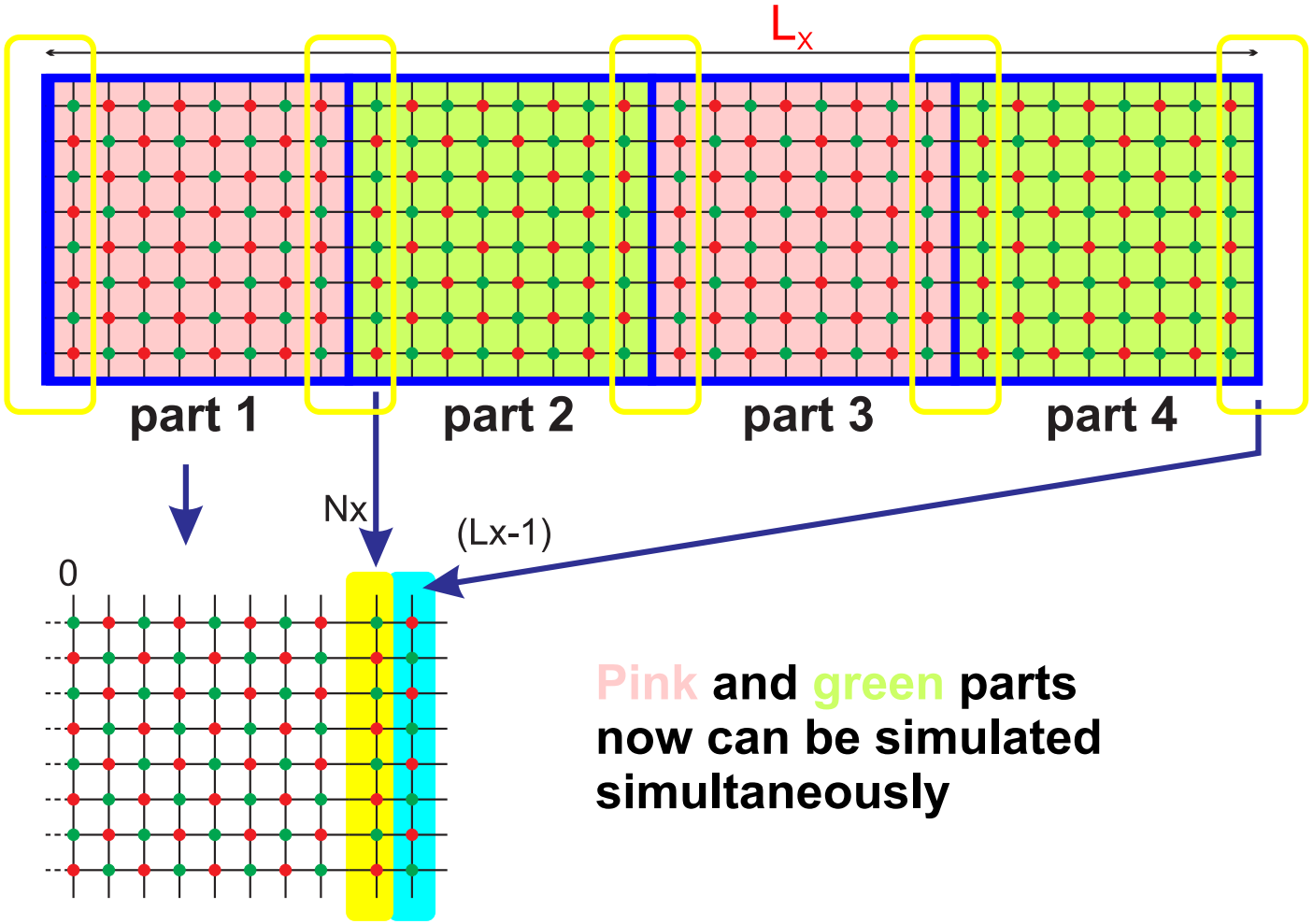

Pink and green parts now can be simulated simultaneously

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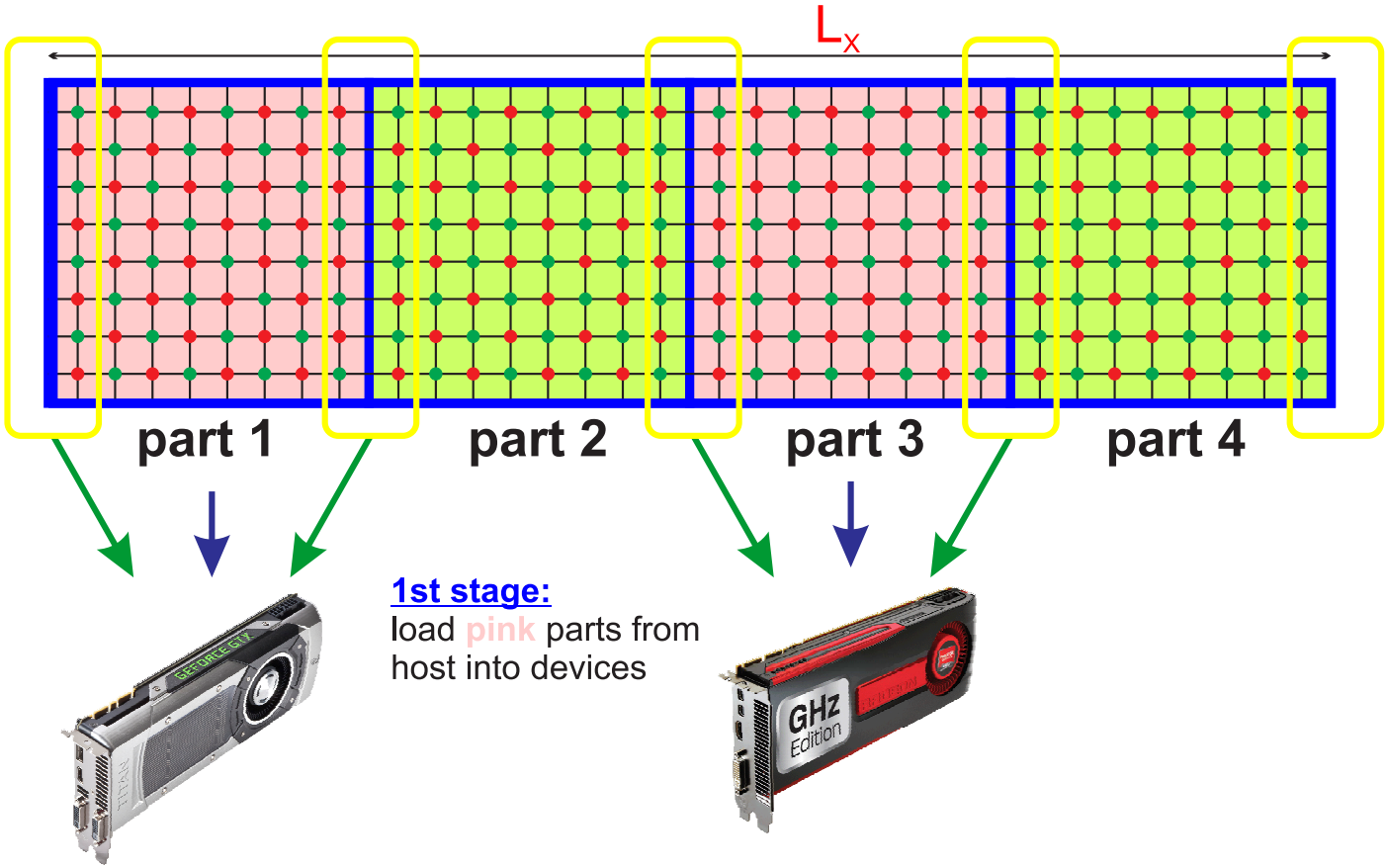

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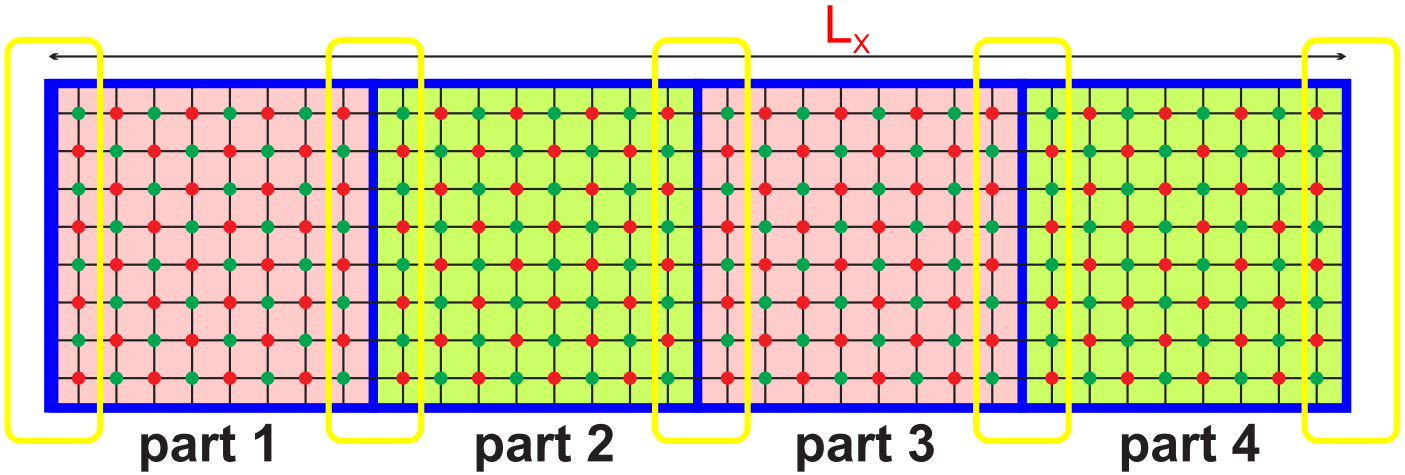

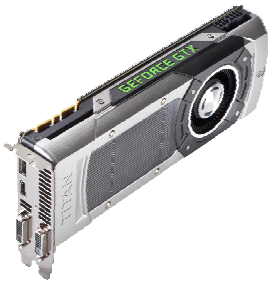

2nd stage:
update internal lattice sites/links

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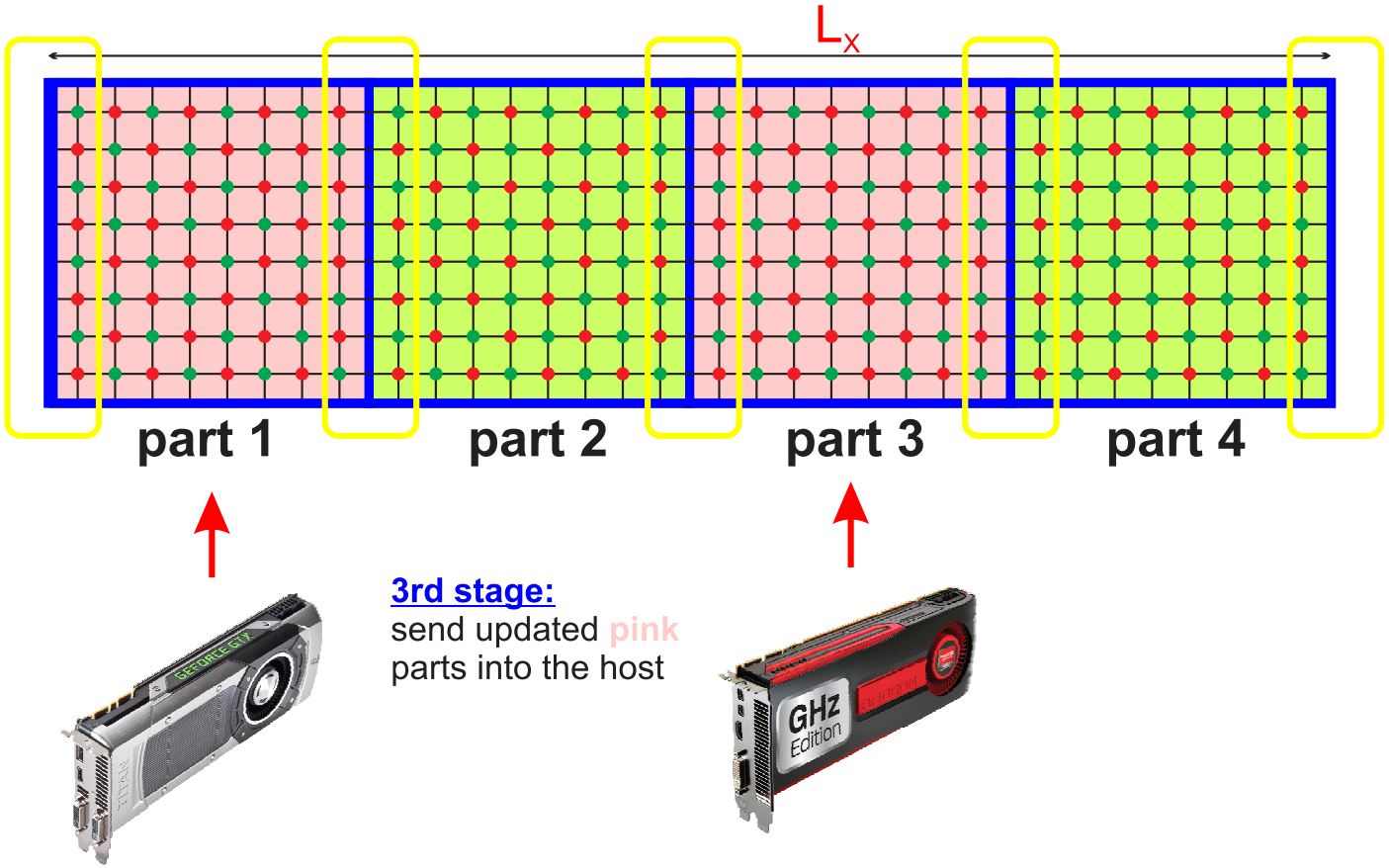
Second level checkerboard scheme



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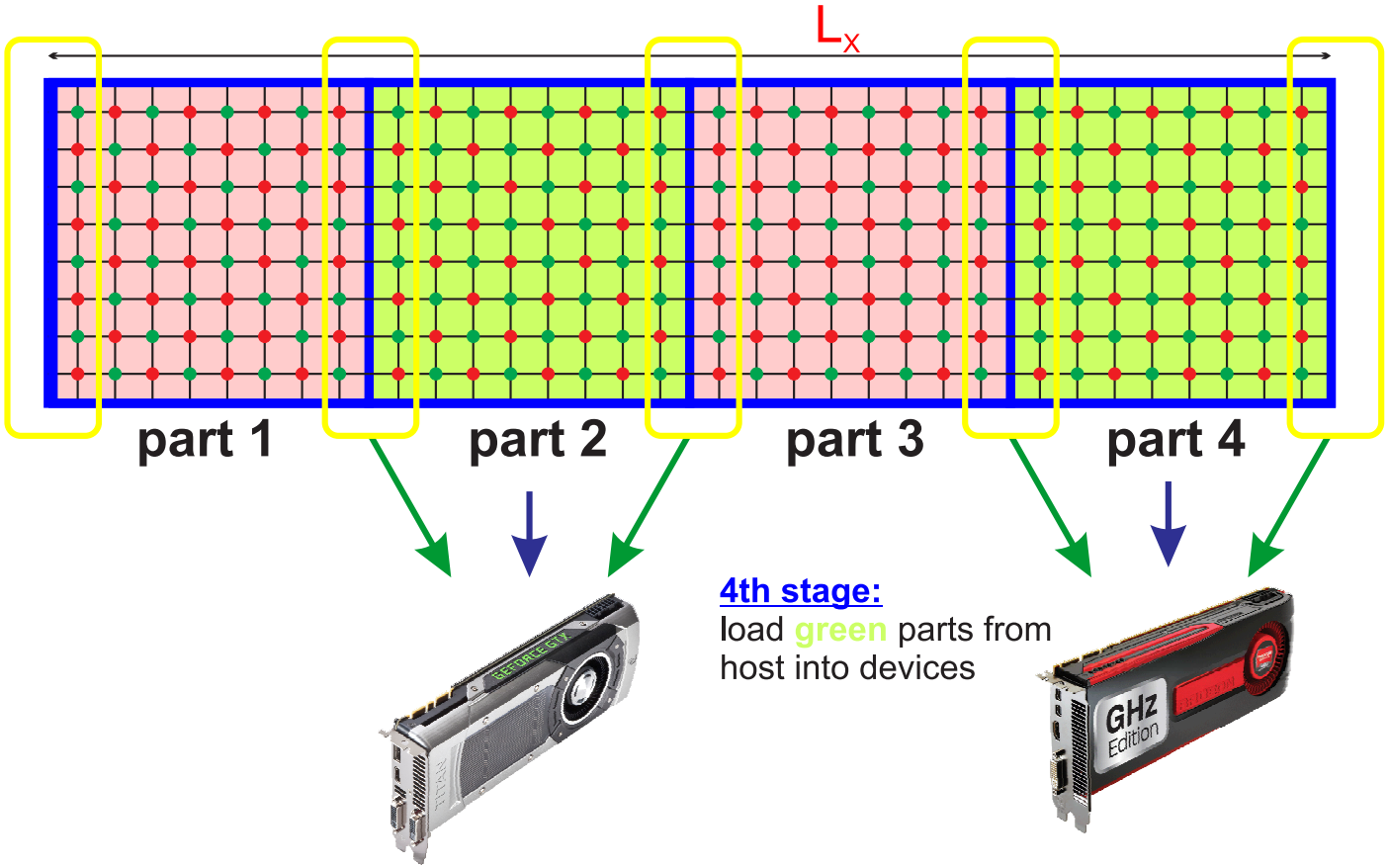
Second level checkerboard scheme



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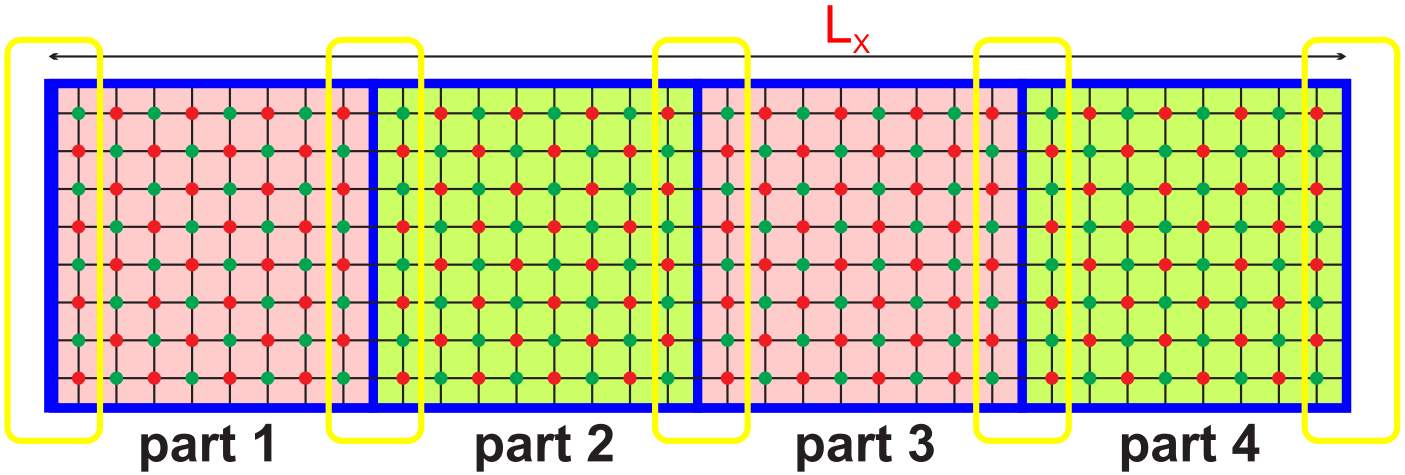
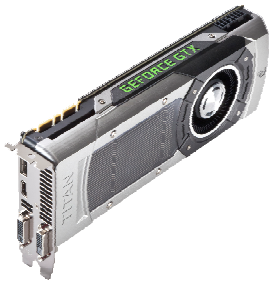
Second level checkerboard scheme





5th stage:
update internal lattice sites/links

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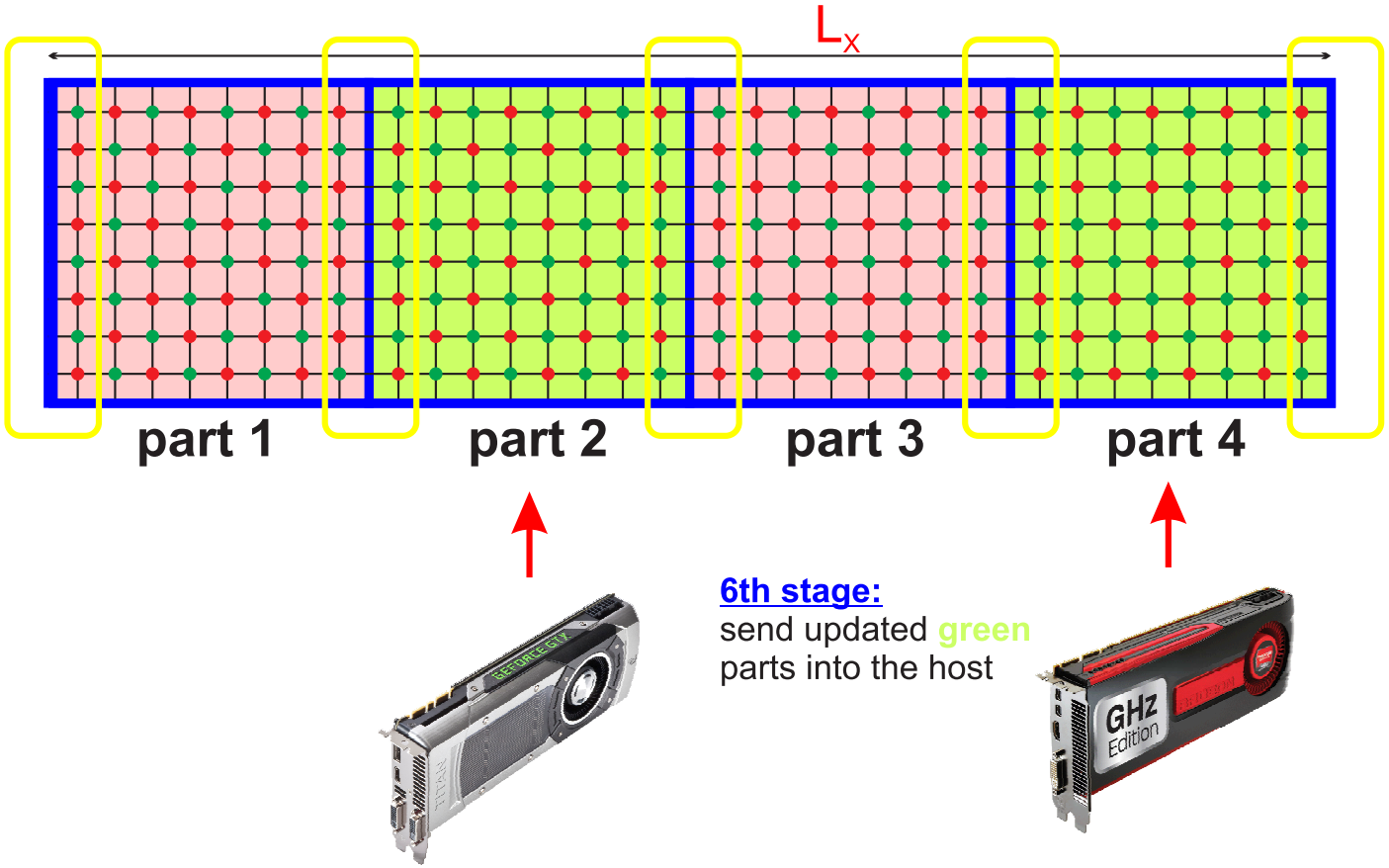
Second level checkerboard scheme



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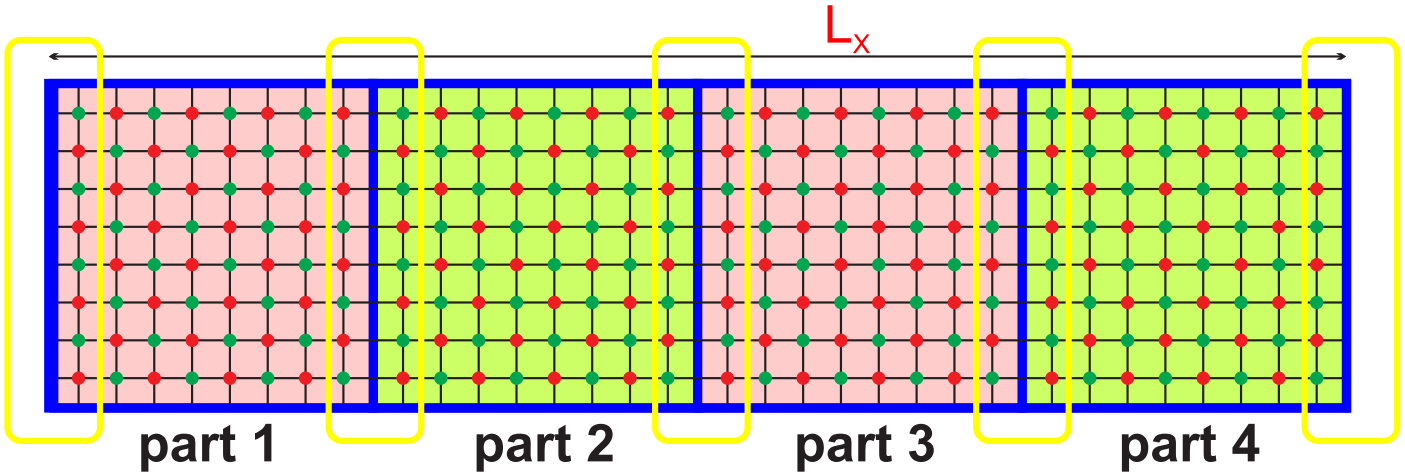
Second level checkerboard scheme



The device performance differences should be hidden by selection of lattice parts with unequal size

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Performance results

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QCDGPU performance results

QCDGPU was tested on NVIDIA GeForce GTX 560 M (Windows 7), NVIDIA GeForce GTX 560 Ti, AMD Radeon HD 7970 (OpenSUSE 12.2), HD 6970, HD 5870 (OpenSUSE 11.4)

Timings of 1 working sweep for O(4), SU(2) and SU(3) models in single- and double-precision (seconds)

Model	Device	Parts	Lattice	Single	Double
O(4)	GTX560M	1	16^4	0.08	0.12
			24^4	0.42	0.6
			32^4	1.31	1.87
		4	48^4	7.79	11.11
	GTX560Ti	1	32^4	0.72	0.99
		4	48^4	4.64	6.10
	HD 5870	2	32^4	0.96	1.56
	HD 6970	2	32^4	0.73	1.3
	HD 7970	2	32^4	0.66	0.95
		12	72^4	20.35	36.2
	HD 7970+GTX560Ti	4	32^4	0.72	0.96
		8	48^4	2.97	4.1
SU(2)	GTX560Ti	1	44^4	0.95	1.14
	HD 5870	1	30^4	0.22	0.24
	HD 6970	1	30^4	0.20	0.22
	HD 7970	1	48^4	4.64	6.10
SU(3)	GTX560Ti	1	32^4	0.56	1.17
			36^4	0.90	1.86
	HD 6970	1	24^4	0.24	0.23
	HD 7970	1	28^4	0.13	0.22

"Hot" start, RANLUX PRNG (luxury level 3). For O(4) model NHIT = 100 tries were used to update each lattice site (this provides acceptance rate up to 50%). For SU(2) and SU(3) models NHIT = 10 and reunitarization were used. One bulk sweep was performed to decorrelate configurations to be measured.

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QCDGPU performance results comparison

Cardoso and Bicudo reported in [1] the following timings (seconds per single sweep) on lattice 8^4 for SU(2) and SU(3) models (one lattice sweep with reunitarization, without any measurements).
The authors [1] used NVIDIA GeForce GTX 580 and NVIDIA CUDA

	SU(2)		SU(3)	
	single	double	single	double
[1]	$6x10^{-4}$	$7x10^{-4}$	$2x10^{-3}$	$4x10^{-3}$
GTX 560 Ti	$6x10^{-4}$	10^{-3}	$1.3x10^{-3}$	$4.9x10^{-3}$
HD 7970	$2x10^{-3}$	$2.6x10^{-3}$	$3.4x10^{-3}$	$5.1x10^{-3}$

* For large lattices AMD HD 7970 demonstrates better performance than NVIDIA GTX 560 Ti

[1] N. Cardoso and P. Bicudo: Generating SU(Nc) pure gauge lattice QCD configurations on GPUs with CUDA and OpenMP. *Comput. Phys. Commun.* 184: 509-518, 2013

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Availability

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QCDGPU is available online

https://github.com/vadimdi/QCDGPU

PRNGCL library for pseudo-random numbers generation on OpenCL-ready devices is available online

https://github.com/vadimdi/PRNGCL

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Conclusions

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Some papers in which QCDGPU was used :

- V. Demchik and A. Strelchenko: Monte Carlo simulations on Graphics Processing Units. *arXiv:0903.3053 [hep-lat]*, 2009 (ATI Stream version)
- V. Demchik: Pseudo-random number generators for Monte Carlo simulations on ATI Graphics Processing Units. *Comput. Phys. Commun.* **182**, 692, 2011
- S. Antropov, M. Bordag, V. Demchik and V. Skalozub: Long range chromomagnetic fields at high temperature. *Int. J. Mod. Phys. A* **26**, 4831, 2011
- M. Bordag, V. Demchik, A. Gulov and V. Skalozub: The type of the phase transition and coupling values in $\lambda\phi^4$ model. *Int. J. Mod. Phys. A* **27**, 1250116, 2012
- V. Demchik, A. Gulov and N. Kolomoyets: Spontaneous generation of chromomagnetic fields at finite temperature in the SU(3) gluodynamics on a lattice. *arXiv:1212.6185 [hep-lat]*, 2012
- V. Demchik, A. Gulov and V. Skalozub: Spontaneous symmetry breaking in the O(4) model on a lattice. *NPQCD*, 2013

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Conclusions:

1. new package QCDGPU for Monte Carlo simulations of SU(N) gluodynamics in external field and O(N) model on OpenCL-compatible devices is developed
2. QCDGPU allows to carry out the simulations for very big lattices in single- or multi-GPU mode
3. simulations can be run with single or double precision
4. QCDGPU allows to investigate most popular LGT models in N-dimensional space-time
5. current version of QCDGPU uses trivial parallelization scheme to distribute computing
6. built-in mechanism for saving the computational state while achieving some conditions allows to interrupt long calculations without threat of data loss and to continue them on another available device

Plans for future:

1. implement the automatic adjustments of package start-up parameters via built-in profiling mechanism, as well as additional micro-benchmarks
2. realization of RHMC algorithm for including fermionic fields on a lattice
3. running of one simulation on several hosts at the same time on the base of MPI, which is very important in case of accounting of fermionic fields

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Thank you for your attention!

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