Simulating Lattice Quantum Chromodynamics on the Govorun Supercomputer

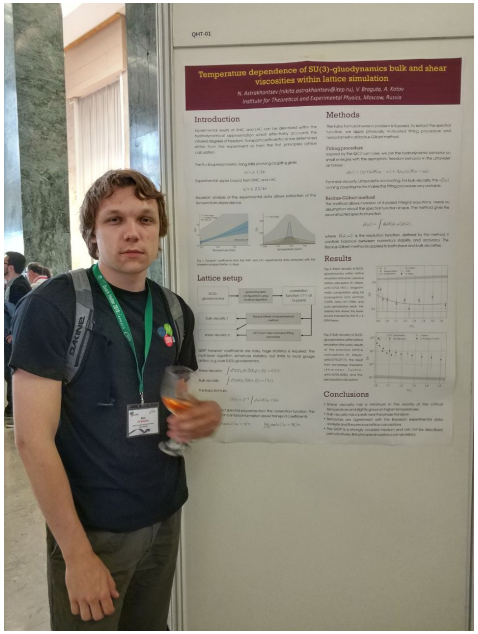
A.Yu. Kotov

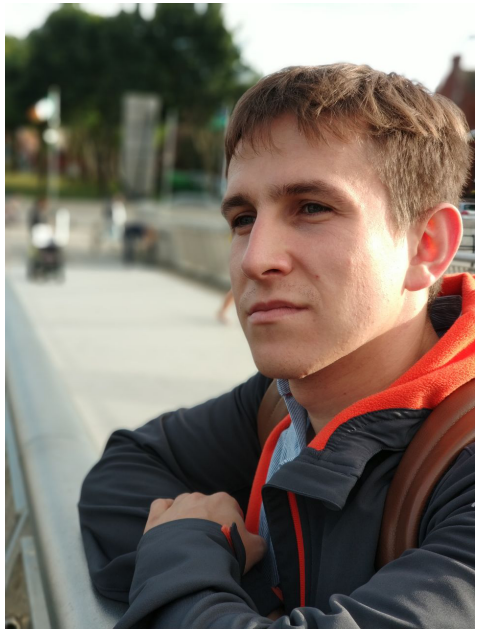
BLTP Bogoliubov Laboratory of Theoretical Physics

XXVII International Symposium on
Nuclear Electronics & Computing NEC'2019

30 Sept - 4 Oct, 2019

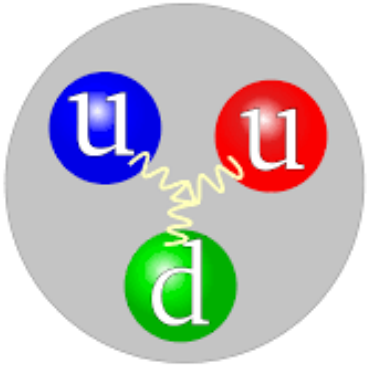
Our group

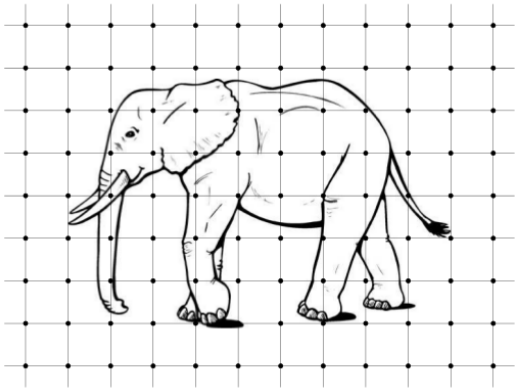




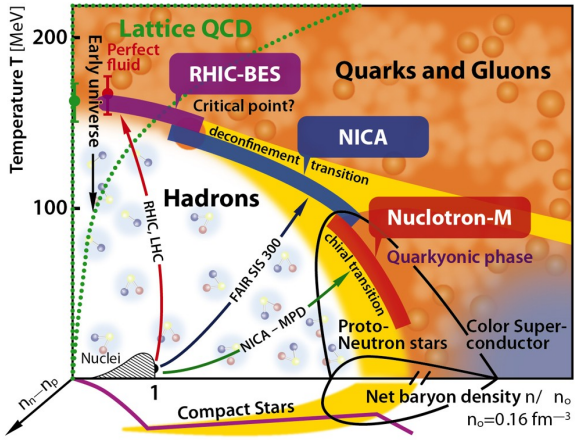
- N.Yu. Astrakhantsev
- V.V. Braguta
- A.Yu. Kotov
- A.A. Nikolaev

Outline

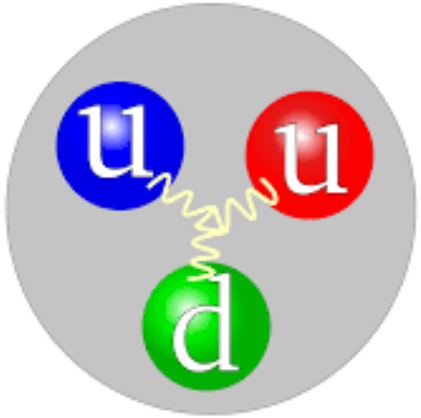




1. Quantum Chromodynamics and Lattice
2. Lattice QCD and Govorun
3. Physical applications
4. Conclusions



Theory of strong interactions (QCD)



proton

- Degrees of freedom
  - Quarks
  - Gluons

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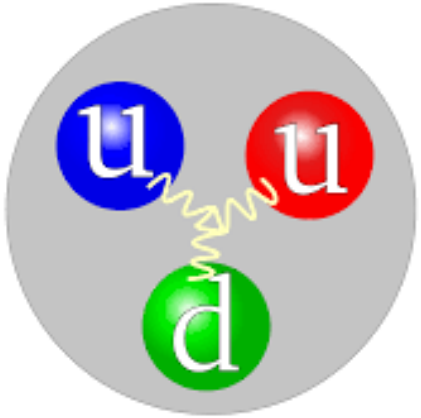

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- Confinement: The Millennium Problem!

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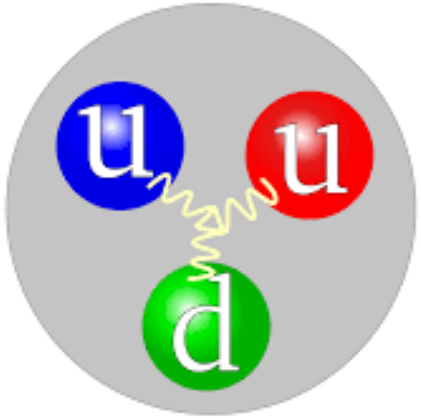

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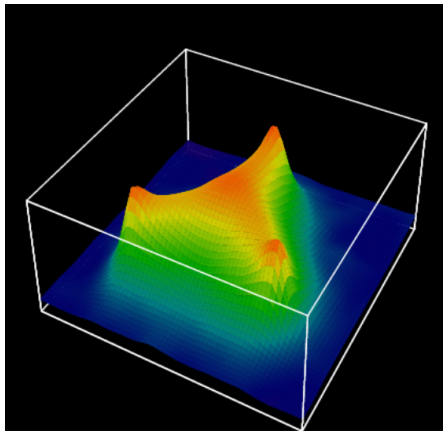

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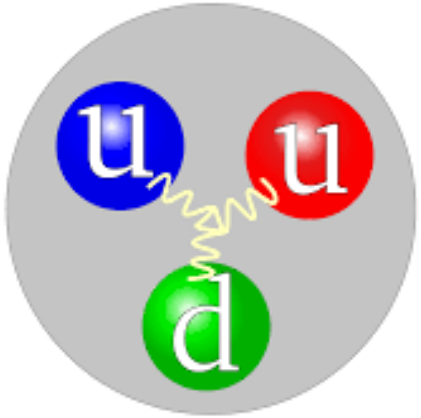

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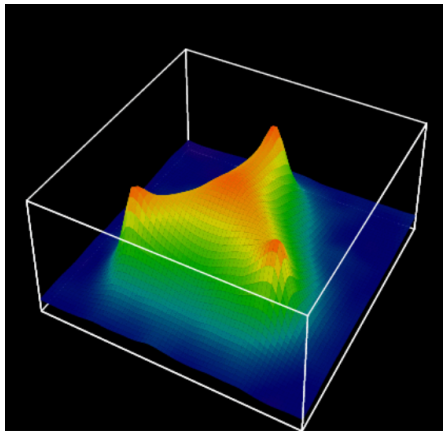
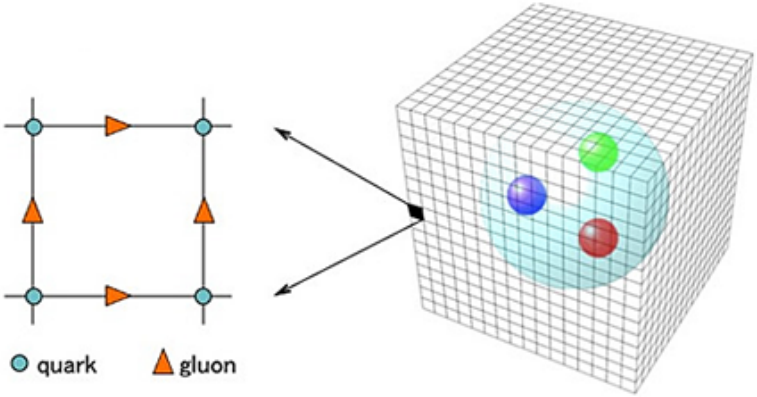


Lattice QCD allows to study QCD from the first principles!

Building Lattice QCD



Path integral:

$$Z = \int DU_{x,\mu}\ D\bar{q}_x\ Dq_x\ \exp\left(-S[U,\bar{q},q]\right)$$

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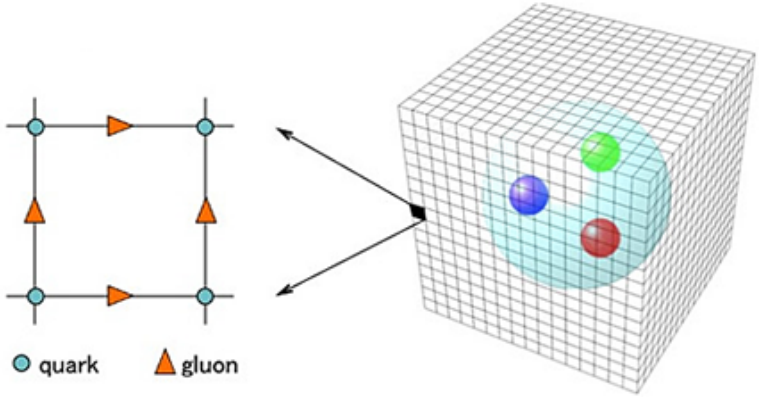

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Typical sizes:

- Number of variables U: $40^4 \times 4 \times 8 \sim 10^8$
- Number of variables q, $\bar{q}$: $40^4 \times 4 \times 3 \sim 3 \cdot 10^7$

Large number of variables $\Rightarrow$ Monte Carlo integration

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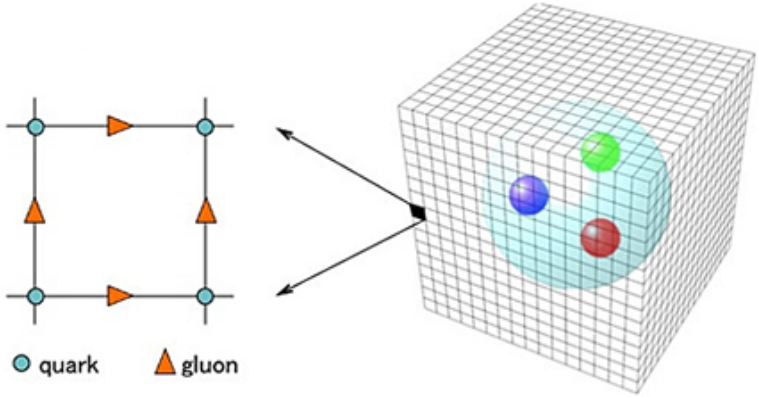

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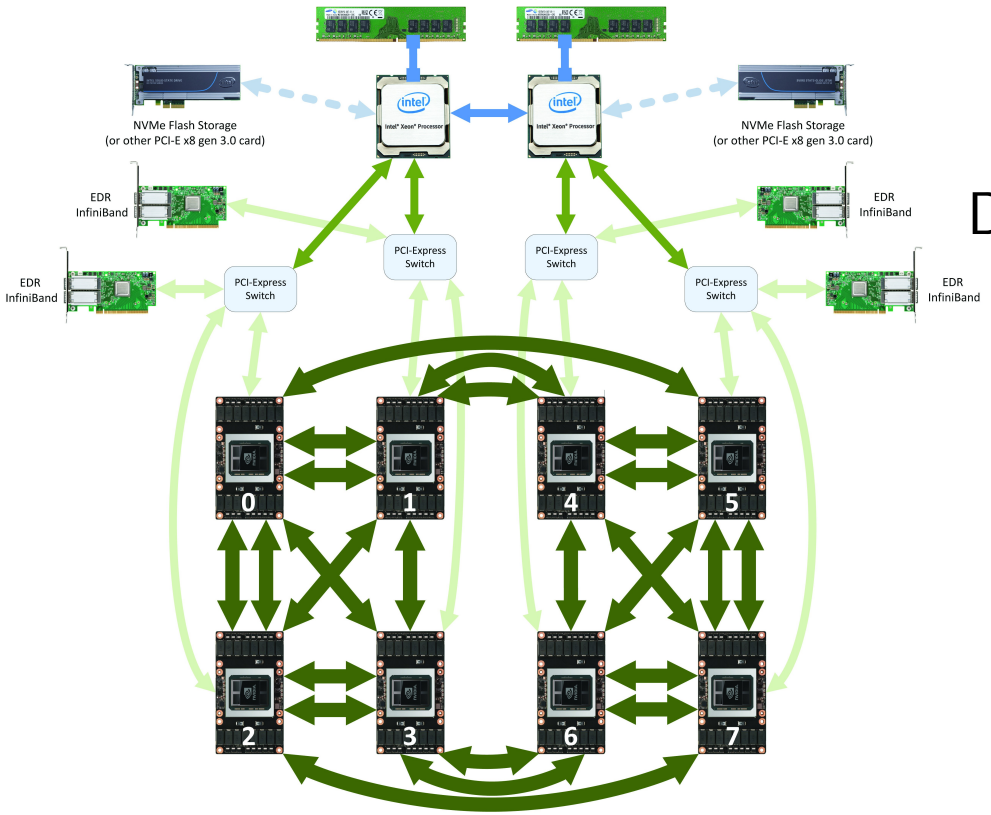
Can be efficiently parallelized on GPU!

Govorun DGX high-performance nodes



DGX-1 node:

- **8 GPU Tesla V100**
- P2P direct GPU–GPU memory transfer
- PCI-Express CPU–GPU transfer

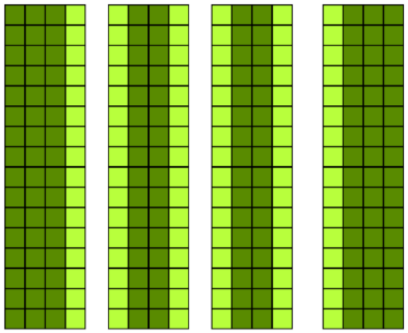
The DGX-1 nodes open wide opportunities for **multiGPU**

Single GPU problems:

- GPU Memory limitation
- Large wall time

MultiGPU strategy (1D splitting)

Lattice size $L_s^3 \times L_t$ (often $L_s > L_t$) and N GPUs:

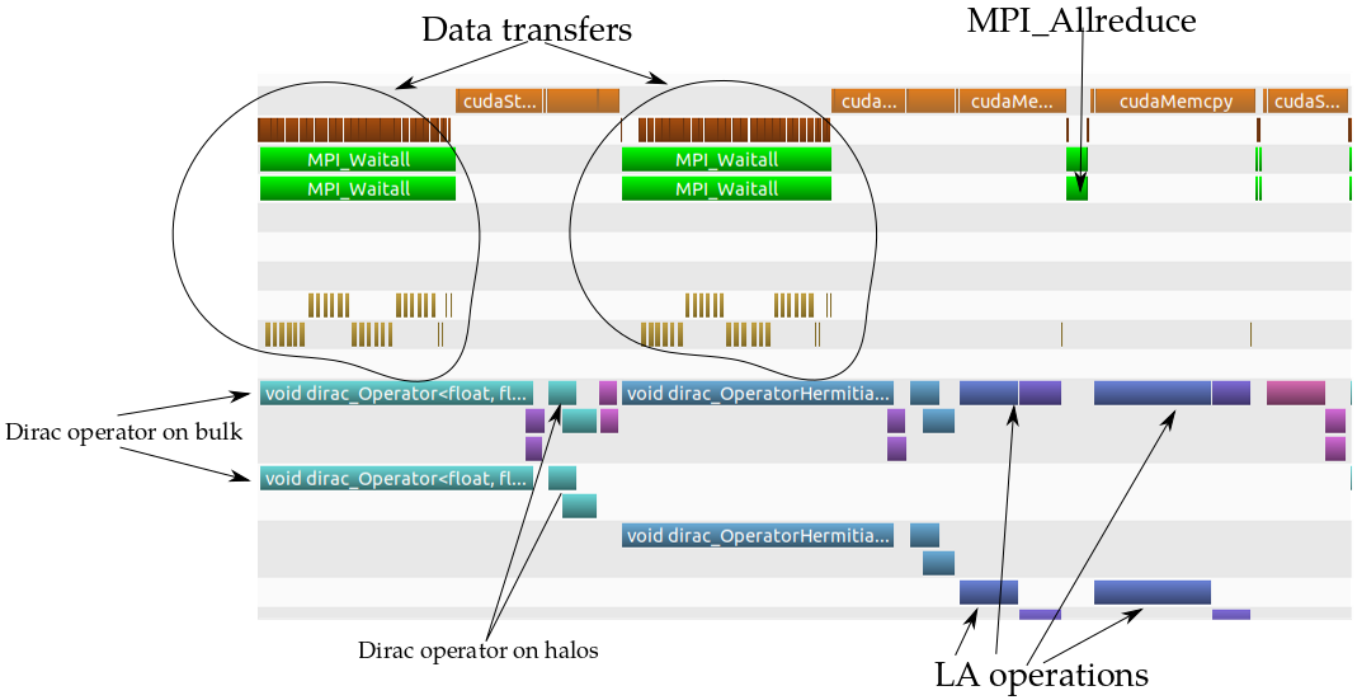


1. N slices of the size $(L_s/N) \times L_s^2 \times L_t$;
2. Data on the edge - *halos* (1 layer), the other - *bulk* ($L_s/N - 2$ layers);
3. Need neighbors from both sides: enlarge $L_s/N \to L_s/N + 2$ (creates overhead)
4. Need to transfer halos of neighbors (huge overhead);

Idea: we need to *overlap* computation of bulk with the transfer of halos.

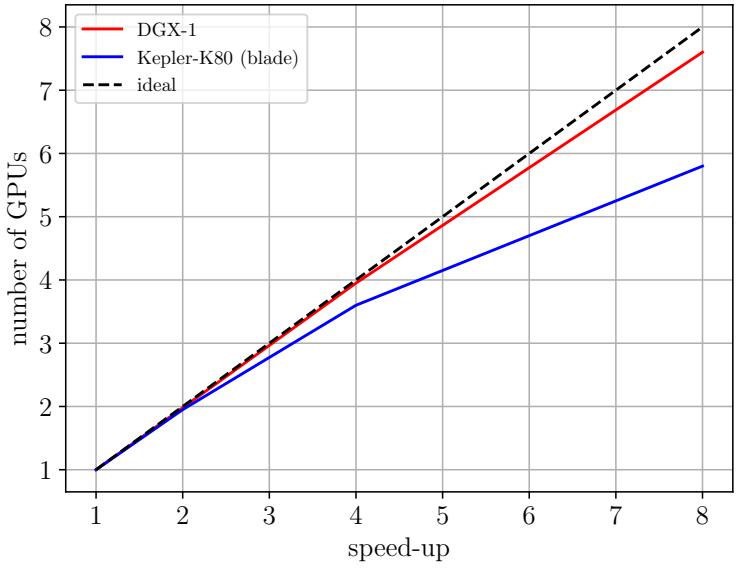
Transfer-computation overlap

DGX-1 fast P2P transfer: *completely overlap transfer with computation*.



MultiGPU performance

Lattice size $64^3 \times 16$ (commonly used), strong scaling analysis



- DGX-1 and blade: good scaling up to 4 GPUs
- DGX-1: well even at 8 GPUs (1 node)
- Blade: worse on 8 GPUs (2 nodes) due to inter-node communication

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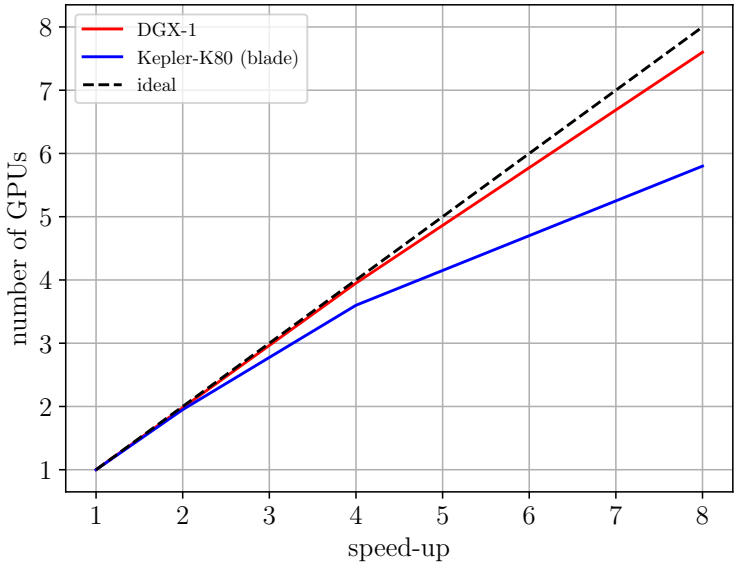

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Scaling is (almost) perfect up to 8 GPUs!

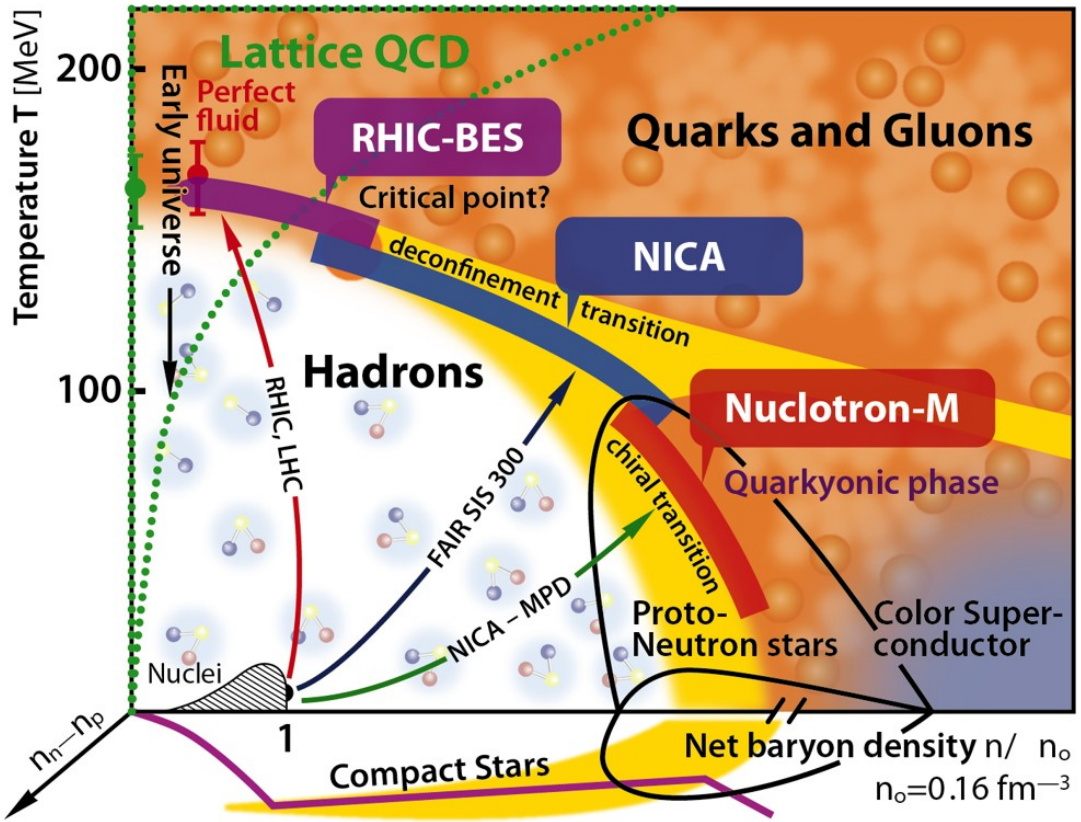
Physical results

QCD and QCD-like theories in various extreme conditions:

- Temperature T
- Baryon density ρ_B
- Isospin density ρ_I
- Chiral density ρ_5
- Magnetic field eB

Selected results

QCD phase diagram in T, μ plane

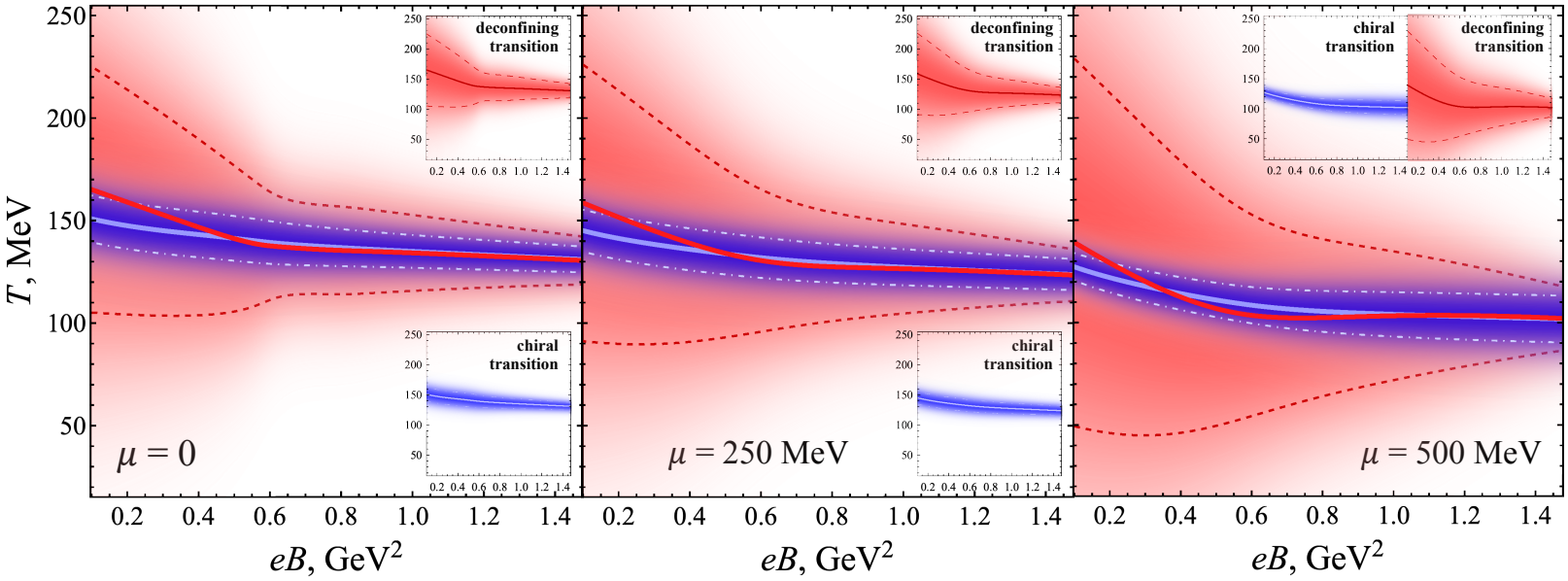


CEP estimation: $(T^{\mathrm{CEP}}, \mu_B^{\mathrm{CEP}}) \sim (100, 800)$ MeV

[arXiv:1909.09547]

Selected results

QCD phase diagram in B, T, μ space



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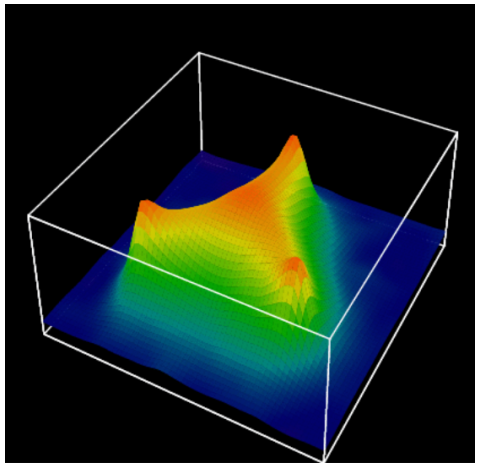
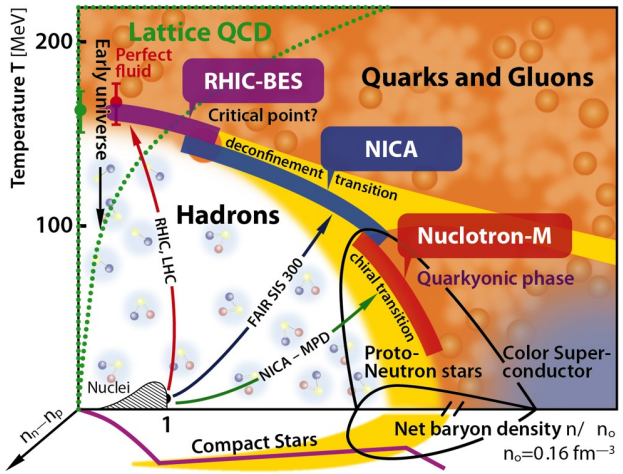
Conclusion





- QCD properties are nontrivial, interesting and important
- QCD is very complicated and can be studied reliably only within lattice simulation
- Lattice simulations are very demanding and require modern supercomputers and efficient algorithms
- Govorun Supercomputer gives possibility to conduct world level lattice simulations important for NICA experiment