



Lattice Field Theory + Multigrid + GPUs

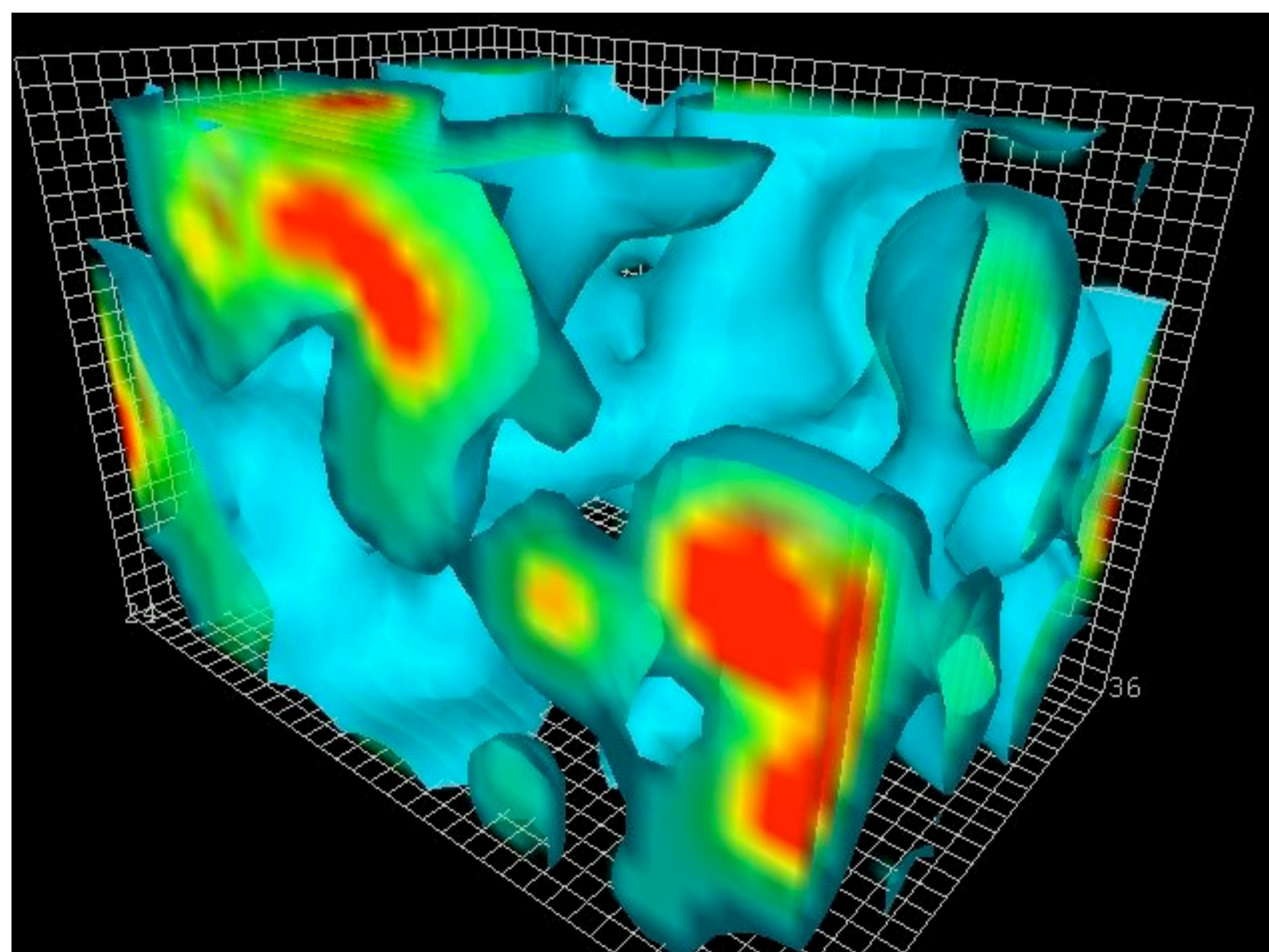
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MULTI-SCALE PHYSICS

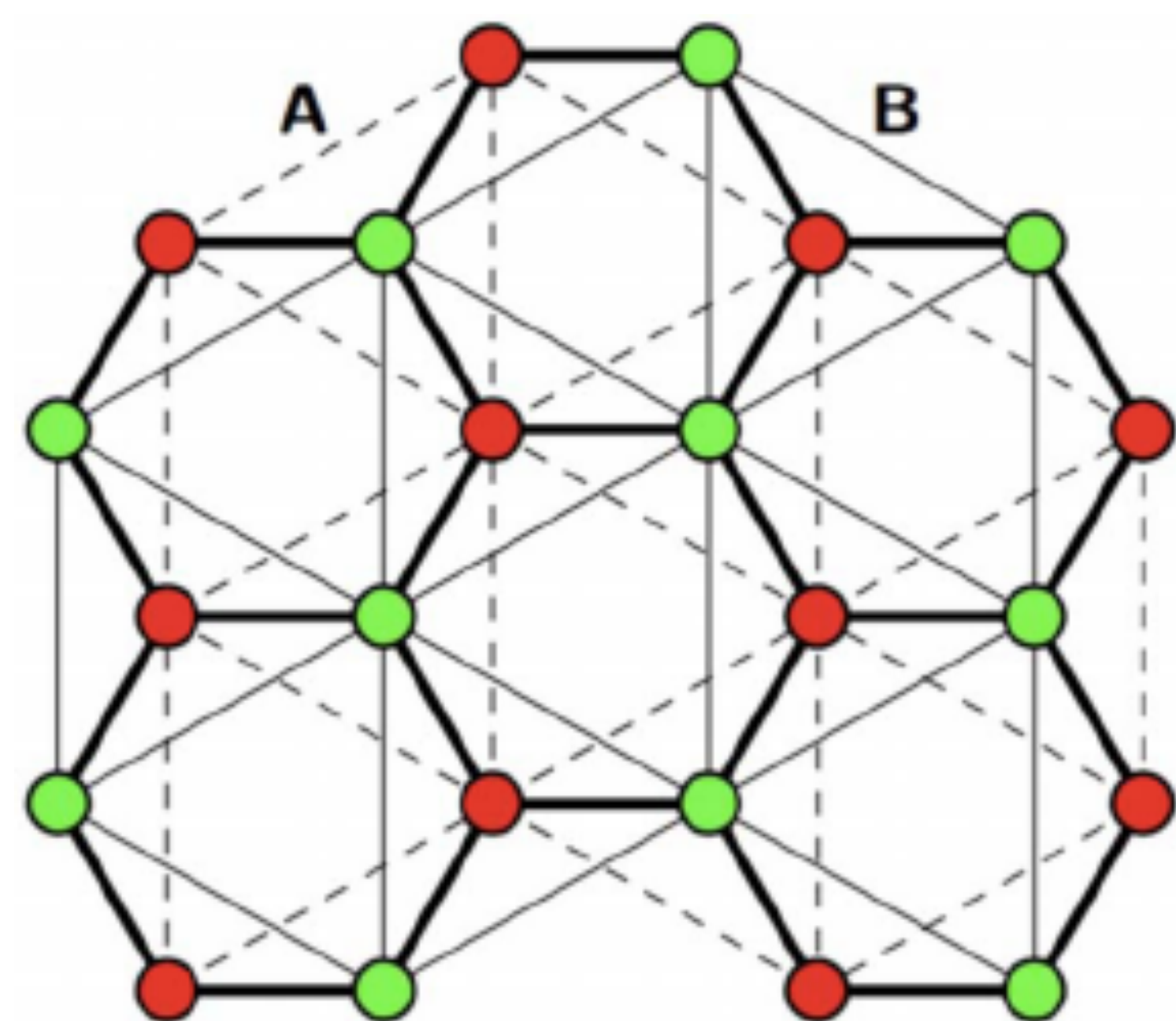
QCD spontaneously breaks scale invariance! Gives Proton its mass!

The classical QCD action (with zero mass quarks) has NO SCALE. From quantum fluctuations one scale (proton mass) arises by “dimensional transmutation” and another (pion mass) by spontaneous chiral breaking. MAGIC of quantum physics! The numerical problem is so difficult that only recently have Petascale computers been able to fully resolve the ratio: $M_{\text{proton}}/m_{\text{pi}} = 7$.



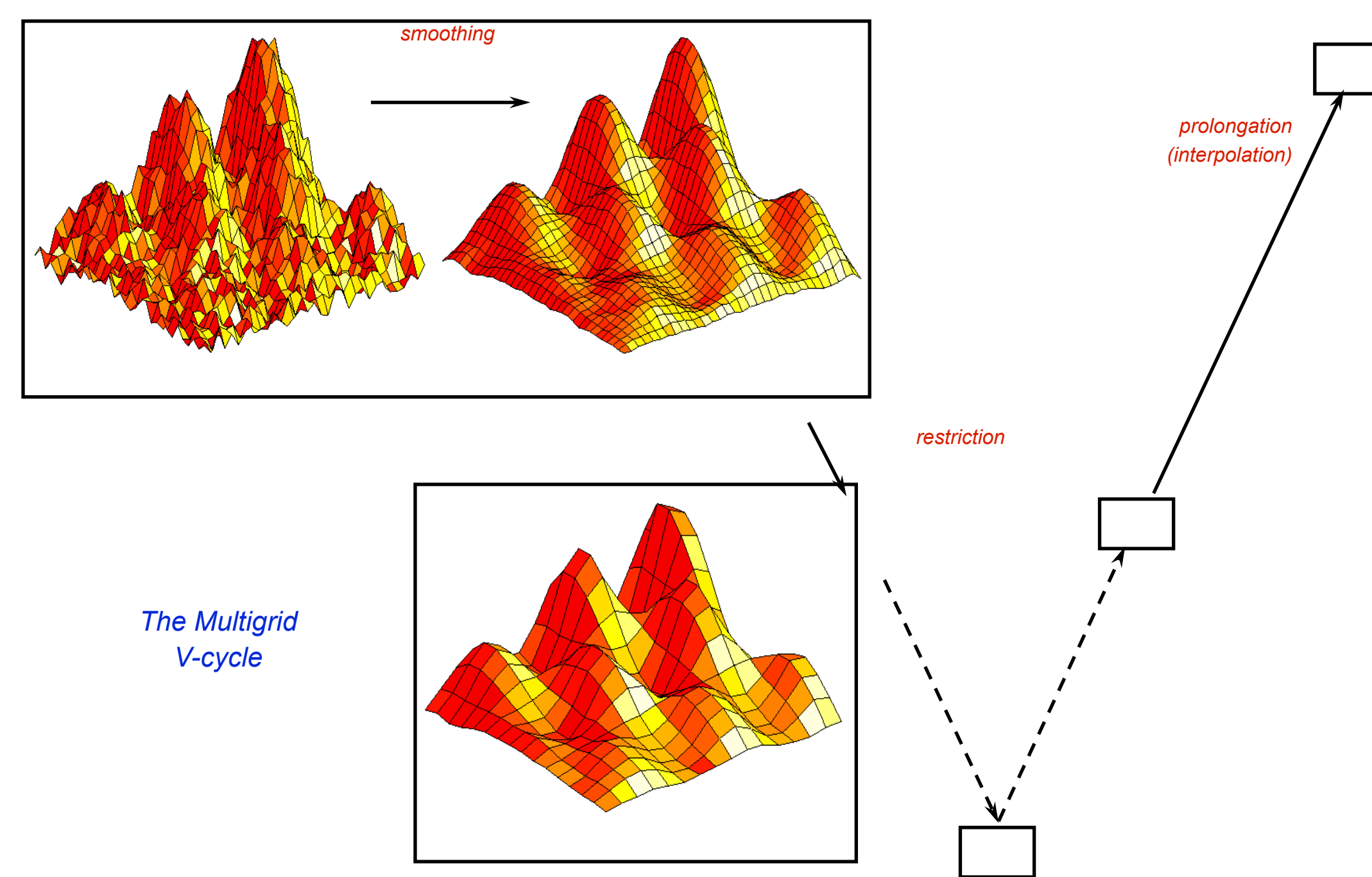
Visualization[1] of the scales in a gluonic ensemble
 $a(\text{lattice}) \ll 1/M_{\text{proton}} \ll 1/m_{\pi} \ll L(\text{box})$

Graphene is also a Lattice Gauge Theory [1] of “relativistic” Dirac Fermion theory!

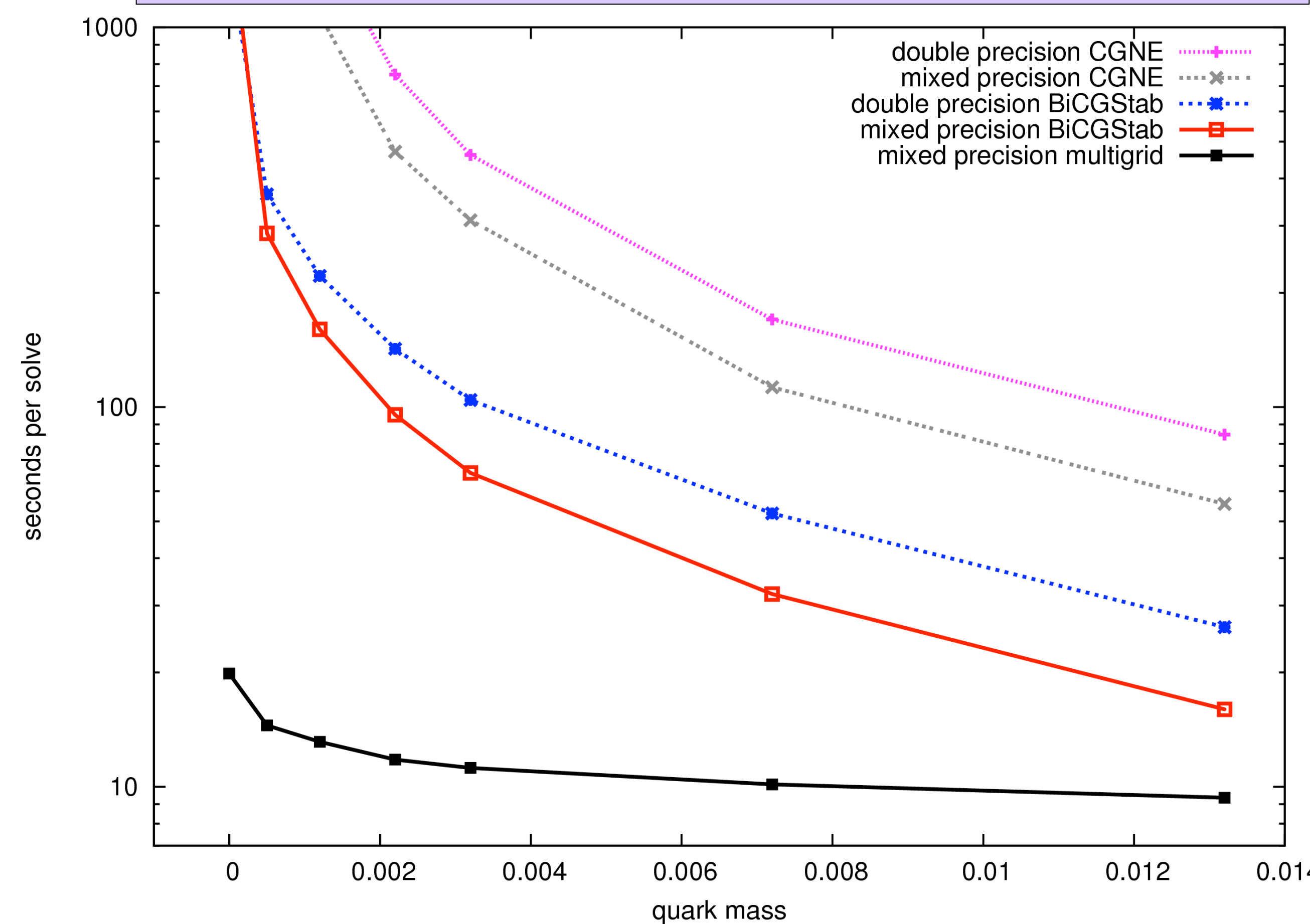


MULTI-SCALE ALGORITHMS

Adaptive Multigrid automatically Finds Slow (near Null) modes



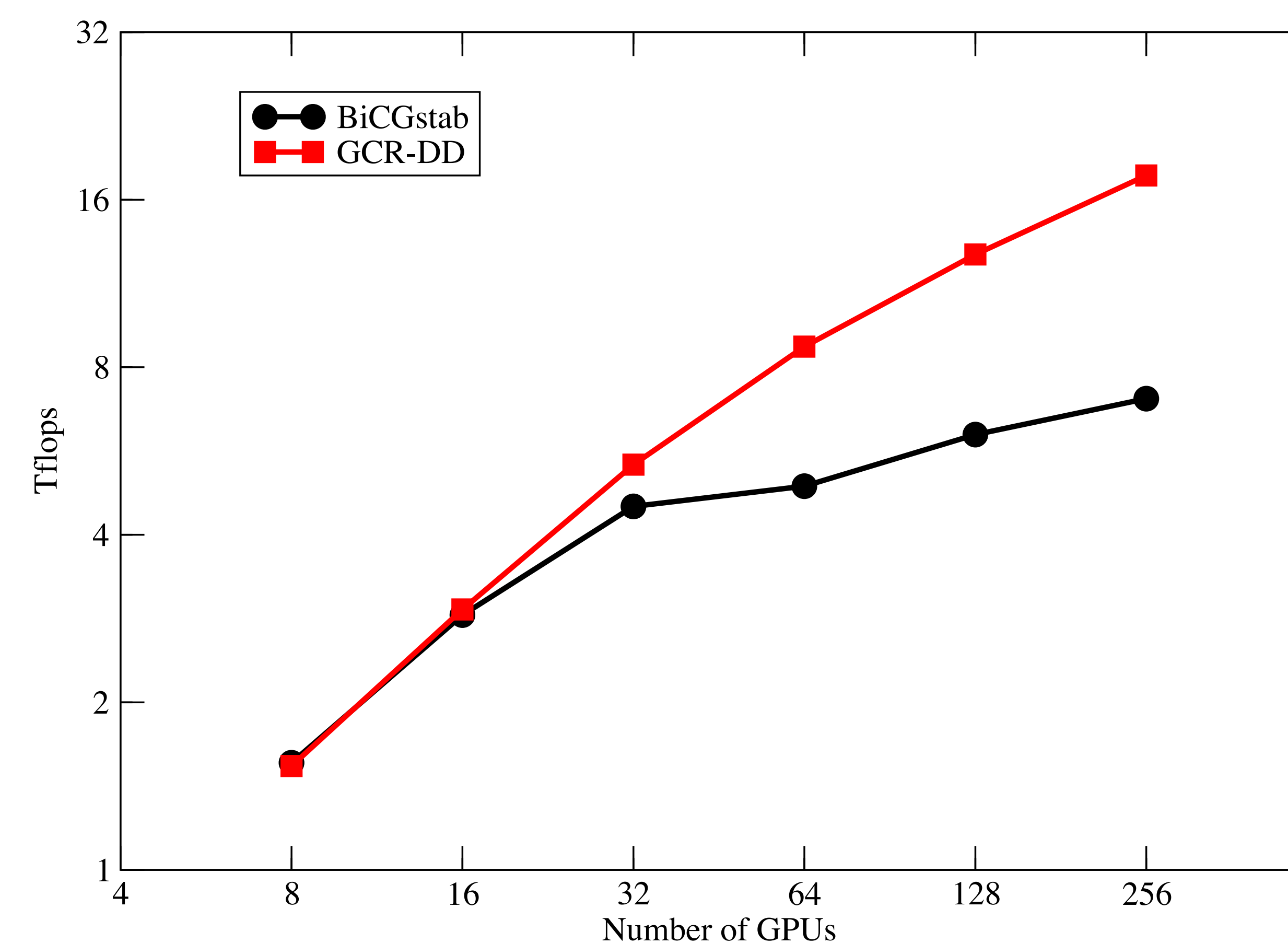
As the inverter slows down it automatically discovers the near null space to construct the coarse grid operator. Applied to the Wilson-clover Dirac inverter, it outperforms uni-grid methods by 20x at light quark masses [2] on the BlueGene/P. Extensions of adaptive MG are under development for Domain Wall and Staggered fermions and its application to Hamiltonian evolution.



Mapping multi-scale algorithms to hierarchical architecture is the software challenge at the Extreme Scale.

MULTI-SCALE ARCHITECTURE

Multi-GPU test bed for Heterogeneous and Hierarchical Extreme scale computing



(1) Development of new algorithms to meet this challenging architecture include communication reduction by (Schwarz) domain decomposition, multi-precision arithmetic, data compression and reconstruction at the core. Above the use of a simple block Jacobi DD algorithm [3] scales to $O(100)$ GPUs.

(2) The QUDA library[4] at Boston University is being used as software platform for these early investigation. Now supports multi-grid primitives and a full Multigrid GPU code is now estimated to drop the price per solver by 100x at least.

(3) Full QCD evolution code is underdevelopment in a USQCD/ Nvidia collaboration. Goal is $O(1/4)$ Petaflops) sustained on single job.

This dramatically expand the ability of lattice field theory to investigate the multiple scales in nuclear physics, the quark-gluon plasma, possible dynamics beyond the standard model

[1] R. Brower, C. Rebbi, D. Schaich, *Hybrid Monte Carlo Simulation of Graphene on the Hexagonal Lattice* (2011).
[2] R. Babich, J. Brannick, R. Brower, M. Clark, T. Manteuffel, S. McCormick, J. Osborn, C. Rebbi, *Adaptive Multigrid algorithm for the lattice Wilson-Dirac operator*. Phys. Rev. Lett. 105, 201602 (2010)
[3] R. Babich, M. A. Clark, B. Joo, G. Shi, R. C. Brower, S. Gottlieb, *Scaling Lattice QCD beyond 100 GPUs*, SuperComputing 2011.
[4] M. A. Clark, R. Babich, K. Barros, R. C. Brower, C. Rebbi, *Blasting through lattice calculations using CUDA*, (2008) <https://github.com/lattice/quda>