LGT Software & Multigrid

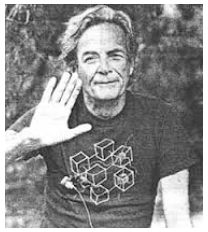
Rich Brower
Boston University

Lattice QCD Computational Science Workshop
Oak Ridge
April 30, 2013

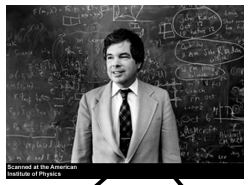
“Algorithms” for “solving” Quantum Field Theory

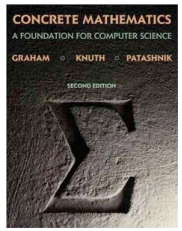
Path Int = Integral[exp[- Action]

Feynman Diagrams



Wilson Lattice QCD



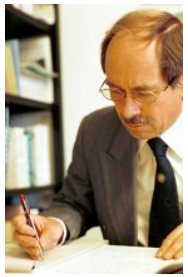


PDE/FEM
Schwartz
Schurs

Renormalization Group

Real-Space GR

Multi-Grid



‘tHooft Dim Reg

Twisters Bootstrap

OPE

AdS/CFT

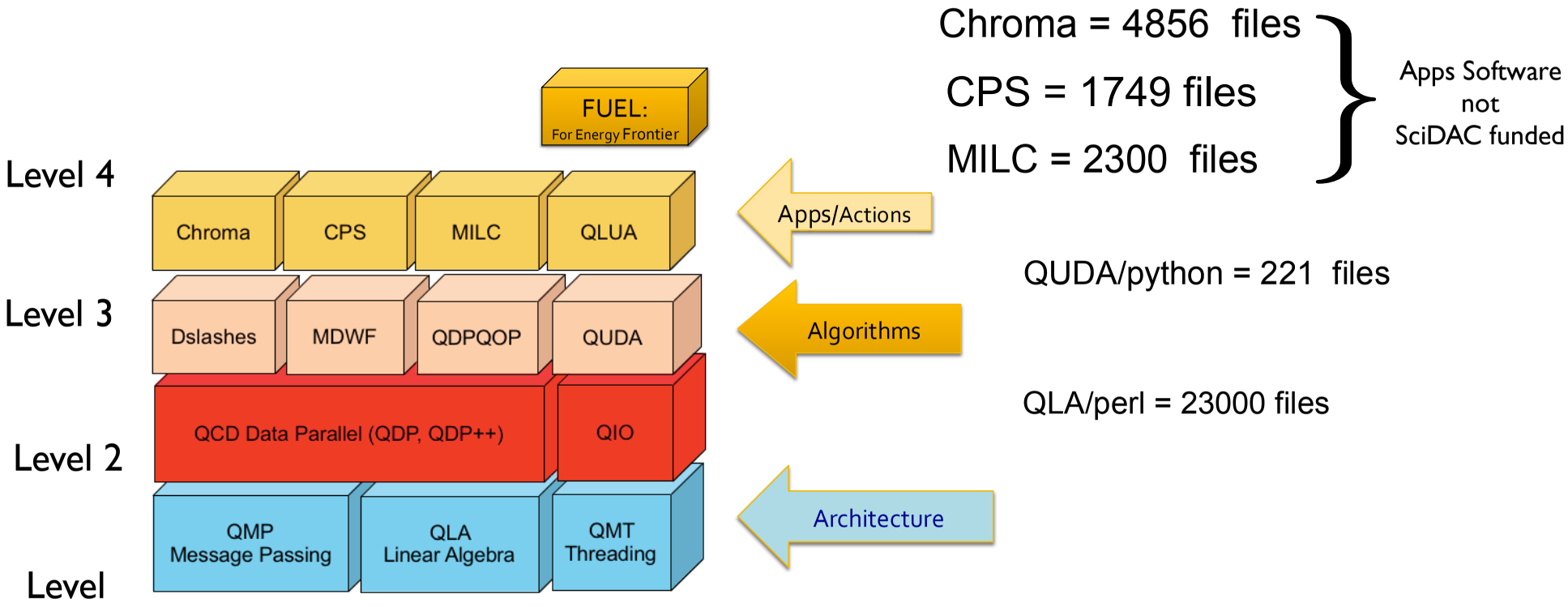
Domain Wall

Wilson Flow

DD

USQCD Software Stack Stack

On line distribution: http://usqcd.jlab.org/usqcd-software/



The application codes Chroma/CPS/MILC and a new QDP LUA code base provide a rich set of tools.

SciDAC LGT contributors

- ANL: James Osborn, Meifeng Lin, Heechang Na, (George T. Fleming)
- BNL: Frithjof Karsch, Chulwoo Jung, Hyung-Jin Kim,Yu Maezawa
- Columbia: Robert Mawhinney, Hantao Yin
- FNAL: James Simone, Alexei Strelchenko, Don Holmgren, Paul Mackenzie
- JLab: Robert Edwards, Balint Joo, Jie Chen, Frank Winter, Chip Watson
- W&M/UNC: Kostas Orginos, Andreas Stathopoulos, Rob Fowler (SUPER)
- LLNL: Pavlos Vranas, Chris Schroeder, Rob Faulgot (FASTmath)
- NVIDIA: Ron Babich, Mike Clark
- Arizona: Doug Toussaint, Alexei Bazavov
- Indiana/NCSA: Steve Gottlieb, Ran Zhou
- Utah: Carleton DeTar, Justin Foley
- BU: Richard Brower, Michael Cheng, Oliver Witzel
- MIT: Pochinsky Andrew, John Negele,
- Syracuse: Simon Catterall, (David Schaich in fall)
- Washington: Martin Savage, Saul Cohen
- Others: Peter Boyle, Jim Hetrick, Massimo Di Pierro, Patrick Dreher, et al
- “Team of Rivals” (apologies to contributors and projects *NOT* mentioned in 6 slides!)

Highest Priority is moving to 3 new architecture!

Chroma | CPS | MILC | QLUA

Dslashes | MDWF | QDPQOP | QUDA

QCD Data Parallel (QDP, QDP++) | QIO

QMP Message Passing | QLA Linear Algebra | QMT Threading

Argonne NATIONAL LABORATORY

IBM

OAK RIDGE National Laboratory

NVIDIA

TACC

intel

(May you live in Interesting Times!)

NCSA

CRAY X1

K. Wilson (Lattice 1989 Capri)

"One lesson is that lattice gauge theory could also require a 10^8 increase in computer power AND spectacular algorithmic advances before useful interactions with experiment …"

vs

- *ab initio Chemistry*

1. *1930+50 = 1980*
2. *0.1 flops ➔ 10 Mflops*
3. *Gaussian Basis functions*

- *ab initio QCD*

1. *1980 + 50 = 2030?**
2. *10 Mflops ➔ 1000 Tflops*
3. *Clever Collective Variable?*

Lattice Field Theory is just now meeting the Wilson criterion for relevance to Experimental Physics!

New Algorithms: Crucial for both New Physics & Architectures

We are just now able to resolve the pion scale!

$$a(lattice) \ll 1/M_{proton} \ll 1/m_\pi \ll L(box)$$

$$0.06 \text{ fermi} \ll 0.2 \text{ fermi} \ll 1.4 \text{ fermi} \ll 6.0 \text{ fermi}$$

$$\Longrightarrow L = O(100) \text{ or Minimum Lattice Volume } 100^4!$$

Many more scales are waiting in line:

quarks masses: (udscbt = 2, 5, 100, 1300, 4190, 200000 MeV)

Electromagnetism (proton-nucleon splitting, g-2)

Binding energy of nuclei (2.2 Mev for deuteron)

TeV Strong Gauge BSM (near conformal) dynamics for composite Higgs

Multigrid: Case History in Algorithm Development

- History Lessons (1989-1992) *
  - Cause of early failure for 20 years!

* *"MG is always the Future": Joke from JLab 2008*

** *"The future has arrived!": Message at Oak Ridge 2013*

- Modern Era (2008-2013)
  - 5 years to put into production the QCD MG Solver for Wilson-clover

- Future** (2013-2018)
  - Domain Wall & Staggered Solvers, HMC evolution, etc
  - Adaptation to heterogeneous architectures, etc.

Past History

QCD MG attempts in 1990's

See Thomas Kalkretuer
hep-lat/9409008
review on "MG Methods
for Propagators in LGT".

Israel: Ben-Av, M. Harmatz,
P.G. Lauwers & S.Solomon

Boston: Brower, Edwards,
Rebbi & Vicari

Amsterdam: A. Hulsebos,
J Smit J. C. Vick

Amsterdam: A. Hulsebos,
J Smit J. C. Vick

group	operator to be inverted	gauge field	lattice sizes
"Israel	$\not{D} + m$	2-d $U(1)$	$\leq 256^2$
[3, 13, and references therein]	staggered fermions	2-d $SU(2)$	$\leq 256^2$
1989–ongoing		2-d $SU(3)$	$\leq 128^2$
"Amsterdam"	$-\not{D}^2 + m^2$	2-d $SU(2)$	$\leq 128^2$
[14, and references therein]	staggered fermions		
1990–1992	staggered fermions	2-d $SU(2)$	$\leq 128^2$
	and Wilson fermions		
"Boston"	$-\Delta + m^2$	2-d $U(1)$	$\leq 64^2$
[7, and references therein]		4-d $U(1)$	$\leq 16^4$
1990–1991		2-d $SU(2)$	$\leq 32^2$
	$(\gamma_\mu + 1)D_\mu + m$	2-d $U(1)$	64^2
	Wilson fermions		
[29]	$(\gamma_\mu + 1)D_\mu + m$	2-d $U(1)$	64^2
1990–1992	Wilson fermions	4-d $SU(3)$	16^4
"Hamburg"	$-\Delta + m^2$	2-d $SU(2)$	$\leq 128^2$
[21, 18, 22, 23, 1, 17, 19, 20, 2, 24]		4-d $SU(2)$	$\leq 18^4$
1990–ongoing	$-\not{D}^2 + m^2$	2-d $SU(2)$	$\leq 162^2$
	staggered fermions	4-d $SU(2)$	$\leq 18^4$

Table 1: *Overview of works on MG methods for propagators in lattice gauge theories.*

QCD MG "failure" in 1990's:

SUPERCOMPUTER
COMPUTATIONS
RESEARCH INSTITUTE

PROJECTIVE MULTIGRID FOR
WILSON FERMIONS

by

Richard C. Brower, Robert G. Edwards,
Claudio Rebbi, and Ettore Vicari

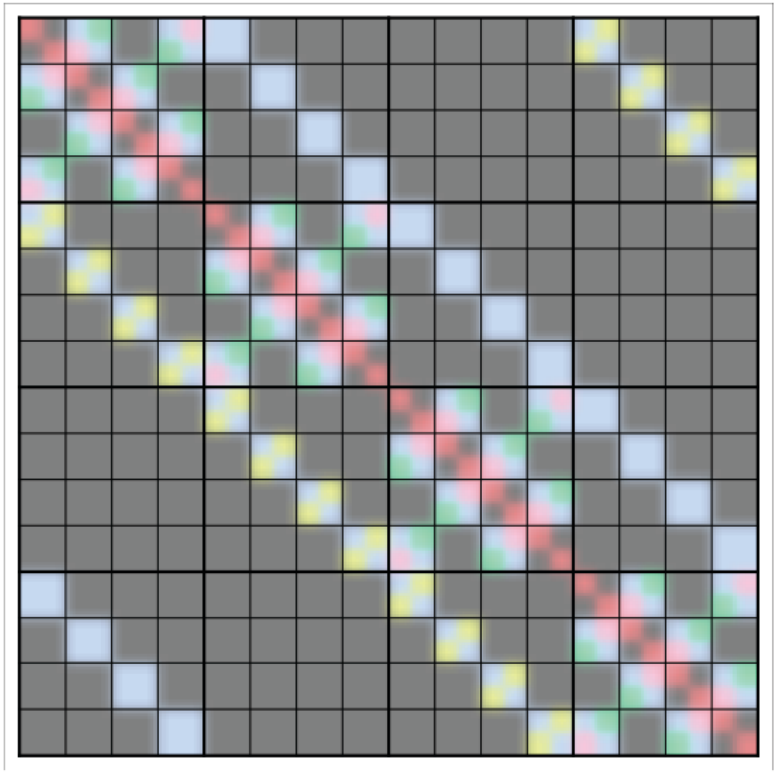
FSU-SCRI-91-54

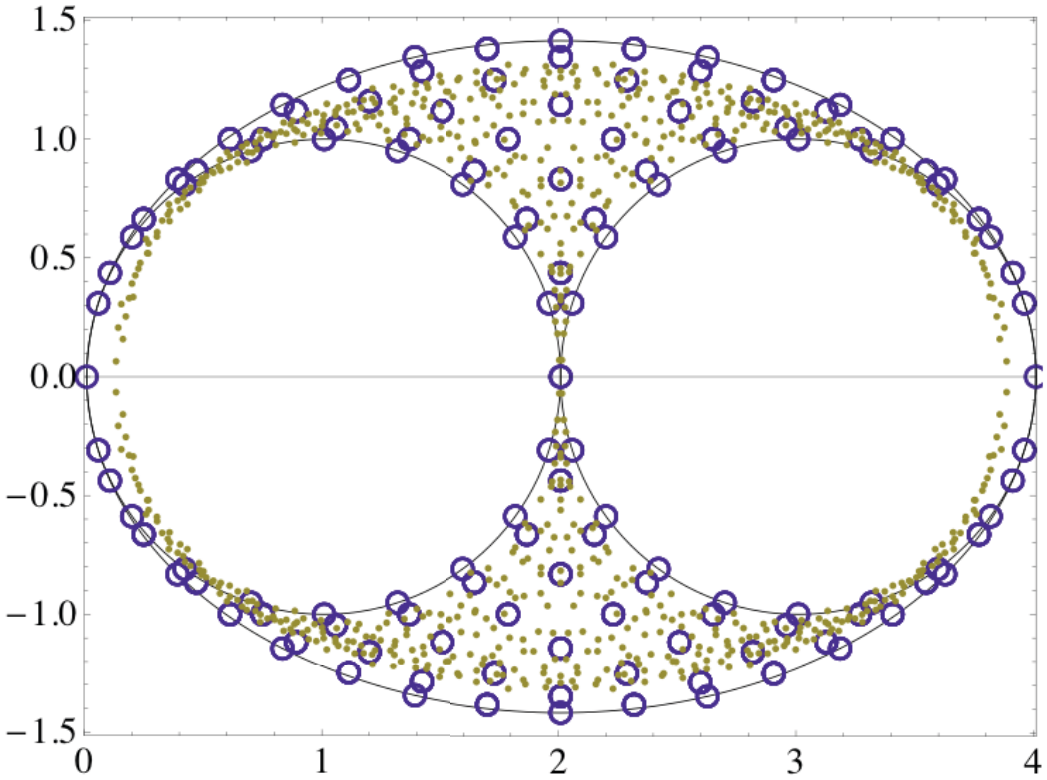
Wilson Operator

2-D Wilson Dirac Operator

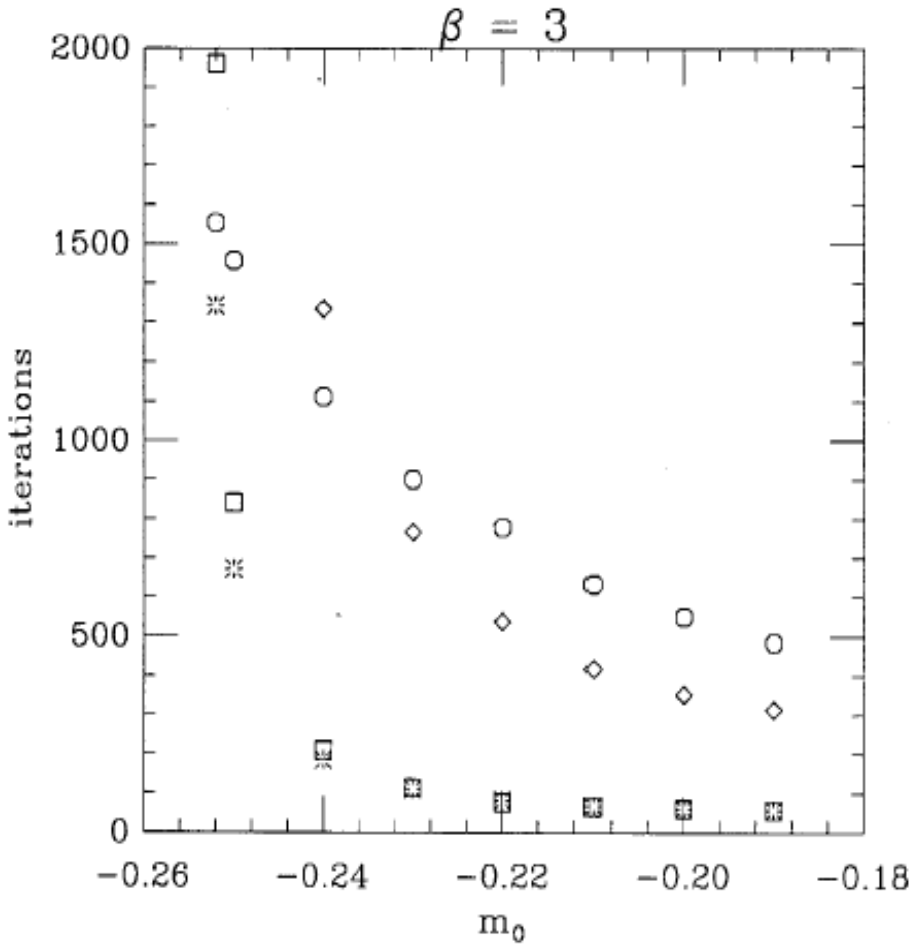
$$D^{\text{Wilson}}_{x,x'} =$$

$$(m+d)\,\delta_{x,x'} - \sum_{\mu} \frac{1}{2}\left[(1+\gamma_\mu)\,U_{x,\mu}\,\delta_{x+\hat{\mu},x'} + (1-\gamma_\mu)\,U^{\dagger}_{x,\mu}\,\delta_{x,x'+\hat{\mu}}\right]$$

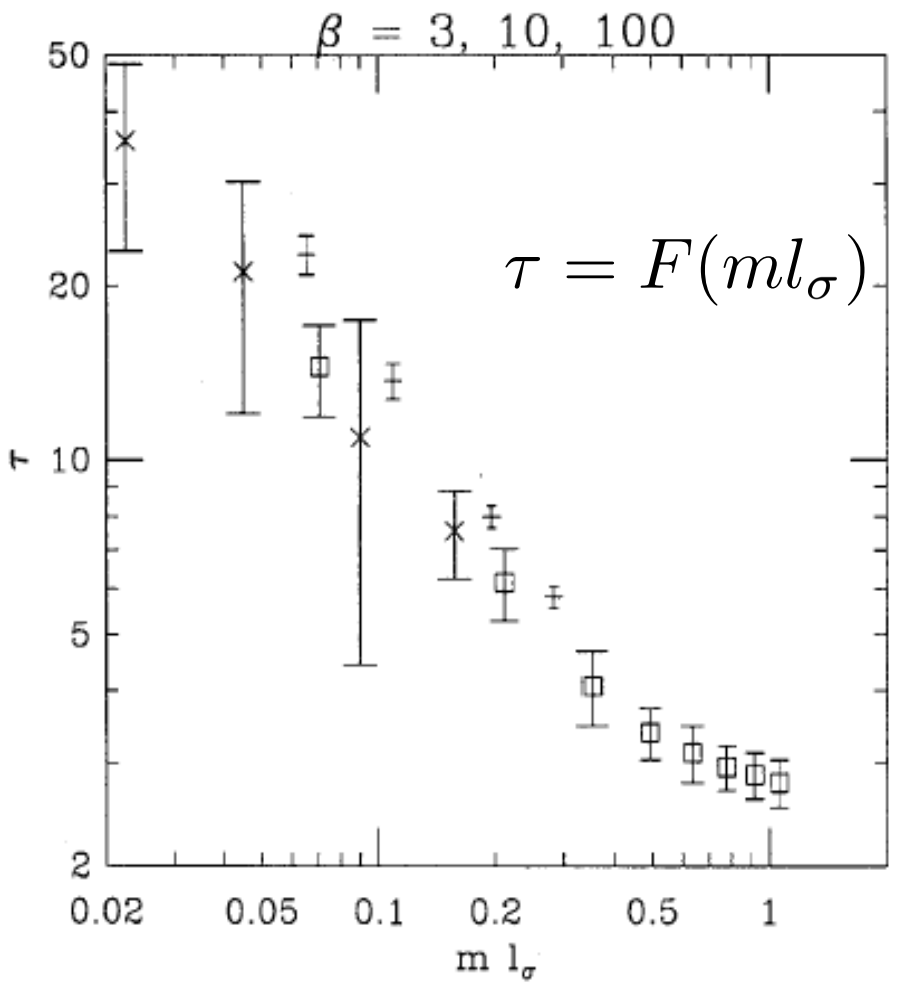




Universal "failure" of Critical Slowing down:



Gauss-Jacobi (Diamond), CG (circle), Multi-Grid 3 levels (square star)

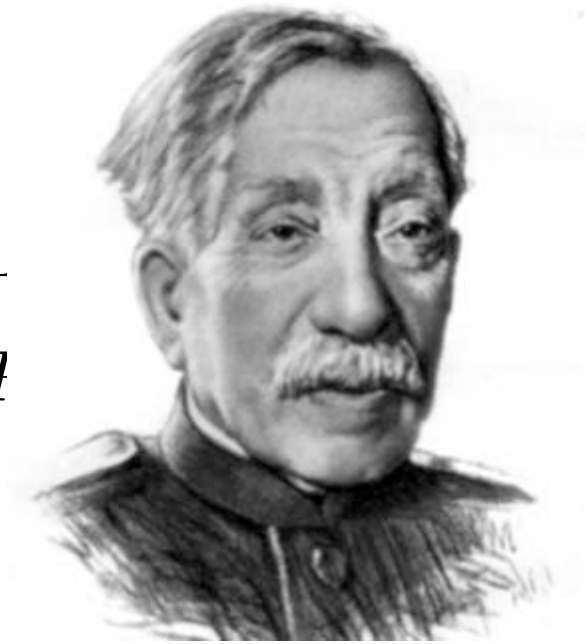


$\beta = 3(cross), 10(plus), 100(squares)$

Success & Failures of MG attempts in 1990's : Why?

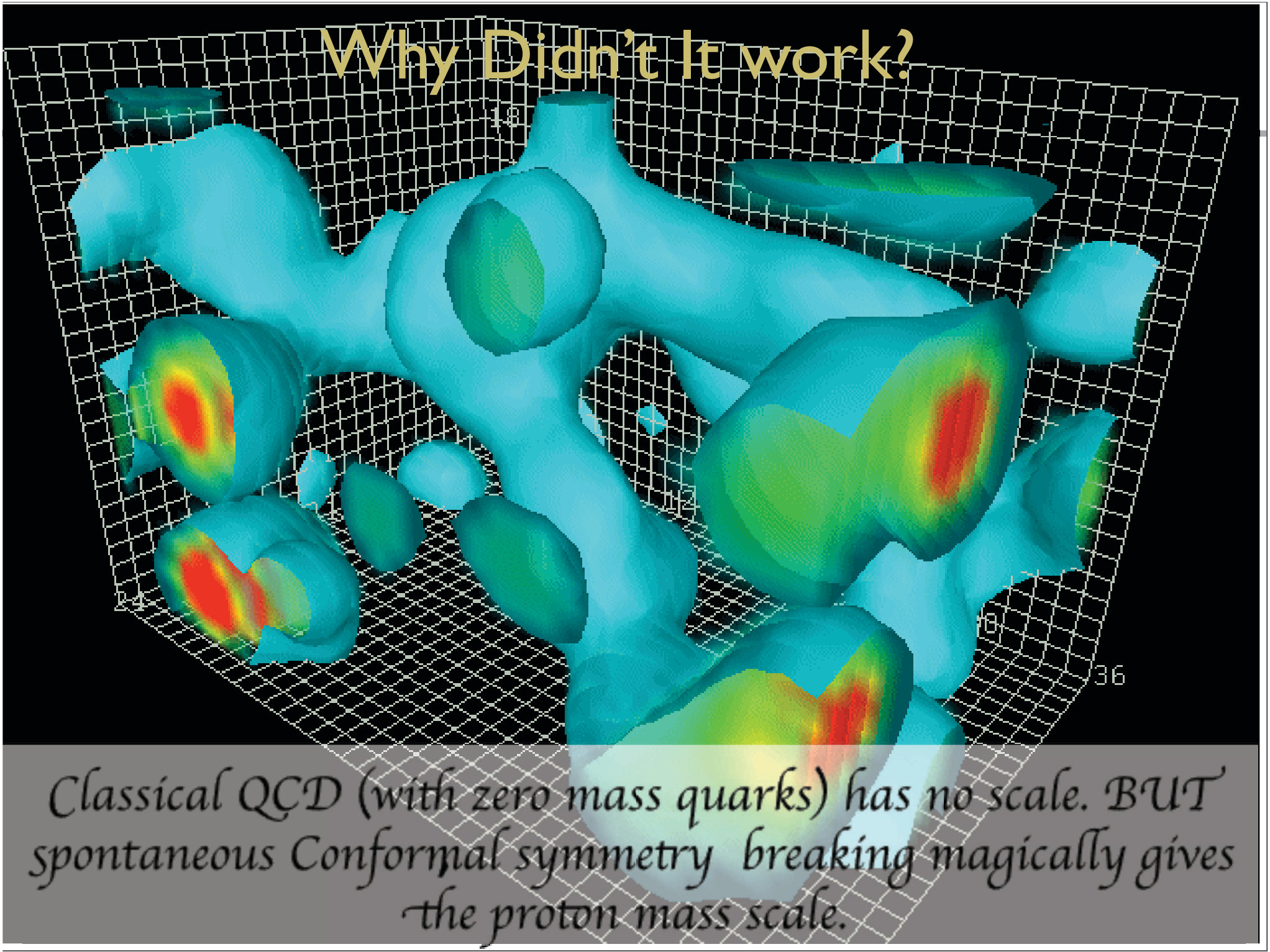
- Success:
- Maintain Gauge Invariance
- Maintained Gamma-5 Hermiticity $H = \gamma_5 D = D^\dagger \gamma_5$
- Local adaptive blocking (with Projective MG)
- Partial success with (RG) at weak coupling
- Failed at strong coupling.
- Galerkin form corse operator: $\mathrm{D}_c = R$

Prolongator $P \implies$ Restrictor $R = I$



Boris Grigoryevich Galerkin (Russian: Бори´с Григо´рьевич Галёркин, surname more accurately romanized as **Galyorkin**; March 4 [O.S. February 20, 1871] 1871 – July 12, 1945),

Why Didn't It work?



Classical QCD (with zero mass quarks) has no scale. BUT spontaneous Conformal symmetry breaking magically gives the proton mass scale.

First Success: Applied Math/Physics Collaboration Collaboration

Many different people (TOPS, QCD) and institutions involved in the collaboration

- CU Boulder
  - Tom Manteuffel
  - Steve McCormick
  - Marian Brezina
  - John Ruge
  - James Brannick
  - Christian Ketelsen
  - Scott MacLachlan
- Lawrence Livermore
  - Rob Falgout
- Columbia
  - David Keyes

Chris Schroeder

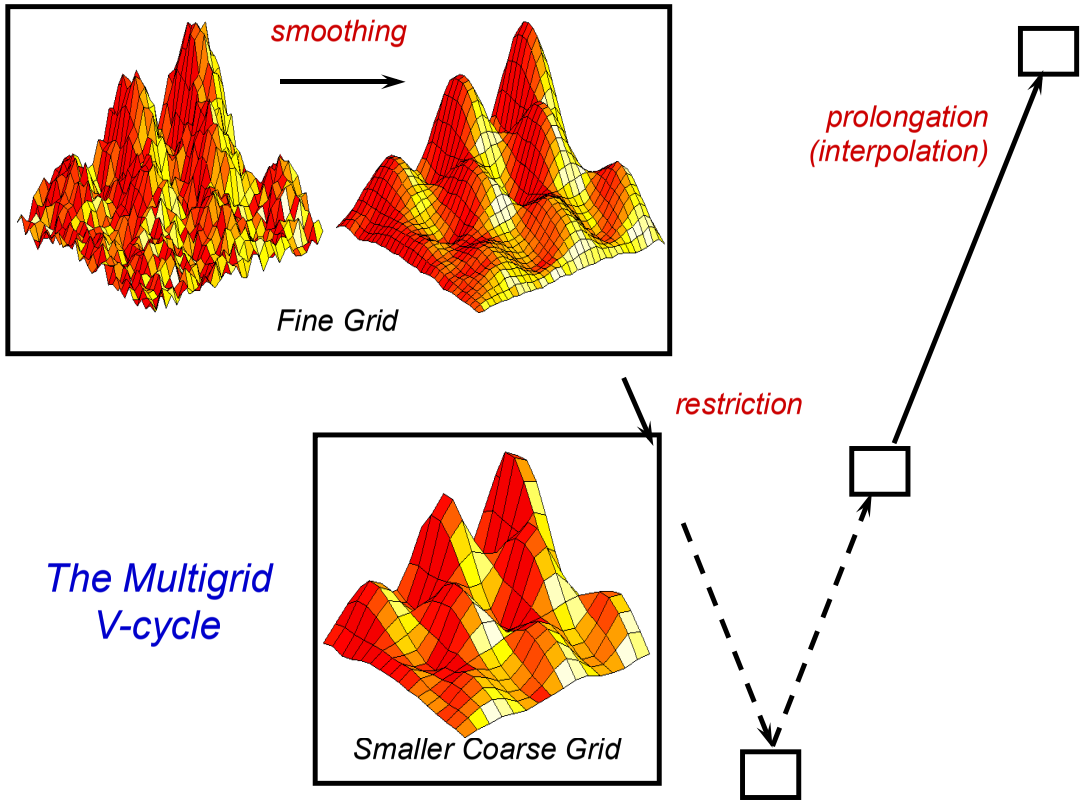
- MIT
  - Andrew Pochinsky

- Ron Babich
- Boston University
  - Rich Brower
  - Claudio Rebbi
  - Mike Clark
  - James Osborn
  - Saul Cohen
- Penn State
  - James Brannick
  - Ludmil Zikatanov
- Tufts
  - Scott MacLachlan
- Argonne
  - James Osborn

- NVIDIA
  - Mike Clark
  - Ron Babich
- Michael Cheng
- Oliver Witzel
- INT Seattle
  - Saul Cohen

Present Break Through

Adaptive Smooth Aggregation Algebraic Multigrid



The Multigrid V-cycle

Spilt the vector space into near null space $\mathcal{S}$ and the complement $\mathcal{S}_\perp$

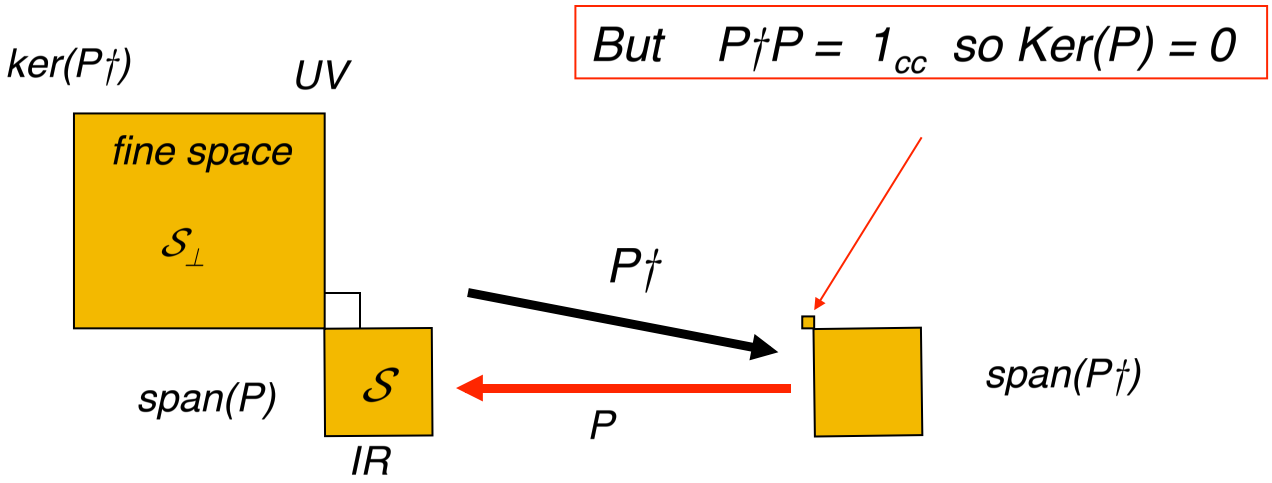
$D: \mathcal{S} \simeq 0$

Slow convergence of Dirac solver is due to small eigenvalues for vectors in near null subspace: $\mathcal{S}$.

What is the New Idea?

- Math Speak: A Schur/Schwarzian DD splitting of the vector space:
  - How do you spit the space into Fine vs Coarse Space?
  - Classical MG vs Adaptive MG

Karl Hermann Amandus Schwarz (25 January 1843 – 30 November 1921)



(see Front cover of Strang's Undergraduate MIT math text!)

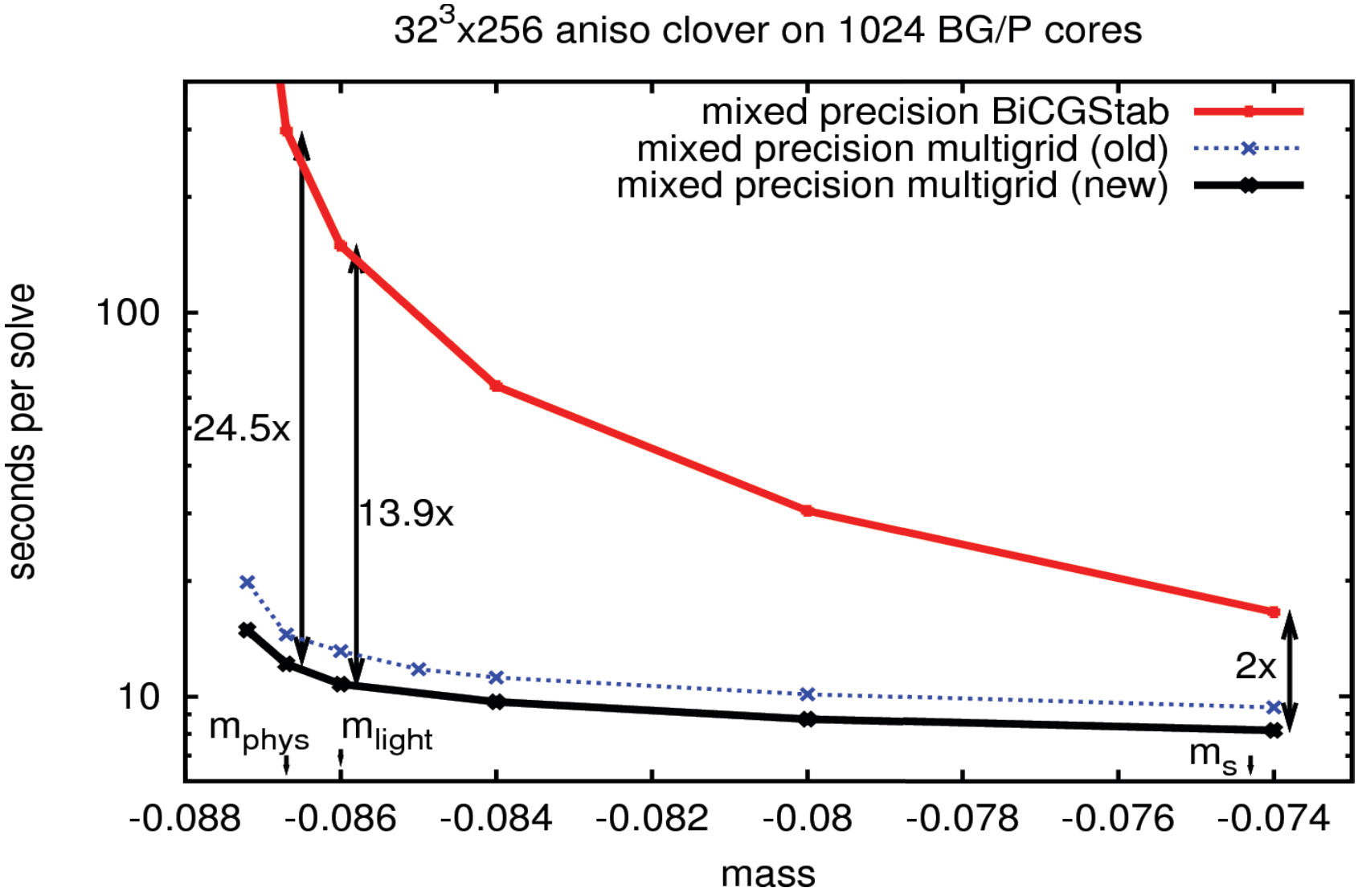
- In Physics Speak: The Wilsonian Renormalization Groups:
  - How to separate UV (short scales) from IR (long scales)
  - Conformal (Scale Inv) vs Non-perturbative RG

Devils in the Details!

- To turn the new Mathematical idea into a competitive MG solver took a lot of work!
  - First in principle demonstration of coarsening used the normal equations: no dependence on the mass (lowest e.v.) but was not competitive.
  - Needed to go to Red/Black precondition non-Hermitian operator -- not conventional MG.
  - O(25) near null vector on 4^4 blocks plus chirality.
  - GCR smoother etc etc.
- See:

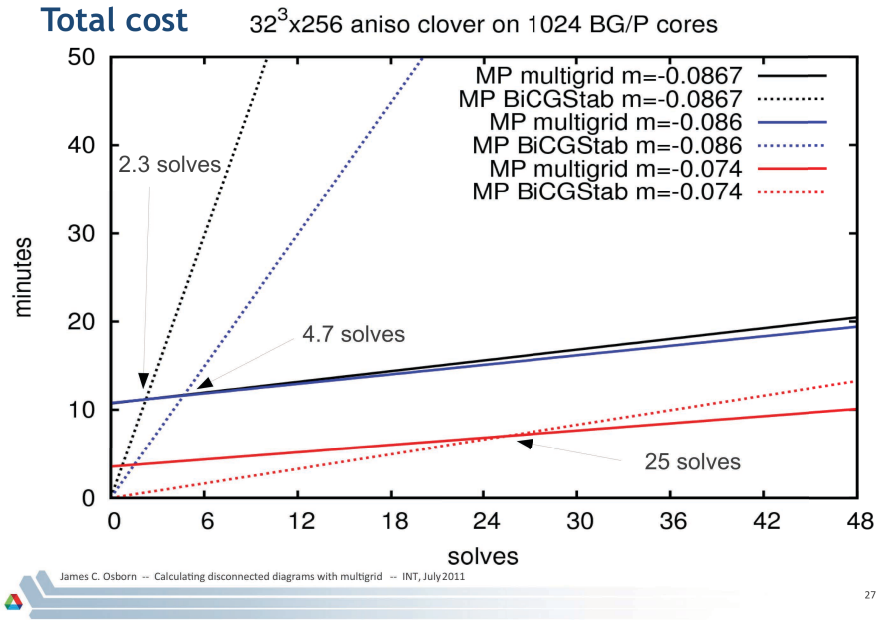
  Adaptive multigrid algorithm for the lattice Wilson-Dirac operator, R. Babich, J. Brannick, R. C. Brower, M. A. Clark, T. A. Manteuffel, S. F. McCormick, J. C. Osborn and C. Rebbi, Phys. Rev. Lett. 105 (2010) 201602.
- Code is available: Documentation this sumer?

Adaptive Smooth Aggregation Algebraic Multigrid



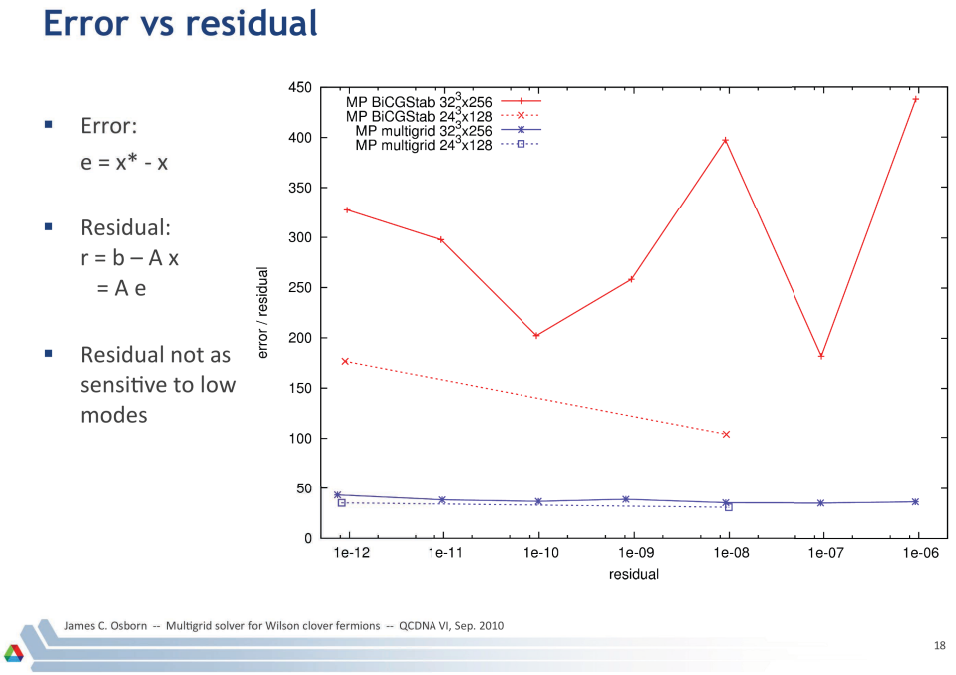
SciDAC compliant production code on BG/P

Good News/Bad News



More Data: Should Save MG projectors with lattice

Actually MG error is smaller at fixed Residual



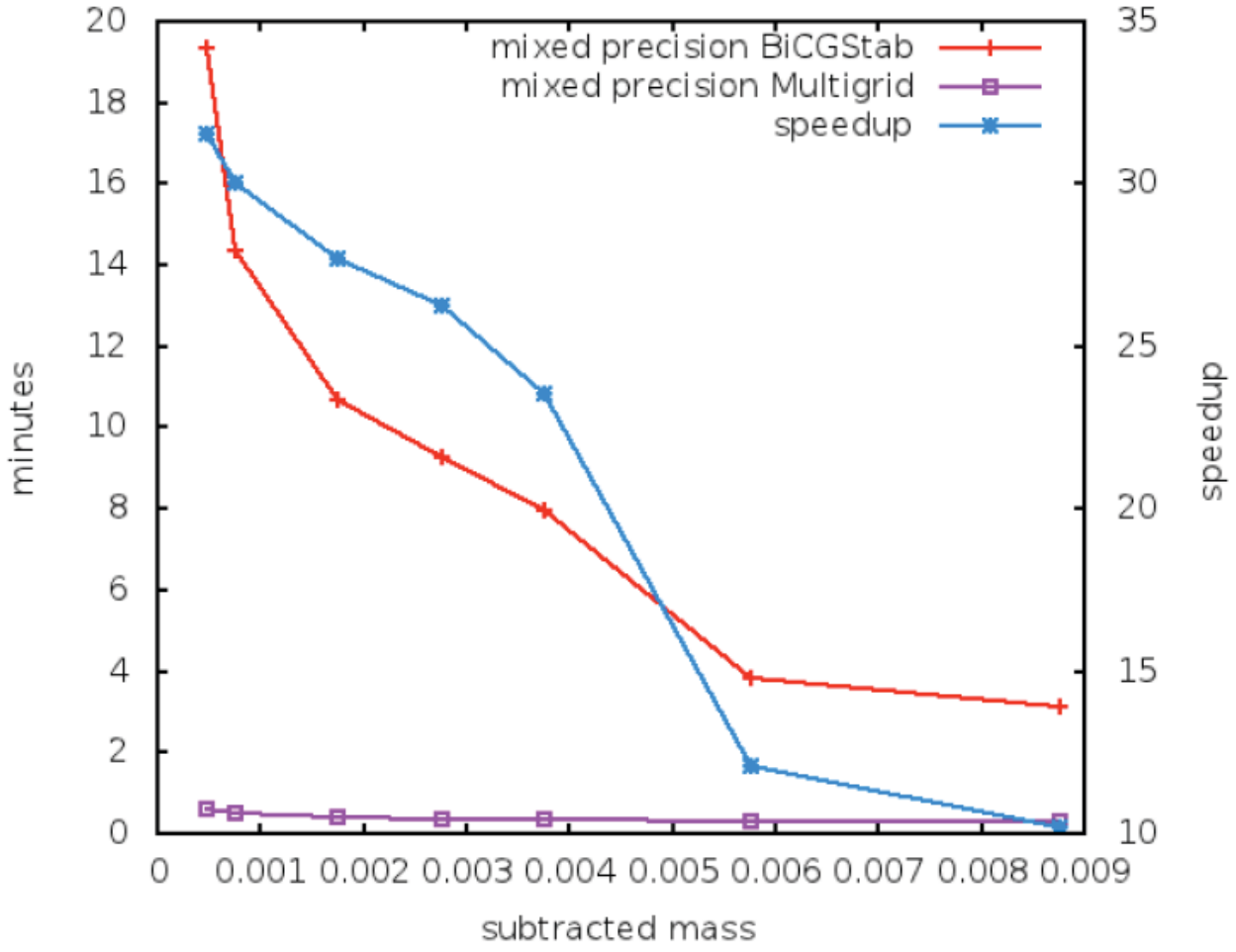
Wilson clover multigrid (3 level)

128^3x96 quenched lattice (Karsch+collabs.)

512 BG/Q nodes (64 ranks/node), plain C, xlc -O3, QMP-MPI

BiCGStab total speed
~ 5.8 Tflops
(5.6% peak)

Multigrid effective rate
~ 184 Tflops
(176% peak)

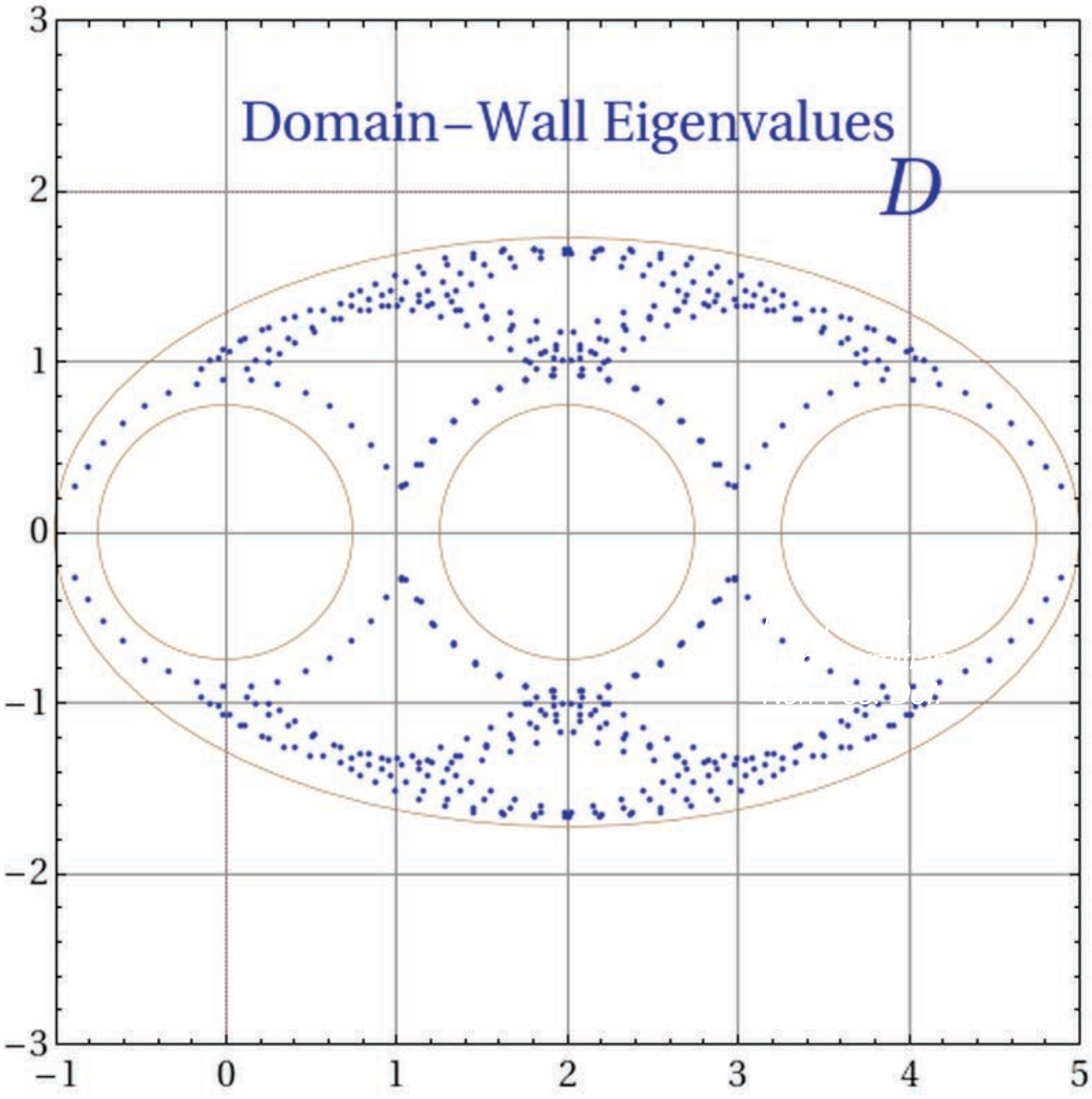


Near Future Projects

What about Domain Wall and Staggered?

- Domain Wall attempt Saul Cohen, M. Clark and J. Osborn
  - Must use Normal Equations (so far).
  - But Blocking eliminate 5th dimension!
  - The algorithm is still not tested.
  - New effort with Oliver Witzel and Andrew Pochinsky in QLUA
- Staggered.
  - Red/Black precondition is the Normal Eq.
  - Theoretical straight forward
  - BUT “double” is a 4 fold increase in near null space.
  - May have to have blocks preserving the tastes?
  - Carleton ?

Multigrid Algorithms for Domain-Wall Fermions, S. D. Cohen, R. C. Brower, M. A. Clark and J. C. Osborn, PoS LATTICE 2011, (2011) 030



Non-normal
non-Hermitian
Non Pos. Def.

$$D = U\sqrt{D^\dagger D}$$

$$D^\dagger D = H^2$$

$$(\Gamma_5)^n D$$

Saul's Video!

What about Multigrid HMC?

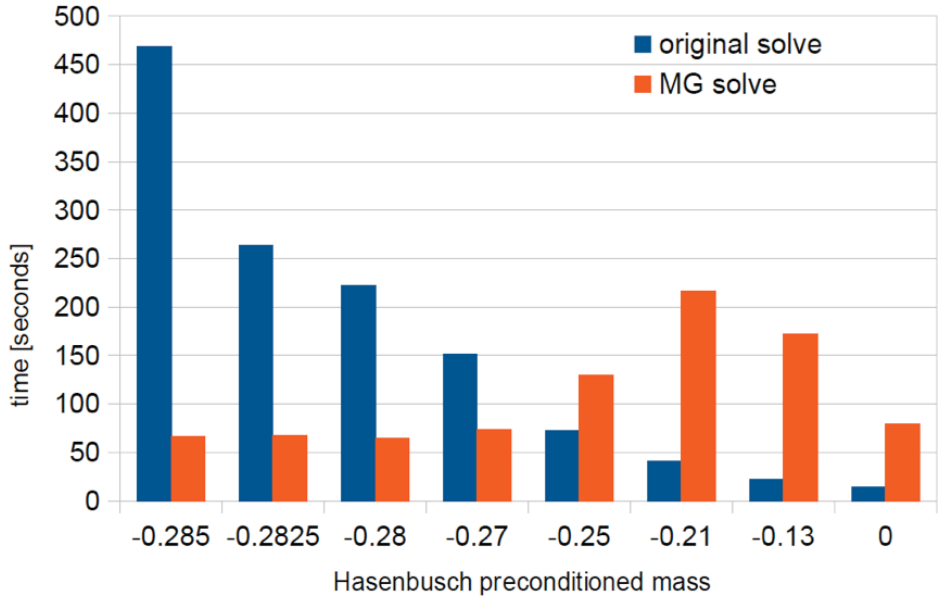
New Project with Meifeng Lin and James Osborn: VERY EARLY TESTS on Wilson Lattice from Kostas.

- Looks promising with much development
- Chronological Preconditioner
- Retuning HMC algorithm
- Bigger Lattices
- Note: Lattice will be stored WITH the near NULL vector so there is no set up cost to MG in analysis

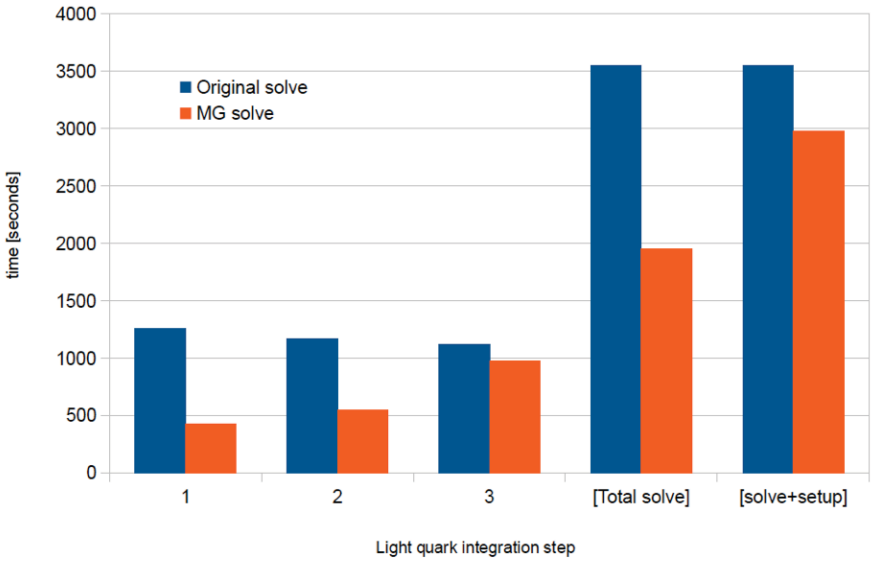
MG-HMC Test Case

- 2+1 Clover fermions, with 1-level Stout smearing
- Lattice size: 32^3x64
- Light quark mass: -0.285 => pion mass ~ 300 MeV
- MD residual: 1e-10.
- Original HMC evolution:
  - 7 Hasenbusch mass preconditioners for light quark
  - Multi-scale integrator:
    - gauge field integration inner-most
    - Light quark integration outer-most

Solve time vs Hasenbusch mass



Total light quark solve time vs. integration step



Herterogeneous Architecture

- Problem: Wilson Clover for Light Quark is FASTER on the CPU than using the QUDA solver on GPUs!
- Solution put MG on GPU of course
  - Cost in $s reduced by a factor of at least

O(100+)

GPU O(10+) MG O(10+)

Ron Babich
and
Mike Clark
and
SciDAC
and
Nvidia

(now with Mike Clark at NVIDIA and Michael Cheng on NSF grant)

Rapid Prototyping and Tuning?

- HYPER in FastMath with Pavlos Vranas, Chris Schroeder, Rob Faulgot (FASTmath)

Integration of HYPRE and Qlua is well underway. Rob Falgout, Christopher Schroeder and Andrew Pochinsky have completed an overall design of a HYPRE/USQCD interface (HQL) and begun its implementation. RF is largely finished extending HYPRE to handle more than 3 dimensions and fully expects to finish implementing complex numbers on schedule. CS and RF are making progress on the implementation of the HQL interface, and RF and AP are proceeding with the HQL-Qlua interface. AP is finishing extending Qlua to handle data types and procedures required to support HQL.

- QLUA = QCD + LUA is FUN
  - **https://usqcd.lns.mit.edu/w/index.php/QLUA_tutorials**

FUEL: James Osborn for BSM HMC development

New FUEL HMC framework (Framework for Unified Evolution of Lattices)

- High level layer focused on gauge configuration generation
  - motivation is to have flexible HMC framework to support wide range of beyond standard model theories
  - algorithmic abstraction: generation algorithm independent of gauge group, action, etc.
  - easy to write new high-level algorithms, tune parameters
  - serves as wrapper for efficient "level 3" routines
  - easy to plug in new routines
  - new routines can be written in any other language/framework

- Uses scripting language Lua
  - Small
  - Easy to port (ANSI C89)
  - Easy to use, yet powerful
  - Easy to embed and interface with libraries

RxSherical Lattice: R x S3

- Radial Quantization requires “spatial” spheres!
  - Conformal Fix Points for BSM theories
  - (or partial wave expansion & Scattering Length?)
- Need Finite Elements Method to do 3d Ising on curves space!

ELSEVIER

Contents lists available

Physics

www.elsevier.c

Lattice radial quantization: 3D Ising

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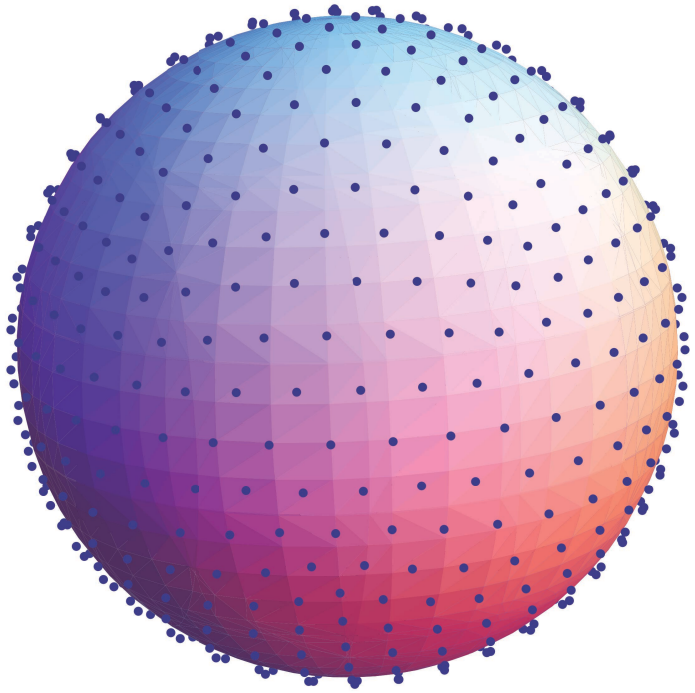
ABSTRACT

Lattice radial quantization
Euclidean conformal field
example, we employ a lat
dilatations in the 3D Ising
two descendants ($l = 1, 2$),
from integer spacing for tl
lattice action will be requi
continuum limit.



exact icosahedral symmetry

Conclusions: "The Sun is But a Morning Star*"!

Much more Algorithmic Develop is a critical investment

- * MG Domain Wall &Staggered
- * Multi-grid/HMC Evolution
- * Multi-grid QUDA on GPUs
- Research Area for "real" DD
- MultiGrid/DD "deflation"
- *Wilson Flow
- Disconnected Diagrams
- EigCG Deflation & All mode averaging (48^3 96 24: Big Data, 600 ev 7.2TBytes)
- Multi-quark contraction codes
- *Radial Quantization: Conformal Theory
- LOTs MORE to DO.

- Algorithmic advances are difficult and time consuming

Need separate Development and Optimization Software Environment

Need Modularity to move new algorithm into Application Codes.

* *Henry David Thoreau in Conclusion to Walden, 1845*