PLQCD

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CAPACITIES

e-infrastructure

Partners

- C. Alexandrou, A. Abdel-Rehim, G. Koutsou (CyI, CaSToRC)
- I. Liabotis, N. Anastopoulos, N. Papadopoulou (GRNET)

PLQCD

- Software developed under PRACE 2IP, WP8.
- Main focus is on scaling of community codes on large number of cores.
- Two community codes are considered: tmLQCD by ETMC and Chroma by USQCD.
- Partnetrs: CaSToRC, GRNET, U. of Coimbra

Selected Activities

- Wilson Dirac operator with MPI+openMP (PLQCD).
- Implementing efficient linear solvers for tmLQCD.
- Other contributions by U. of C.

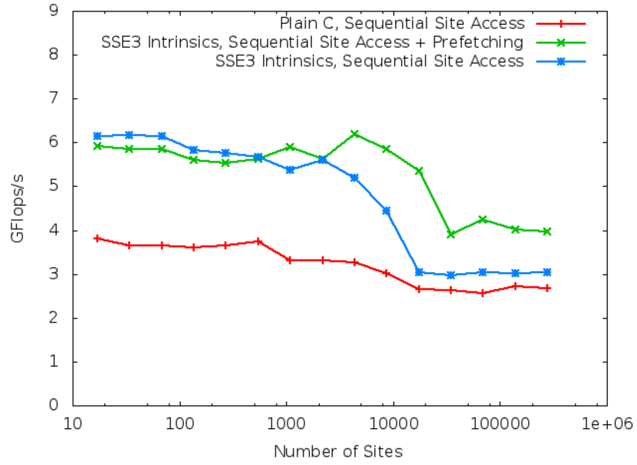
Dirac operator work

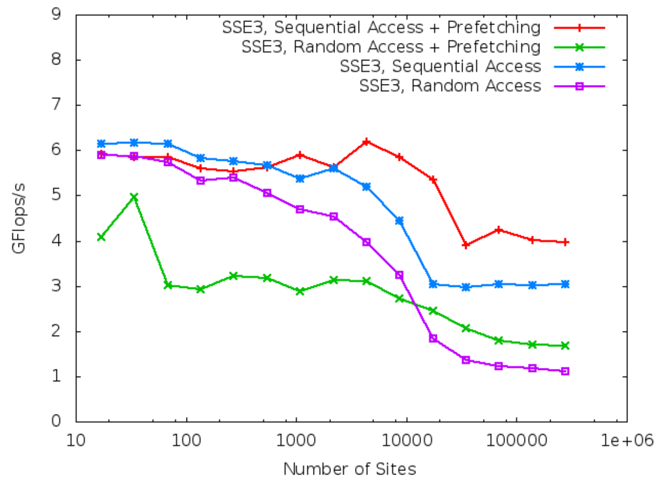
- Overlap communications and computations.
- Use MPI+openMP to improve scaling.
- Use a compact representation of the Gauge links.
- Using AVX instructions.
- Improving SIMD parts using compiler intrinsics.

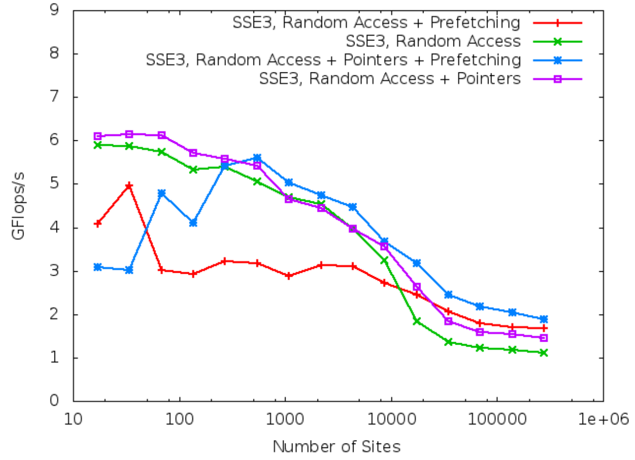
Overlap of Communications and computations

- Compute $(1-\gamma_\mu)\varphi(x)$ and $\left(U_\mu(x)\right)^{-1}(1+\gamma_\mu)\varphi(x)$ on the boundaries and send/recieve them to neighbouring processes using non-blocking MPI send/recv.
- Compute $(1-\gamma_\mu)\varphi(x)$ and $\left(U_\mu(x)\right)^{-1}(1+\gamma_\mu)\varphi(x)$ on the bulk.
- Wait for communications to finish.
- Compute results on all sites.

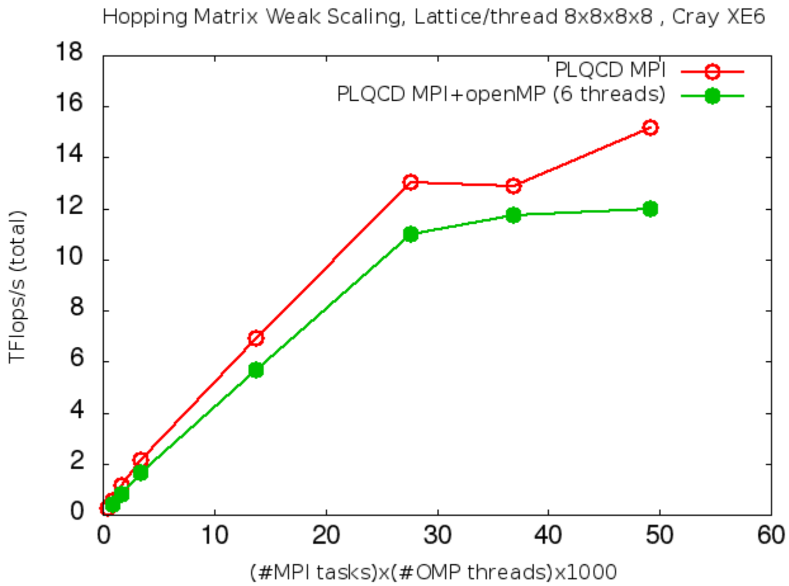
Effect of Random Access of Sites

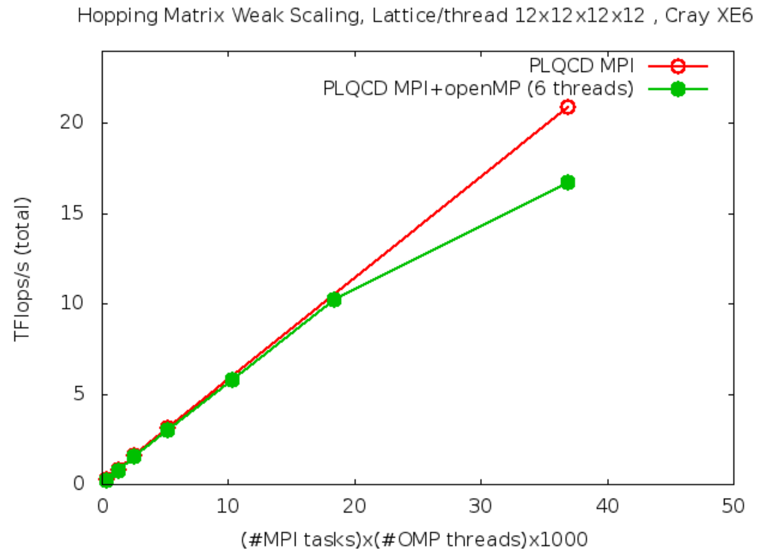




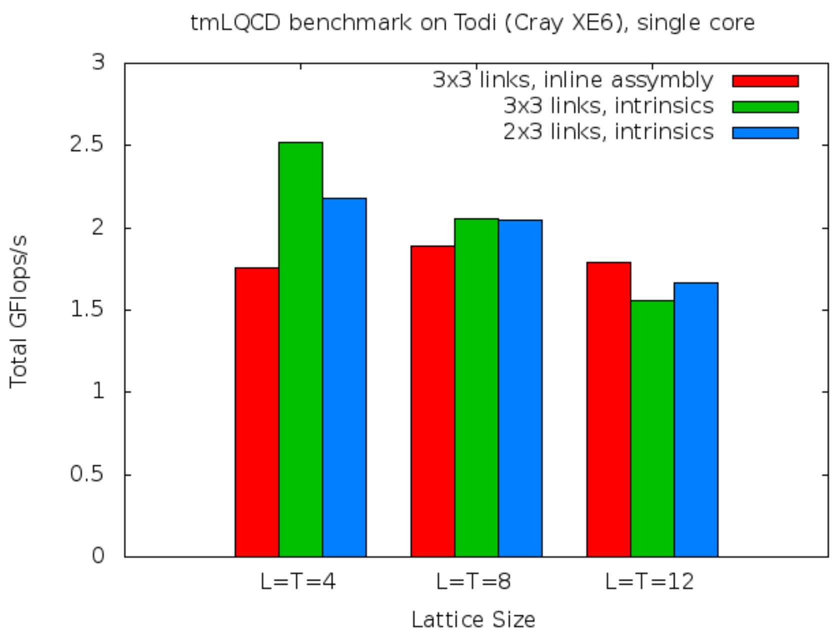


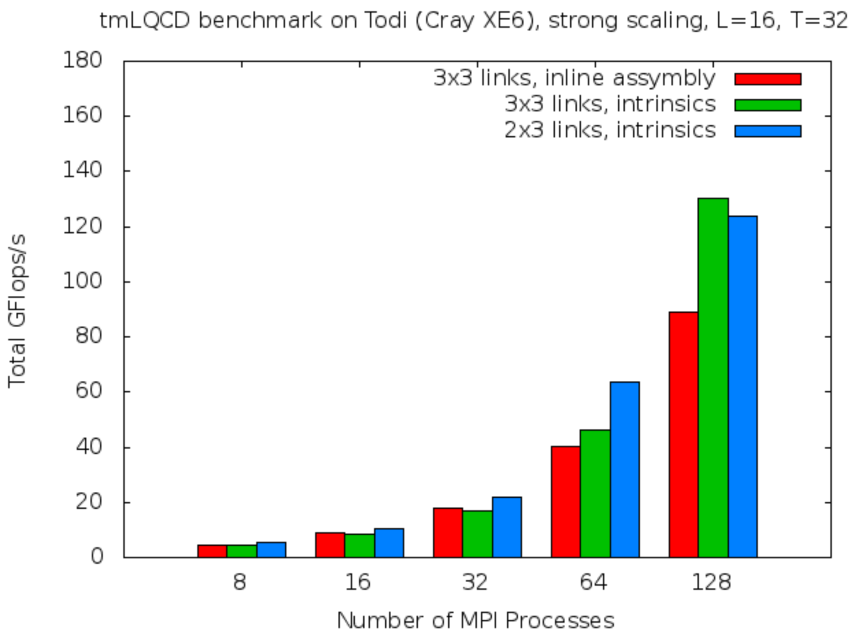
Weak Scaling Tests

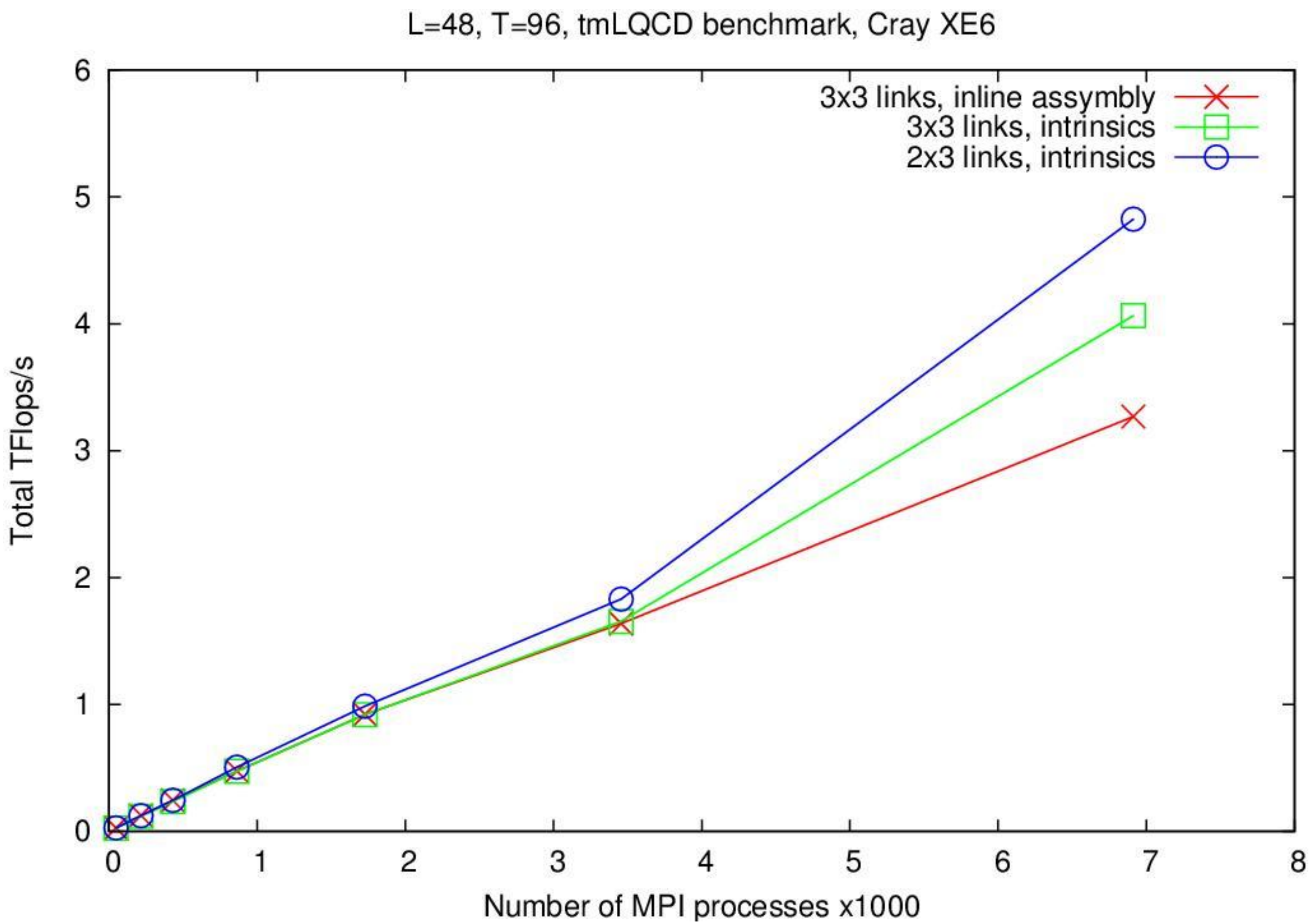




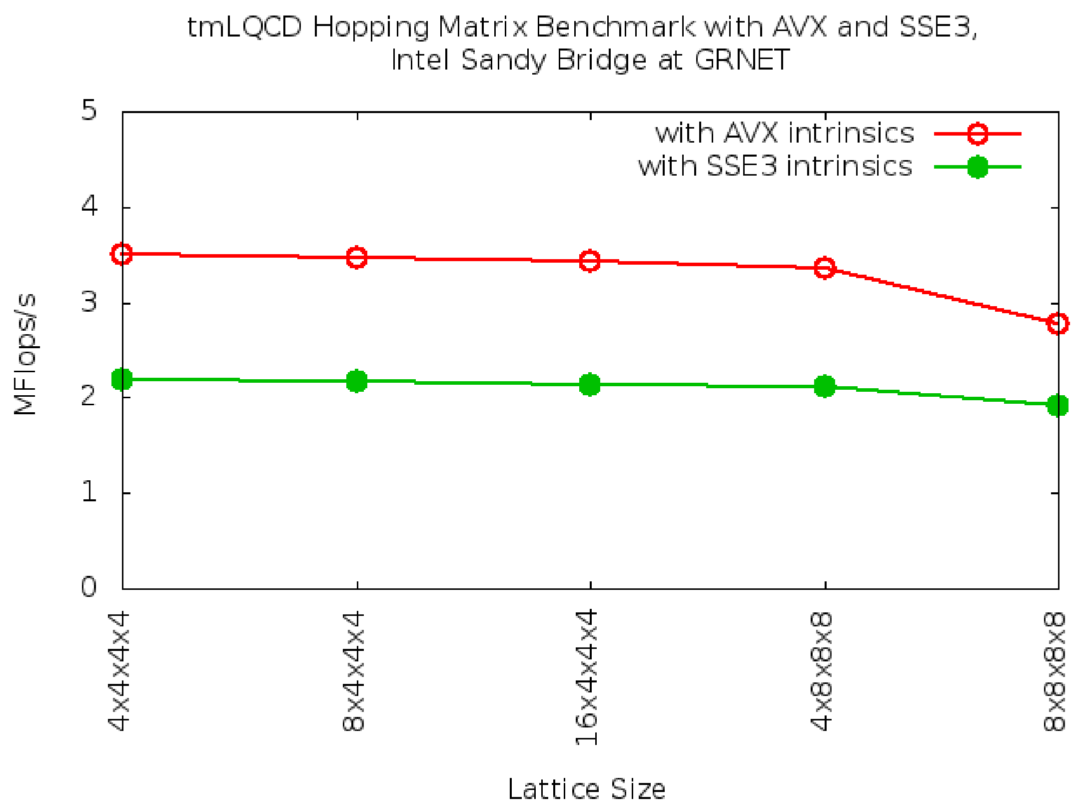
Using Intrinsics and 2x3 Links






L=48, T=96, tmLQCD benchmark, Cray XE6
3x3 links, inline assymbly
3x3 links, intrinsics
2x3 links, intrinsics
Total TFlops/s
Number of MPI processes x1000
0
1
2
3
4
5
6
7
8

Using AVX


tmLQCD Hopping Matrix Benchmark with AVX and SSE3,
Intel Sandy Bridge at GRNET
with AVX intrinsics
with SSE3 intrinsics
MFlops/s
0
1
2
3
4
5
4x4x4x4
8x4x4x4
16x4x4x4
4x8x8x8
8x8x8x8
Lattice Size

Implement New Efficient Linear Solvers

- Incremental EigCG: CG+deflation for SPD case

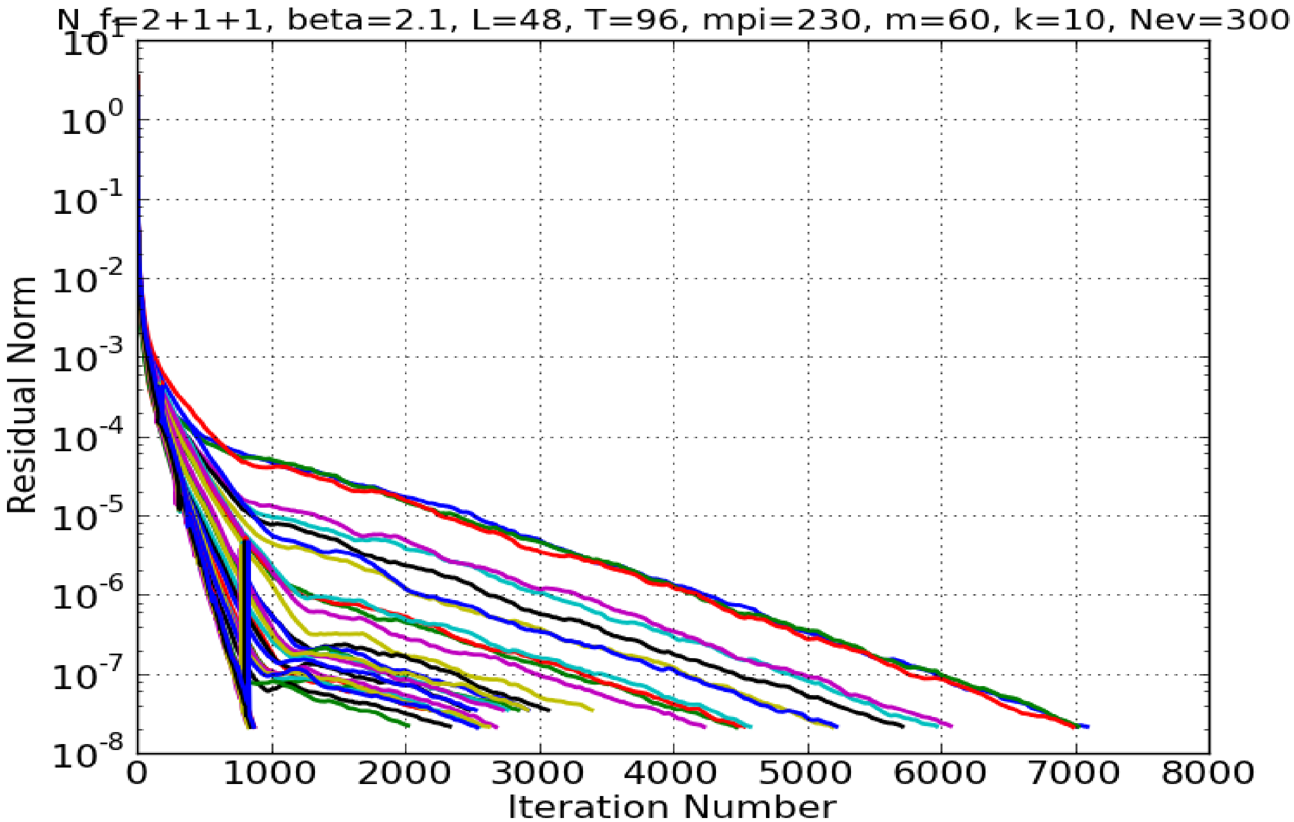
(found to be efficient for Twisted-Mass LQCD)

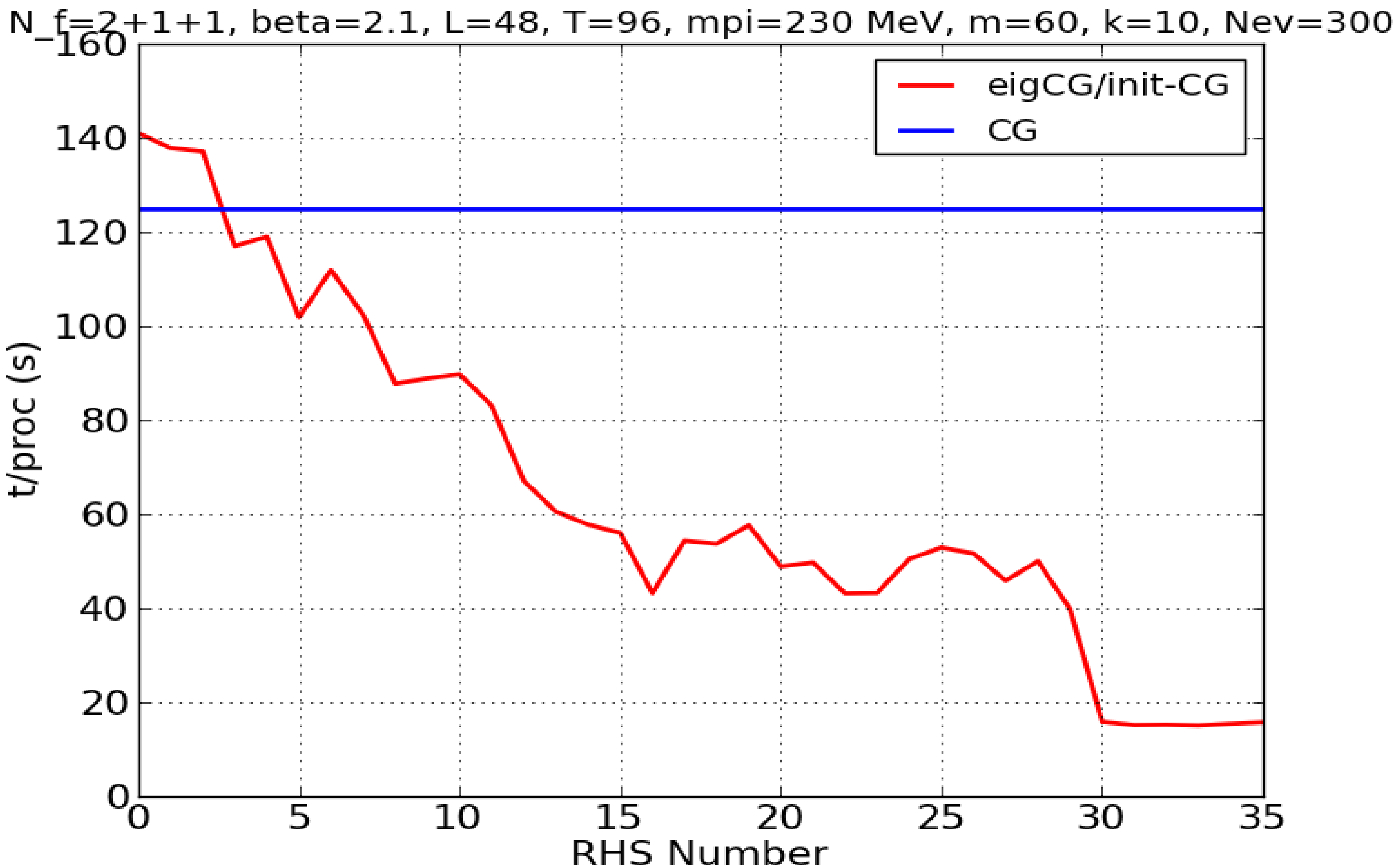
- Incremental EigBiCG: BiCG/BiCGStab+ deflation for Non-symmetric case.

(Worked on small lattices but was less efficient on large volumes).

- GMRES-DR/BiCGStab (under development).

Eig-CG Linear Solver Results




N_f=2+1+1, beta=2.1, L=48, T=96, mpi=230 MeV, m=60, k=10, Nev=300
eigCG/init-CG
CG
t/proc (s)
RHS Number
0
20
40
60
80
100
120
140
160
0
5
10
15
20
25
30
35

Comparing EigCG with GMRES-DR

Incremental EigCG

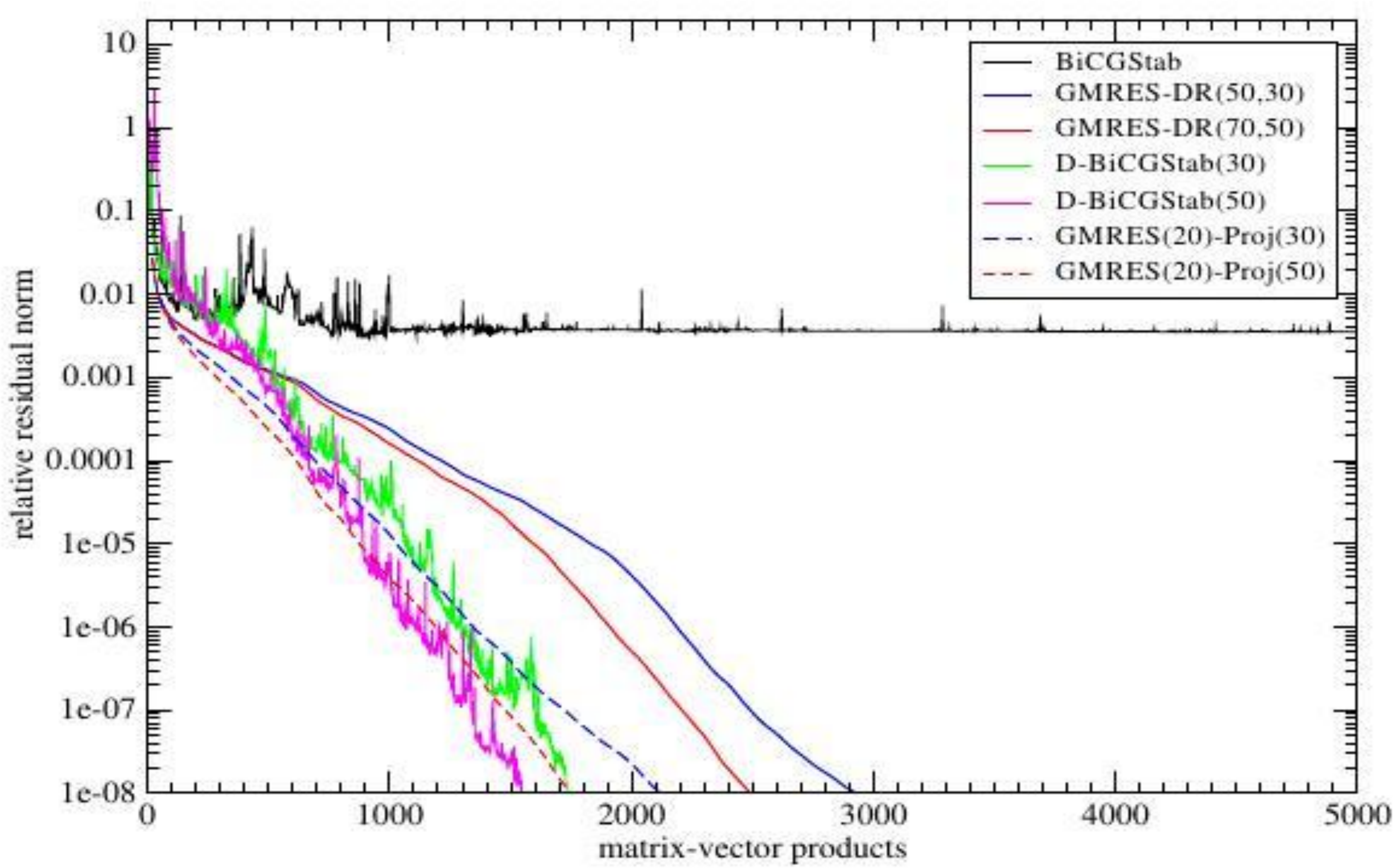
- System has to be converted to a Hermitian Positive Definite
- Eigenvectors needed for deflation are collected incremental while solving few linear systems (10-20)

GMRES-DR/ D-BiCGStab

Original non-Hermitian system solved directly with GMRES or BICGStab.

Eigenvectors needed for deflation are computed while solving the first linear system.

GMRes-DR and Deflated BiCGStab on a ETMC configuration with two dynamical flavors
L=24, T=48, Kappa=0.160859, mu=0.004, arXiv:0710.1831

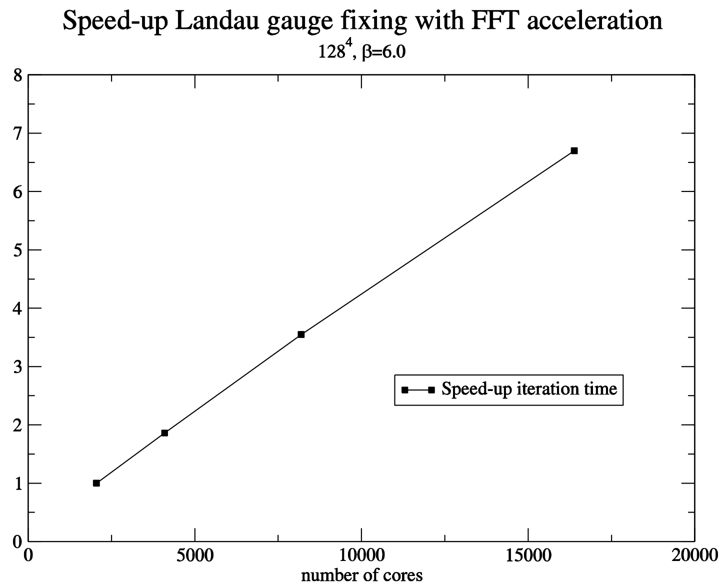


Other Contributions to PLQCD

Landau gauge fixing (Paulo Silva, in collaboration with Orlando Oliveira)

- On the lattice, gauge fixing is usually formulated as a numerical optimization problem
- Local optimization methods usually suffer from critical slowing down.
- Critical slowing down can be reduced by Fourier acceleration.
- We have implemented a MPI parallel version of the Fourier accelerated Steepest Descent method using the Chroma library http://usqcd.jlab.org/usqcd-docs/chroma/
- For FFT's we use the PFFT library allows parallelization up to L^3 processors http://www-user.tu-chemnitz.de/~mpip/software.php

- results show a good strong scaling up to 16000 cores for lattice sizes up to 128^4



HMC integrator tuning using Poisson brackets

(Paulo Silva, in collaboration with Balint Joo, Mike Clark, Tony Kennedy)

- Main goals: provide Poisson bracket measurements to the users, as well as force-gradient integrators

  A. D. Kennedy, P.J. Silva, M. A. Clark, Phys. Rev. D 87, 034511

- We rely on a modified version of Chroma, which involves - rewriting force calculation routines - a driver routine to compute all PB before/after MD step
- Integrator tuning allows a reduction in computational cost
- Force-gradient integrators are also expected to decrease computational cost for large volume simulations
- At present: working with Clover action

Summary

- We worked on certain important components of tmLQCD and Chroma.
- We obtained encouraging results which we hope will benefit the community.
- Codes developed are publically available.
- More fine tuning will be implemented in the future.