tmLQCD Software Suite

recent developments

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Outline

1. General Overview
2. Available Operators and Inverters
3. Available Actions
4. IO Formats and Performance
5. Parallelisation Strategy
6. Performance Examples

General Overview

- tmLQCD originates from a code of Martin Hasenbusch (2004)
- standard C99 code
- freely available under GPL
- access via `github.com`

  https://github.com/etmc/tmLQCD

- publication:

  [K. Jansen, CU, Comput.Phys.Commun. 180 (2009)]

General Overview

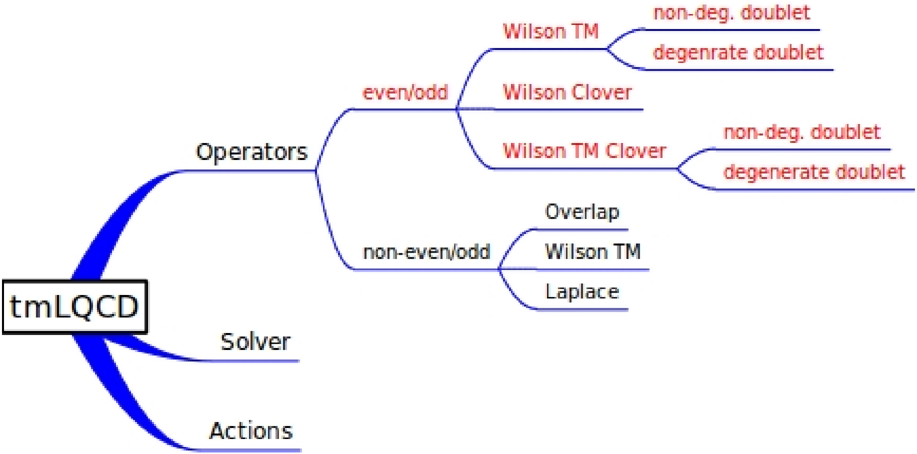
- started as a simple $N_f = 2$ Wilson twisted mass HMC code
- offers now a variety of actions and operators
- optimisation for various modern platforms available
    - Blue Gene family
    - Intel chips (SSE, AVX in preparation)
    - NVIDIA GPUs
- fully parallelised using openMP and MPI
- autoconf configuration framework

Input Example General

- human readable input file format
- lattice size specified at run time
- restarting possible
- general twisted boundary conditions
- reversibility checks can be performed
- set of online measurements
  - basic correlators
  - Polyakov loops
  - ...

```
L=4
T=4
Measurements = 1000
StartCondition = hot
NSave = 5
ThetaT = 1
ReversibilityCheck = yes
ReversibilityCheckIntervall=1
BeginMeasurement CORRELATORS
  Frequency = 2
EndMeasurement
```

Available Operators and Inverters

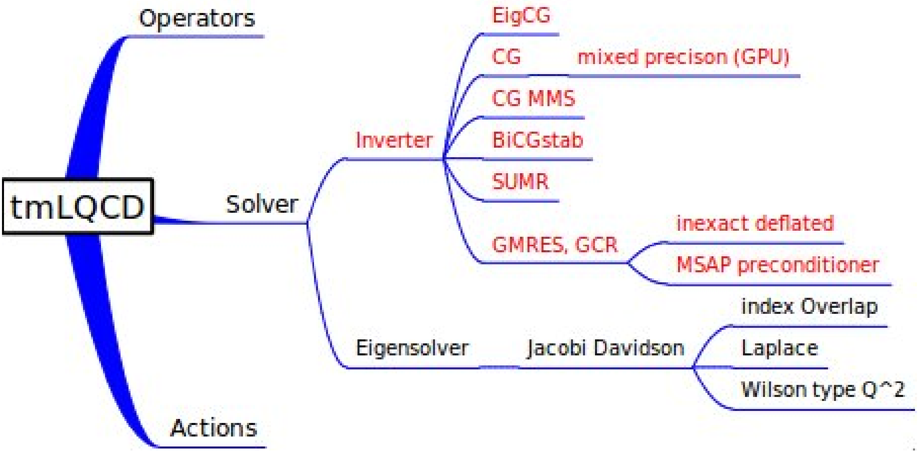


Input Example Operator

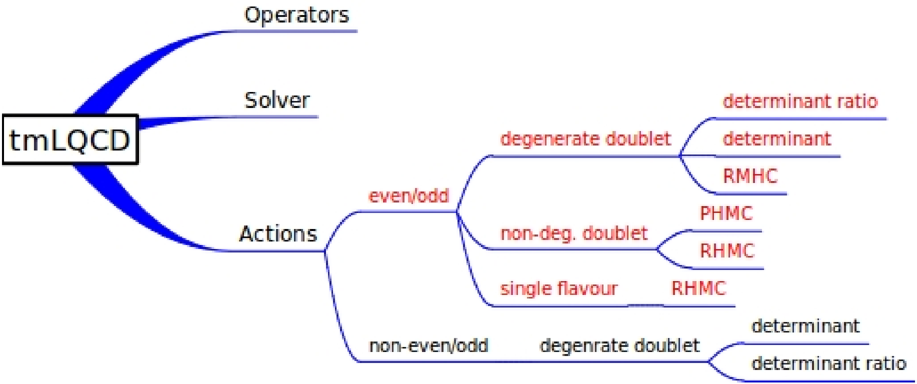
- example for a twisted mass Dirac operator
- even/odd preconditioning
- specify solver and parameters
- invert also with $-\mu$

```
BeginOperator TMWILSON
  2kappaMu = 0.05
  kappa = 0.177
  UseEvenOdd = yes
  Solver = CG
  SolverPrecision = 1e-14
  MaxSolverIterations = 1000
  AddDownPropagator = yes
EndOperator
```

Available Operators and Inverters



Available Actions



Action Input Example

- example for a simple $\det(Q^2_{\mathrm{tm}})$ momomial
- run on timescale 1
- acceptance and MD force precision different
- use even/odd preconditioning
- use CG solver

```
BeginMonomial DET
  Timescale = 1
  2KappaMu = 0.177
  kappa = 0.177
  AcceptancePrecision =1e-20
  ForcePrecision = 1e-12
  Name = det
  Solver = CG
  UseEvenOdd = yes
EndMonomial
```

Action Input Example

- a rational monomial for non-degenerate twisted doublet
- approximation interval

$$[\tilde{s}_\mathrm{min}, \tilde{s}_\mathrm{max}]$$

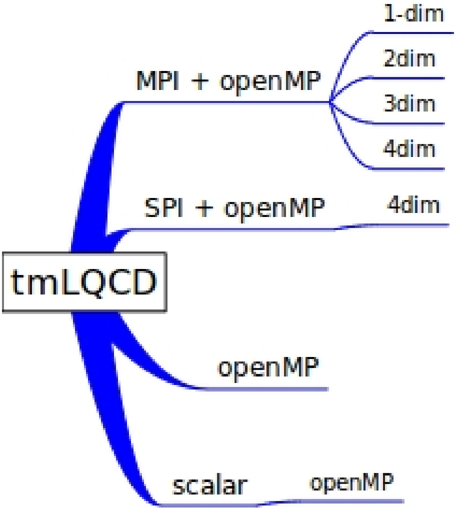
- rational degree $= 12$
- simulate only 7 first roots
- compute lowest eigenvalue every trajectory
- name `rat` will appear in output

```
BeginMonomial NDRAT
  Timescale = 1
  kappa = 0.170
  AcceptancePrecision =1e-20
  ForcePrecision = 1e-12
  StildeMin = 0.013577
  StildeMax = 3.096935
  Name = rat
  DegreeOfRational = 12
  Cmin = 0
  Cmax = 6
  ComputeEVFreq = 1
  2KappaEpsBar = 0.0935
  2Kappamubar = 0.1105
EndMonomial
```

Link Smearing

- dynamical link smearing
- any `monomial` can be defined link smearing
  - in the input file
- available smearings
  - stout smearing
  - HEX smearing
- also 3d smearing possible (source smearing)
- not in the master branch yet

Parallelisation Strategies

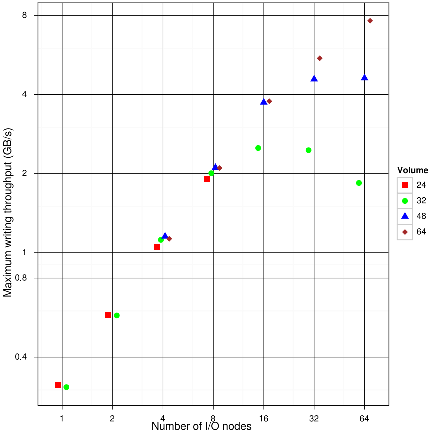


- tmLQCD flexible parallelisation strategy
- should run on as many as possible architectures
- e.g. a special version for AURORA
- important new feature: openMP threads

→ talk by B. Kostrzewa

IO Formats and Performance

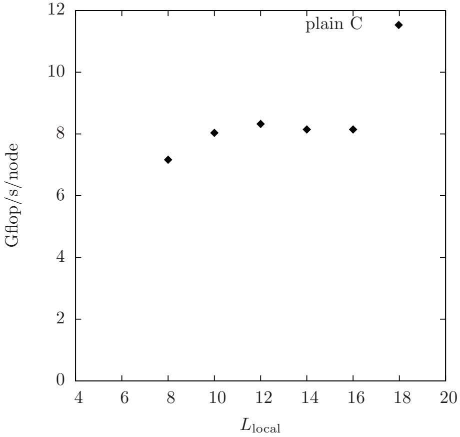
- ILDG format for gauge files
- Scidac format for propagators
- Scidac checksums
- parallel IO using Lemon
  [Deuzeman, Reker, CU, (2012)]
  - standard MPI II IO
  - collective calls
  - writes lime format
- plot: write performance on BG/P



Starting Point on BG/Q

- hopping matrix performance
- hybrid openMP+MPI code
- no optimisations yet
- initial performance on BG/Q
  - MPI communication switched off
  - 64 openMP threads per node
  - 1 MPI process per node
- local volume L_{local}^4

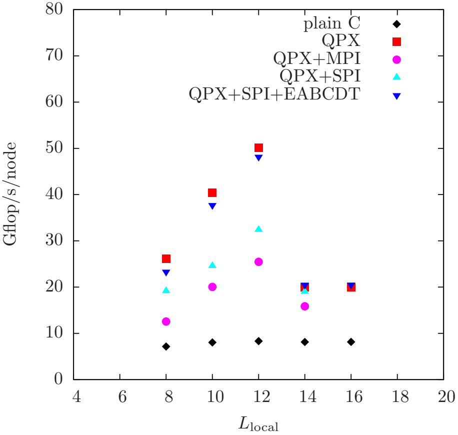
⇒ not even 5% of peak



BG/Q Performance (double precision)

- XLC QPX compiler intrinsics
- IBM SPI instead of MPI (works in parallel to MPI)
- proper mapping to the physical 5d torus
- strong dependence on L_{local}

⇒ sweet-spot:
comm/nocomm= 0.95!
24% of peak



GPU Performance

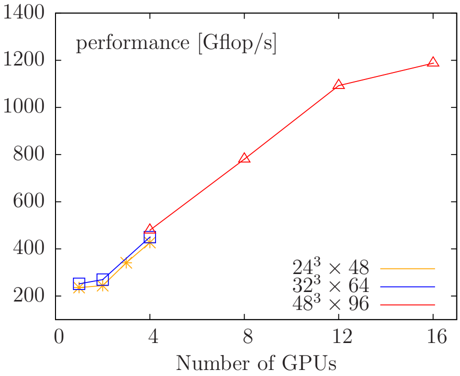
- NVIDIA CUDA extension
- mixed precision CG solver
- parallelised for multi-GPU
- scaling of operator reasonable

⇒ $>$ 1 TFlop

- also HMC available

⇒ in particular force computation

- ... but not yet in main branch



Summary

- tmLQCD now a general tool for simulating Wilson type fermions
- $N_f = 2$, $2 + 1$ and $2 + 1 + 1$ flavours
- mass preconditioning, PHMC, RHMC
- many solvers for propagator generation
- optimisation for many architectures, including BG/Q and GPUs