Chroma: An Application of the SciDAC QCD API(s)

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Soon to be moving to the JLAB

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An Overview of Chroma

- An Open Source Lattice QCD Toolbox
- Designed to be
  - Portable
  - Efficient
  - Standards/Buzzword Compliant
- Achieved through
  - Utilizing SciDAC QCD APIs
  - Modern Software design techniques
  - Portable third party libraries

Where Chroma Fits in the API layers

Level 3:

Wilson Dirac Operator (SSE and BAGEL), SSE DWF Inverter, and more yet to be defined ....

Chroma:

Actions, Linear Operators, Inverters, Eigensolver, Monomials, MD Integrators, HMC, RHMC, Propagators, Sources, Spectroscopy, Three Point Functions and more

SciDAC Level 2: QDP++ and QIO

SciDAC Level 1: QMP Message Passing & QLA

Key Components...

- Action Factories
  - Fermion
    - Produce Linear Operator objects
    - Compute Propagators
    - Compute Force for Linear Operators
    - Produce SystemSolver objects for computing propagators
  - Gauge
    - Compute action
    - Compute Forces

Key Components...

- Monomials
  - Fermion
    - Abstract flavour information for Fermion Action
      - eg: 2 flavour: $\varphi^{\dagger}(M^{\dagger}M)^{-1}\varphi$
      - eg: Rational 1 flavour: $R(M^{\dagger}M) \approx [\ \varphi^{\dagger}(M^{\dagger}M)^{-1}\varphi\ ]^{1/2}$
    - Applies chain rule to compute relevant force
      - can be overridden for optimisations
    - Computes action as relevant
    - Can use Chronological Predictor for force
  - Gauge
    - Forwards force calculation to GauaeActions

Key Components...

- Hamiltonians
  - Sum of monomials
  - Can mix and match monomials as desired
    - eg: Nf=2+1 made up from
      - Gauge Monomial(s)
      - 2 flavour fermion monomial
      - 1 flavour rational fermion monomial
  - Used by MD Integrators
  - Used by HMC algorithms

Key Components…

- InlineMeasurement Tasks
  - Uniform Interface for measurements
  - Specify list of tasks in XML
  - XML converted to a list of function objects
  - Application executes tasks in sequence
  - Can be used to chain measurements either
    - inline in an HMC evolution
    - after the fact through the Chroma Application
  - Allows XML scripting of complex tasks

Algorithms...

- Gauge Update Algorithms
  - HMC (Rational if Rational Monomial is used)
  - Heatbath (Not yet mature)
- MD Integrators
  - PQP Leapfrog, 2 Scale Sexton-Weingarten, Minimal Residual Norm (deForcrand et al)
- Chronological Predictors for solves
  - Zero, Last Solution, Linear Extrapolation, Minimal Residual Extrapolation

Algorithms...

- Inverters
  - Conjugate Gradients
  - Multiple Shift (MultiMass) Conjugate Gradients
  - BiCGStab
  - SUMR and others
- Eigensolver
  - Ritz with or without Kalkreuter Simma acceleration

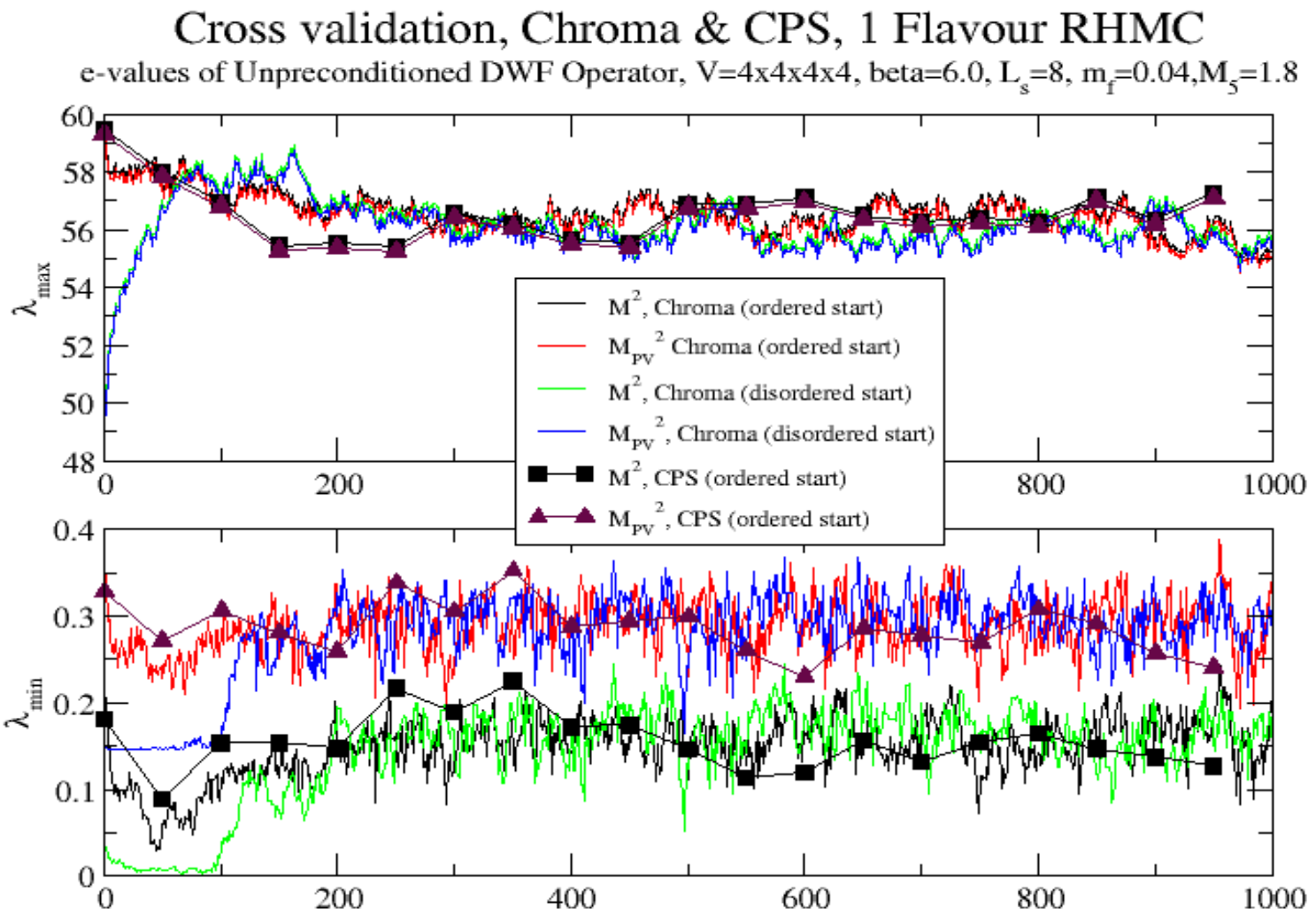
Measurements and Utilities

- Spectroscopy for Wilson Like Fermions
- Hadronic Three Point function s
- Wilson Loops
- Smearing and Fuzzing
- ...

Chroma Production Applications

- `chroma`
  - Post production measurement
  - Executes list of measurements in input file
  - Measurements can communicate via files
- `hmc`
  - Primary gauge production code
  - Flavour choice through Hamiltonians and Monomials
  - Usual bag of tricks...

Chroma RHMC Cross Validation



Platforms Exploited by Chroma

QCDOC, using custom QMP, BAGEL

Intel Clusters, QMP-MPICH,
QMP-MVIA, SSE Assembler

BlueGene/L, QMP-MPI, BAGEL
(QCDOC code used, single FPU only)

IBM Pseries (HPCx), BAGEL
QMP-MPI

Chroma People

- Maintainers and Main Developers
  - Robert Edwards, Bálint Joó
- Contributors
  - S. Basak, G. Fleming, K. Orginos, D. Renner, D. Richards, I. Sato, A. Pochinsky (LHPC)
  - S. Miller, C. McNeile, E. Gregory (UKQCD) – Staggered Fermion Measurements
  - Z. Sroczynski – CPS & Chroma glue (UKQCD)
  - J. Noaki (UKQCD) – Fuzzed Wilson Loops

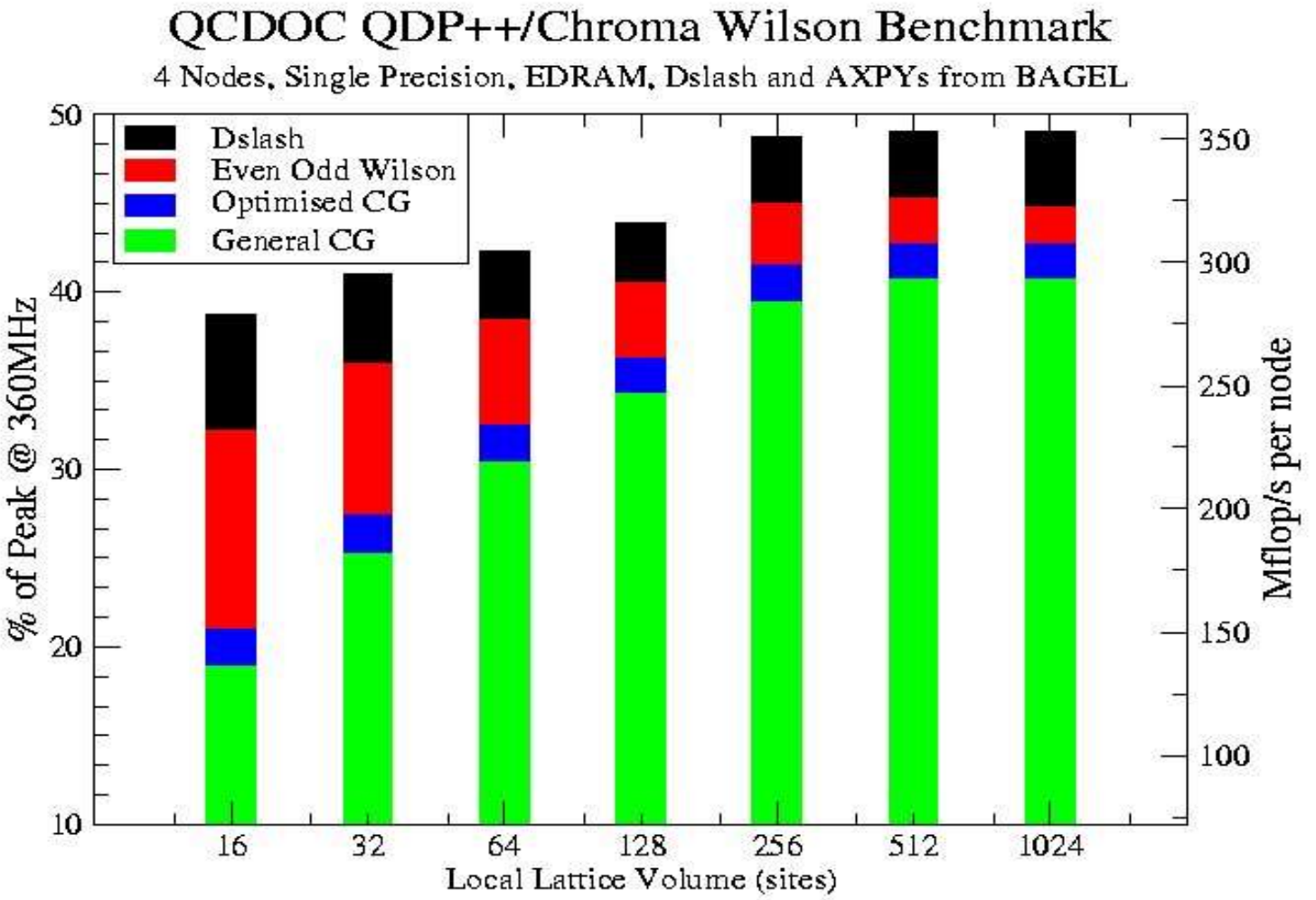
Chroma Penetration & Uptake

- LHPC - Hadron structure project
  - G.T. Fleming et. al. as per previous slide...
- UKQCD
  - DWF locality Study (A. Yamaguchi, P. Boyle)
  - Static Potential (J. Noaki)
  - Staggered Measurement (C. McNeile et al)
- Joint USQCD & UKQCD
  - Chiral fermion algorithms (R. G. Edwards, B. Joó, A. D. Kennedy, K. Orginos, U. Wenger)

Chroma and Efficiency

- Efficiency achieved through
  - Calls to High Performance Libraries
    - Intel SSE
      - Optimized Wilson Dslash (C. McLendon – Jlab)
      - Optimized DWF Inverter (A. Pochinsky – MIT)
    - QCDOC, BlueGene/L, Pseries
      - Optimized Wilson Dslash and Simple BLAS
      - Produced by Peter Boyle's BAGEL Generator
      - PLEASE DON'T ASK ME FOR BAGEL !!! ASK PETER !
        - paboyle@ph.ed.ac.uk
  - Optimized expressions in QDP++

Chroma QCDOC Benchmark (Lat'04)



I/O Timings on 1 QCDOC Rack

I/O Timings (s)

Global Volume	Size (MB)	Singlefile Write time	Singlefile Read Time	Multifile Write Time	Multifile Read Time
16x16x16x32	72	100	124	11	3
24x24x24x32	243	370	458	13	35
24x24x24x64	486	743	918	32	88

I/O Transfer Rates (Mbyte/s)

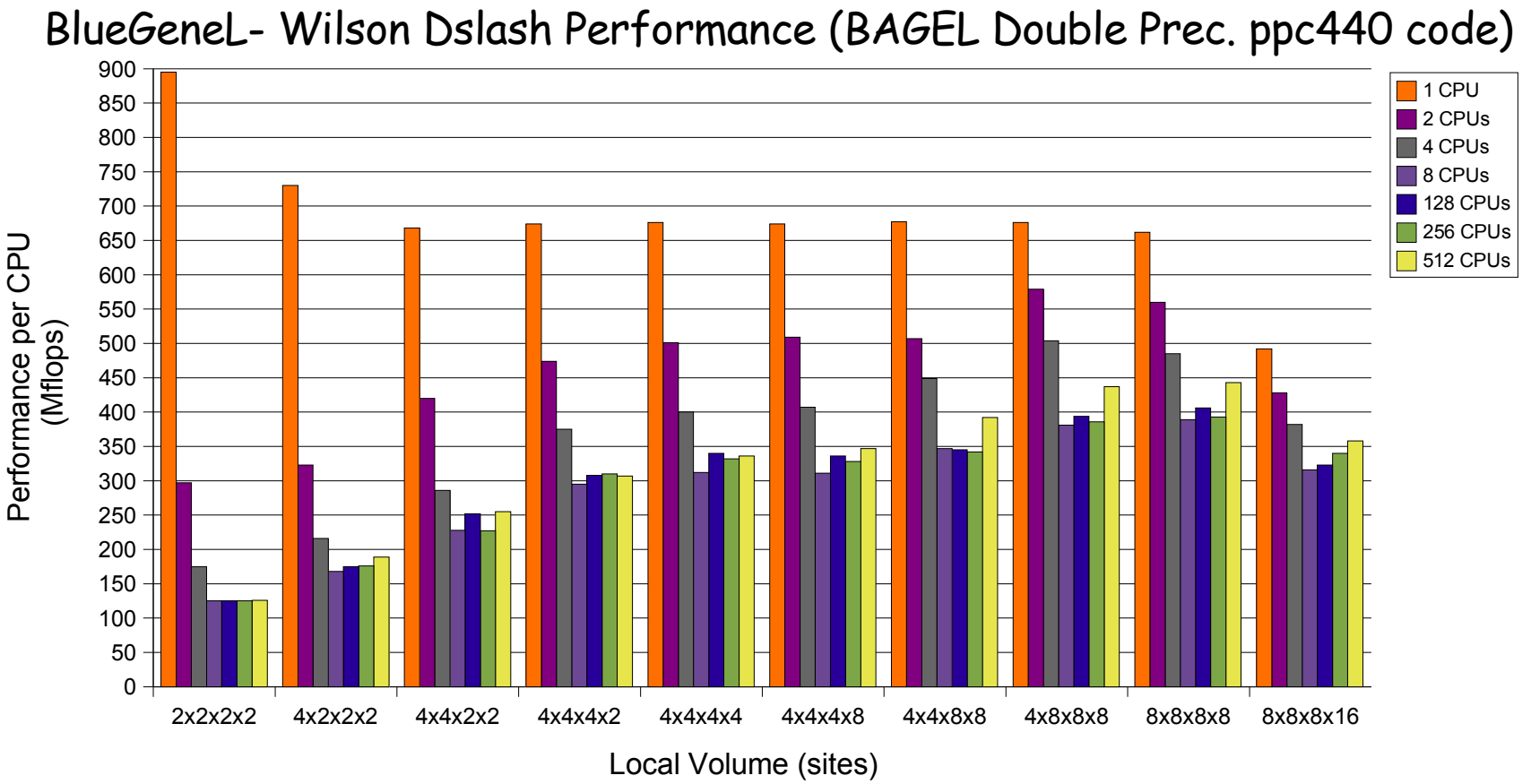
Global Volume	Size (MB)	Singlefile Write Rate	Singlefile Read Rate	Multifile Write Rate	Multifile Read Rate
16x16x16x32	72	0.72	0.58	6.79	23.43
24x24x24x32	243	0.66	0.53	18.86	6.96
24x24x24x64	486	0.65	0.53	15.11	5.54

Singlefile I/O is painfully SLOW. Multifile is OK.

But as QIO's performance will improves so will ours

Quick and Dirty BlueGene Benchmark

- Edinburgh BlueGene/L @EPCC, 1 midplane, Co-processor mode
- 1 CPU Peak Performance=700MHzx2FPUs*2flops=2800 Mflops
- Max attainable with 1FPU=1400Mflops **(Double Prec Mflops)**

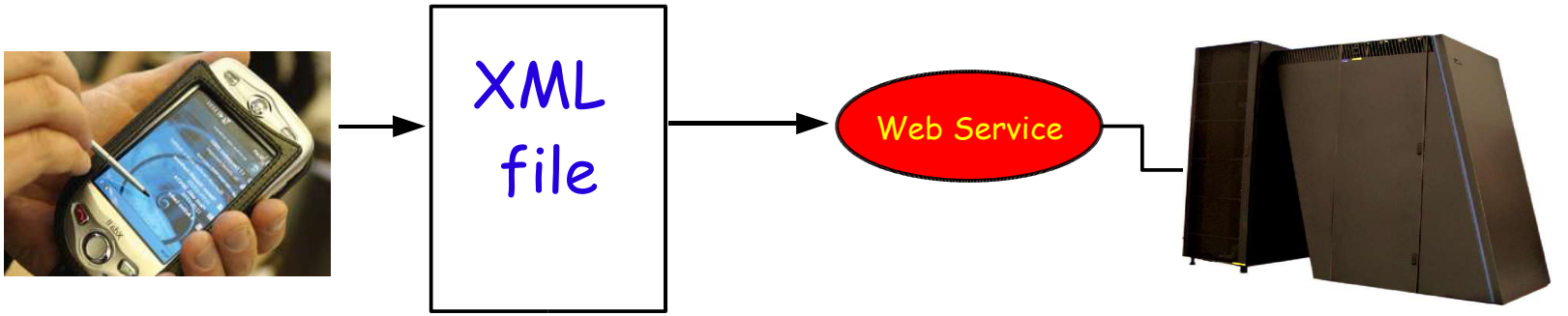


Near Future Work

- Polishing and More Optimization
  - e.g.: more optimization of 5D operators (Level 3 style), more assembler, etc.
- Improved algorithms
  - e.g.: exact handling of low eigenvalues of H in 5D operators and molecular dynamics.
- QDP++/QMP implementation optimization
  - e.g: BlueGene/L native QMP?
  - Help with QIO improvements?

Chroma Dreams … (Nightmares?)

- ChromaGUI – Create XML Files
- ChromaGrid – Grid Enabled Chroma?
  - Send input XML File to remote Web Service
  - Web Service launches `chroma`
  - Web Service sends back URL to output



Conclusions

- Chroma is not just a toy system
- Growing usage worldwide
- Ported to currently interesting systems
- Efficiency may need tweaking on some of the more recent platforms (eg BG/L)
- Beautiful example of how SciDAC APIs enable rapid exploitation of new systems
- Bright and colorful (chromatic) future