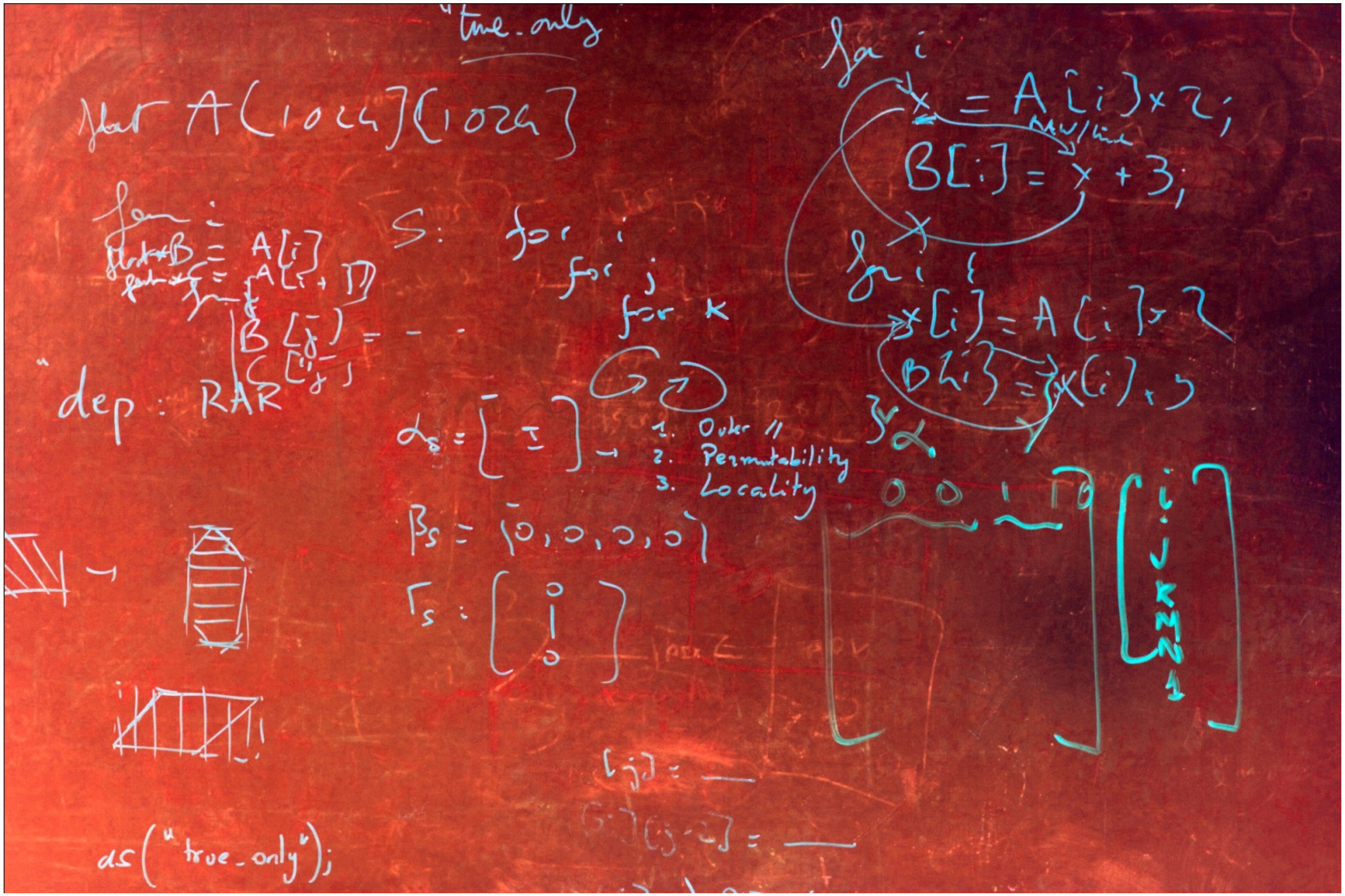
Polyhedral Mapping Assistant and Visualizer (PUMA-V)

Department of Energy Office of Science, Office of Nuclear Physics, SBIR/STTR Exchange Meeting, August 6-7, 2015



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Project and Motivation

- US Department of Energy contract number DE-SC0009678:
  - Phase II STTR, 2014 Award Year.
  - April 15, 2014 – April 15, 2016 term
  - Solic. Number DE-FOA-0001019, Topic Code 39e
  - Reservoir Labs, SUNY StonyBrook, Brookhaven National Lab
- Motivation:
  - Lattice QCD community has traditionally produced very efficient home-grown software and is continuing to do so.
  - However, with the arrival of new hardware architectures, significant efforts are required to optimize the software for the target new architecture.
    - One way to deal with this is to rewrite the software to be "future-proof".
    - Another way is to see if there are any automation tools that are capable of producing efficient code for a target architecture from generic, high-level, user codes.
  - As a Phase II US DOE SBIR/STTR funded program, PUMA-V explores the second approach, seeking to use the R-Stream source-to-source compiler to optimize the Domain Wall Dirac operator implementation as well as develop accelerated solvers and state-of-the-art visualization methods
  - Columbia Physics System (CPS) as initial target.

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Goals for Accelerating Code Production for Nuclear Physics

- Algorithms for automatic generation of highly optimized heterogeneous code based on inherent properties of Lattice QCD problem, providing opportunities for substantial speed-ups in computation.
  - Compiler technology (R-Stream) to help with specific computations, especially those related to the proton size puzzle and muon magnetic moment, of particular interest to our domain expert partners (BNL).
- An automated visualization tool-chain to assist with software optimizations and mappings in high dimensional spaces, of great utility not only to the physics community but to the larger scientic computation enterprise.
  - Performance visualizer and IDE plugin development for intuitive code generation (Stonybrook)
- New opportunities to lower cost and power requirements for large computations needed in fundamental physics, fluid dynamics, computational biology and other scientific disciplines.
  - Faster preconditioners and solvers (CMG, Peng-Spielman, etc.)

PUMA-V Teams

PUMA-V Personnel

- Reservoir Labs, Compiler Technology and Solvers:
  - M. Harper Langston, PhD – PI of PUMA-V project
  - Richard Lethin, PhD - President of Reservoir Labs
  - Paul Mountcastle, PhD - Physicist
  - Benoit Meister, PhD – Managing Engineer
  - Muthu Baskaran, PhD – Managing Engineer
  - Tom Henretty, PhD – Senior Engineer
- Brookhaven National Lab, Domain Experts:
  - Taku Izubuchi, PhD
  - Meifeng Lin, PhD
  - Chulwoo Jung, PhD
- StonyBrook University, Visualization and Compiler Technology:
  - Klaus Mueller, PhD
  - Eric Papenhausen
  - Bing Wang

Reservoir Labs, Inc.

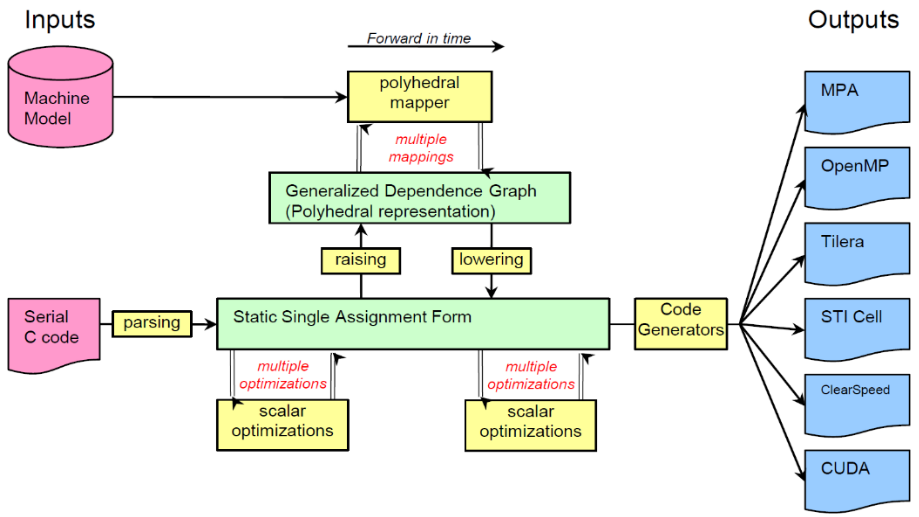
Founded 1990 – Offices in New York City and Portland, OR

- Involved in a variety of research projects to explore ways to solve dynamic systems and effectively compile real-world algorithms. Work for and with numerous government institutions, and collaborate closely with other leading researchers and academics around the world. Sample projects:
  - R-Stream® — advanced compiler technology enables developers to create program logic once and produce optimized code for multiple parallel computing architectures.
  - R-Solve® – An automated reasoning technology that addresses dynamic problems in advanced planning and decision analysis, modeling and simulation.
  - ENSIGN – Cutting-edge hypergraph analysis technology for Big Data applications spanning security, finance and biology.
- Provide services and products to commercial clients through research technologies for organizations working on novel high-performance systems; package those technologies in turnkey commercial and government solutions that address important science and security issues. Sample products:
  - R-Scope Network Security Monitoring — Puts networks under a microscope so customers can respond to both known and zero-day attacks before becoming crises.
  - R-Check® SCA — Simplifies and accelerates SCA-compliance testing for defense communication systems worldwide, shortening the timeframe for checking from weeks and months to hours.
- More than 30 full-time researchers and engineers (half with PhDs) and a mature business development department

R-Stream Polyhedral Model Compiler

Developed by **Reservoir Labs Inc.**

- A high-level source-to-source compiler based on the **polyhedral model**, a mathematical abstraction for analysis and transformation of computer programs:
  - Darte, Schreiber & Villard, 1985
  - Feautrier 1992



- Performs optimizations in terms of parallelization, memory management, locality etc. and can target a range of hardware architectures.
- Accepts a sequential C program as input and produces code in a variety of formats, including C + **OpenMP** and **CUDA**.
  - Meister et. al, 2011
  - Vasilache et. Al, 2013
- Used for PUMA-V in targeting key code kernels in the LQCD formulations

Optimizing the Domain Wall Fermion Dirac Operator Using the R-Stream Source-to-Source Compiler

Domain Experts at BNL Directed Focus

$$M_{x,s;x',s'} = \delta_{s,s'} M^{\parallel}_{x,x'} + \delta_{x,x'} M^{\perp}_{s,s'}$$

$$M^{\parallel}_{x,x'} = -\frac{1}{2}\sum_{\mu=1}^{4}\left[(1-\gamma_\mu)U_{x,\mu}\delta_{x+\hat{\mu},x'} + (1+\gamma_\mu)U^{\dagger}_{x',\mu}\delta_{x-\hat{\mu},x'}\right]$$

$$+ \ (4 - M_5)\delta_{x,x'}$$

Wilson Kernel

$$M^{\perp}_{s,s'} = -\frac{1}{2}\left[(1-\gamma_5)\delta_{s+1,s'} + (1+\gamma_5)\delta_{s-1,s'} - 2\delta_{s,s'}\right]$$

$$+ \ \frac{m_f}{2}\left[(1-\gamma_5)\delta_{s,L_s-1}\delta_{0,s'} + (1+\gamma_5)\delta_{s,0}\delta_{L_s-1,s'}\right].$$

The Wilson Kernel

R-Stream Focus

- We first looked at how R-Stream was able to transform the *single-core version, unimproved*, implementation of the Wilson Dslash operator in CPS.

$$D^{ij}_{\alpha\beta}(x,y) = \sum_{\mu=1}^{4} \Big[(1-\gamma_\mu)_{\alpha\beta} {U_\mu}^{ij}(x)\delta(x+\hat{\mu}-y) + (1+\gamma_\mu)_{\alpha\beta} U^{\dagger ij}_{\mu}(x+\hat{\mu})\delta(x-\hat{\mu}-y)\Big]$$

```
for(x=0; x<lx; x++){
  for(y=0; y<ly; y++){
    for(z=0; z<lz; z++){
      for(t=0; t<lt; t++){
//      printf("wilson_dslash: %d %d %d %d\n",x,y,z,t);
         parity = x+y+z+t;
         parity = parity % 2;
         if(parity == cbn){
```

- At first glance, the nested loops present may be a good candidate for R-Stream.

Code Transformation ***Prior to*** R-Stream

There are, however, a few transformations required on the input code before R-Stream can process it.

- Delinearized array access:
  - In CPS, arrays are linearized. However, the polyhedral model requires that the array indices are **affine functions** of the outer loop indices so that it can perform dependence analysis:
    - chi[NT*NZ*NY*NX/2*4*3*2] → chi[NT][NZ][NY][NX/2][4][3][2]
- Introduction of padding at boundaries:
  - In the original CPS code, the wrap-around at the boundary is handled with array index modulo, e.g., chi[(x+1)%NX], which R-Stream can't analyze directly.
  - For each dimension, padding was added for the two boundaries, leading to new dimensions for the fermion vector arrays:
    - chi[NT][NZ][NY][NX/2][4][3][2] → chi[NT+2][NZ+2][NY+2][NX/2+2][4][3][2]
- Despite several improvements made to R-Stream, it wasn't able to produce optimally efficient code. Some hand tuning was needed to achieve any speedup.

Hand Tuning *After* R-Stream

Hand-tuning necessary for more optimal code

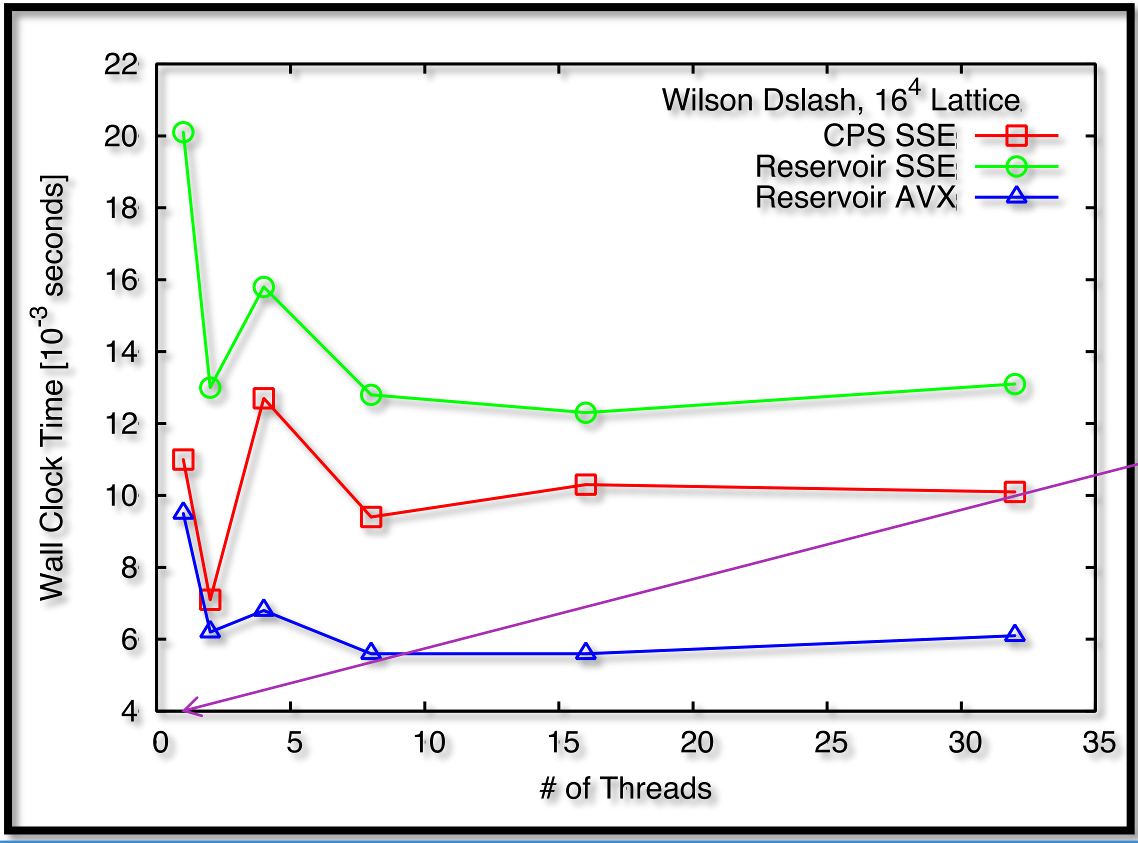
- First hand tuning done was to vectorize the code, with both SSE and AVX intrinsics
  - Intel's **Streaming SIMD Extension (SSE)** can pack **two doubles** into one vector register and perform two double operations per instruction.
  - For Wilson Dslash, the vectorization was done by **packing real and imaginary parts** into one register.

real	imag

- SSE version achieved 2X speedup compared to the input code.
- The **AVX extension** allows to compute 4 doubles with a single instruction:
  - A data layout transform was needed to **pack the four spinor components** into one vector register:
    - chi[NT][NZ][NY][NX/2][4][3][2] -> chi[NT][NZ][NY][NX/2][3][2][4]

Performance of Wilson Dslash

Results from Lattice 2015: M. Lin, "Optimizing the DWF Dirac Operator Using the R-Stream Compiler", Kobe Japan, July 2015



Best performance with 1 thread/core

- CPS-SSE is a heavily hand optimized version of the Wilson Dslash written by Taku Izubuchi.
- Tests were run on Intel i5-2520M dual core @ 2.5 GHz.

Vectorization for the DWF Dslash

The core piece of the DWF Dslash operator is inlining the Wilson Dslash over the loop of NS

- for (s=0; s<NS; s++) //call Wilson Dslash
  - To adapt the code for the AVX instructions, the data layout had to be transformed:
    - chi[NS][NT][NZ][NY][NX/2][4][3][2]➔chi[NT][NZ][NY][NX/2][3][4][NS][2]
  - The AVX register stores the real and imaginary parts of two sites in the s dimension.
    -

s=0, real	s=0, imag	s=1, real	s=1, imag

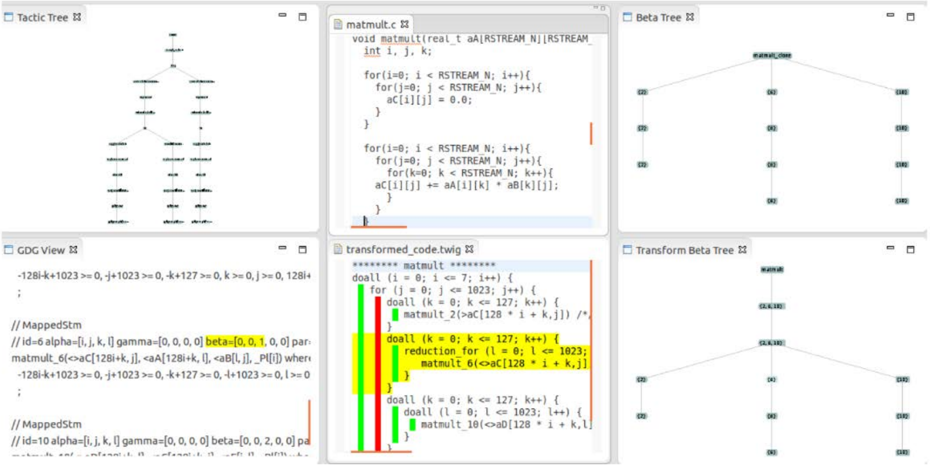
- Initial tests show that the single-core AVX version for the DWF Dslash performs reasonably well.
  - One a single core of Intel Xeon E5-2670 @ 2.60GHz, the 4D DWF Dslash achieved a performance of **5.2 Gflops** in double precision, or **25% peak** (Lattice 2015)
    - Tests were performed with a local volume of 8^4x16.
    - Incorporating MPI communications into the current code creates significant performance drop.
    - We are currently investigating this issue.

# cores	Performance
1	5.2 Gflops
2	4.0 Gflops
16	1.2 Gflops
32	0.7 Gflops

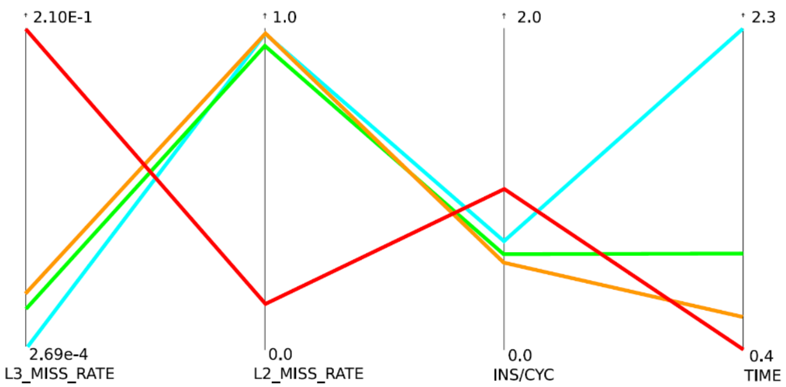
PUMA-V Visualizer

Visualizer Eclipse Plugin with Performance Tuning (Stonybrook Focus)

- Automated toolchain to allow user-in-the-loop to make more intuitive decisions for parallel-ization and R-Stream compiler optimizations. (Video)



- Performance Profiling



- **Tool and results accepted and to be published in Proceedings of IEEE VISSOFT 2015**

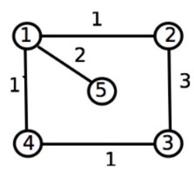
Spectral Support Preconditioning and Nearly-Linear Time Solvers, Combinatorial Multigrid

Solving the linear system Ax = b with actual solution x := A^{-1} b.

- Find B that approximates A in a spectral sense, so solving By = c is easier
- Based on Spielman and Teng (2003-current), solve a system of linear equations with a symmetric diagonally dominant (SDD) discrete operator:

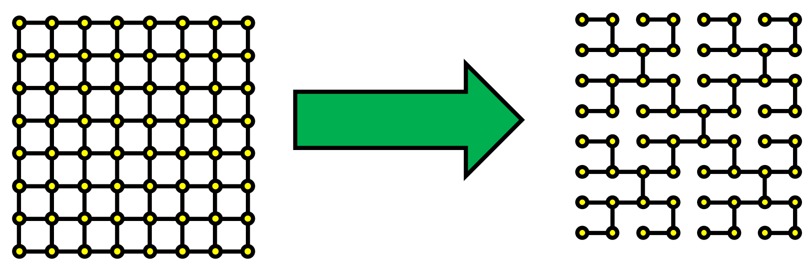
$$A\mathbf{x} = \mathbf{b}, \quad A \in \mathcal{R}^{n\times n} \quad A = A^T, \quad A_{ii} \geq \sum_{i\neq j} |A_{ij}|$$

  – SDD systems have clear connection with graphs and Laplacians:



$$L_G = D - W = \begin{bmatrix} 4 & -1 & 0 & -1 & -2 \\ -1 & 4 & -3 & 0 & 0 \\ 0 & -3 & 4 & -1 & 0 \\ -1 & 0 & -1 & 2 & 0 \\ -2 & 0 & 0 & 0 & 2 \end{bmatrix}$$

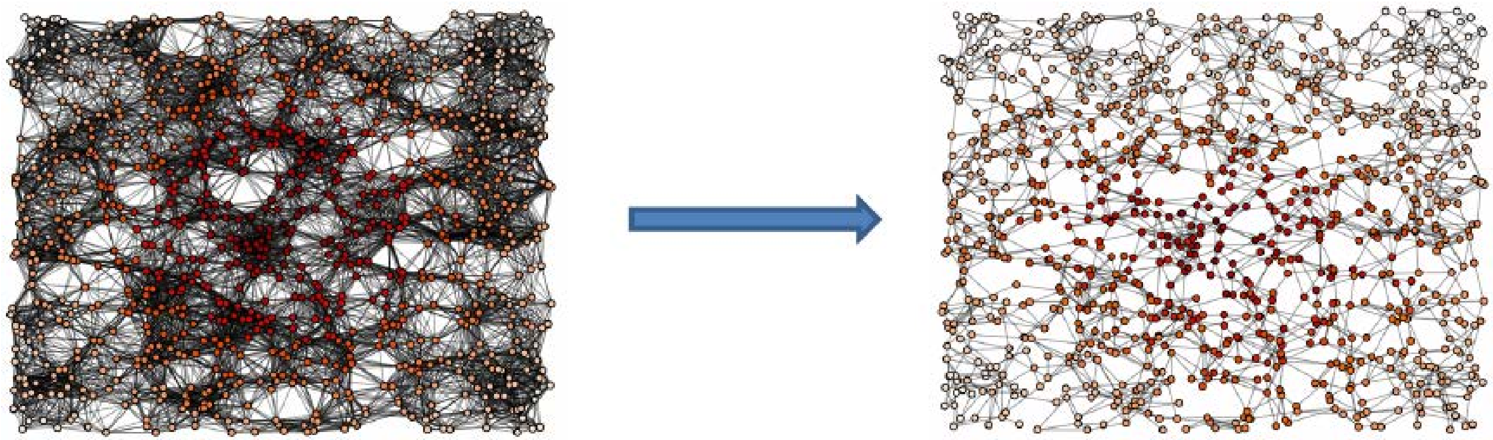
  – Low-stretch trees approximate most distances to within O(log m) using only m-1 edges:



  – Approaches incorporate elements of direct and iterative solvers for class of problems with graph clustering, spectral sparsification, partial factorizations, minimal trees for state of the art towards **O(mlog^{c}n)** solver for m edges and n vertices (Koutis et. al 2009: CMG, Kelner et. al 2013, Peng-Spielman 2014)

Combinatorial Multigrid Issues

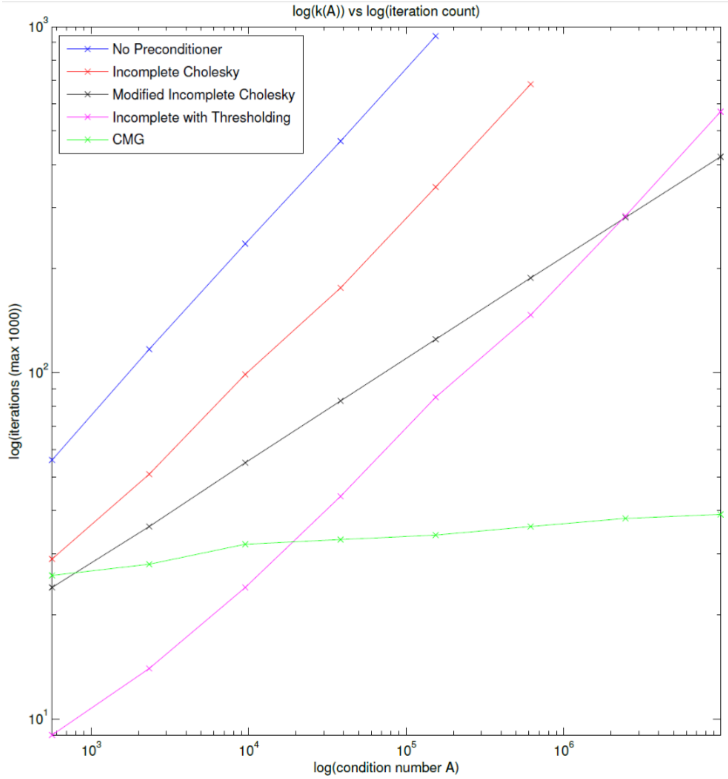
- Sparsifiers generate a “smaller” matrix or analogous graph structure, which preserves many graph parameters.



- Computationally very expensive and only seemingly practical in the theoretical realm! Further, computing on the fly tricky. The idea is to maintain “cliques” and “cycles”.
  - Can be satisfied if the general structure remains in a simpler fashion using simpler strategies.
- Complex-valued data for NP problems
- NP problems not diagonally-dominant, though CMG can still handle this

Preconditioner Sample Results

- Small non-LQCD SDD system for testing MATLAB CMG:
  - Significantly-reduced iteration counts as condition numbers grow



- Incomplete Cholesky-based preconditioners on small LQCD system:

Test Type	N_{iter}	$T(s)$
No Preconditioner ($P = I$)	3352	35
IC(0) (no-fill Incomplete Cholesky)	1780	36
ICT (thresholding with small values)	22	6
IC with diagonal compensation ($\alpha \approx 1e-4$)	652	17

  - IC-based preconditioners show great promise, but LQCD matrices are computed at run-time, so computing incomplete factorization may require too much memory in practice

PUMA-V Conclusions Thus Far

Summary and Ongoing Goals

- In the past year we have explored the possibility of using the R-Stream source-to-source compiler to optimize the Wilson Dslash in CPS.
  - So far R-Stream hasn't been able to produce highly optimized code for CPS.
    - Working on stabilizing R-Stream scheduler to handle more complex codes.
  - Further manual optimizations based on the R-Stream output include incorporating SSE and AVX intrinsics, which give the expected 2X and 4X speedup, respectively, compared to the un-optimized single-core input code.
  - Currently working to fix implementation of the MPI communications causing significant performance drop for DWF Dslash.
  - Single-precision AVX implementation.
  - Incorporate new code into physics production runs.
- Incorporate newer R-Stream versions into Visualizer Tool
  - More performance tuning implementations and auto-tuning/optimizations in tool for more optimal compiler options.
- Preconditioners and Solvers
  - Complete C implementation of CMG and modifiy for LQCD systems.
  - Work on memory-efficient Incomplete factorizations.

Thank You!
Questions/Comments

R-Stream Compiler Additional Slide

R-Stream 3.0 Compiler

Raising
High-Level Dependence Analysis
Parallelization-Fusion
Tiling
Locality Enhancement
Placement
Communication Generation
Synchronization Generation
Thread Generation
…

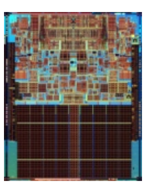
HPEC Application
in C Language

Leveraged Investment

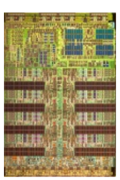
One high-level optimizer leveraged across multiple architectures and implementations.

Virtual Machine Abstractions (language + library calls)

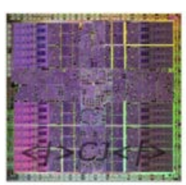
LLC | LLC | LLC | LLC | LLC



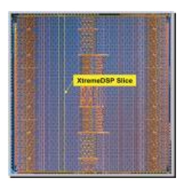
SMP



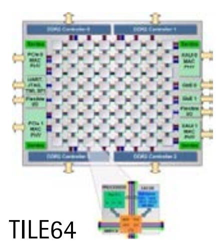
Cell



GPU



FPGA



TILE64

Capabilities beyond previous compilers

Input programs: increased scope of optimizations
- Imperfect loop nests.
- Parametric affine programs.

Out: increased scope of targets
- Optimizations and transformations for multi-core machines.

Based on mathematics:
- Unique implementation of capabilities that would otherwise just be theory.
- Less "magic"
- First opportunity to use theoretical techniques on C

Programming Challenges

Multi-core Hardware:
- 10-100x FLOPS/Watt advantage
- Parallelism
- SIMD
- Heterogeneous Functional Units
- Coarse grain communication ops
- Streaming Engines
- Tiled Chip Multiprocessing
- Distributed local memories
- Starved for pin bandwidth