X-TUNE
Autotuning for Exascale: Self-Tuning Software to Manage Heterogeneity

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Participants

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  - Sam Williams, Lenny Oliker, Brian van Straalen
- Argonne National Laboratory
  - Paul Hovland, Sri Krishna Narayanan, Jeff Hammond, Prasanna Balaprakash, (Stefan Wild), Thomas Nelson (Colorado)
- USC/ISI
  - Jacqueline Chame

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What is Autotuning?

- Definition:
  - Automatically generate a "search space" of possible implementations of a computation
    - A ***code variant*** represents a unique implementation of a computation, among many
    - A ***parameter*** represents a discrete set of values that govern code generation or execution of a variant
  - Measure execution time and compare
  - Select the best-performing implementation (for exascale, tradeoff between performance/energy/reliability)
- Key Issues:
  - Identifying the search space
  - Pruning the search space to manage costs
  - Off-line vs. on-line search

X-TUNE Goals

A unified autotuning framework that seamlessly integrates programmer-directed and compiler-directed autotuning.

- Expert programmer and compiler work collaboratively to tune a code.
  - Unlike previous systems that place the burden on either programmer or compiler.
  - Provides access to compiler optimizations, offering expert programmers the control over optimization they so often desire.
- Design autotuning to be encapsulated in domain-specific tools
  - Enables less-sophisticated users of the software to reap the benefit of the expert programmers' efforts.
- Focus on Geometric Multigrid (ExaCT, BoxLib, Chombo), Nekbone (CESAR) and tensor contractions (NWCHEM)

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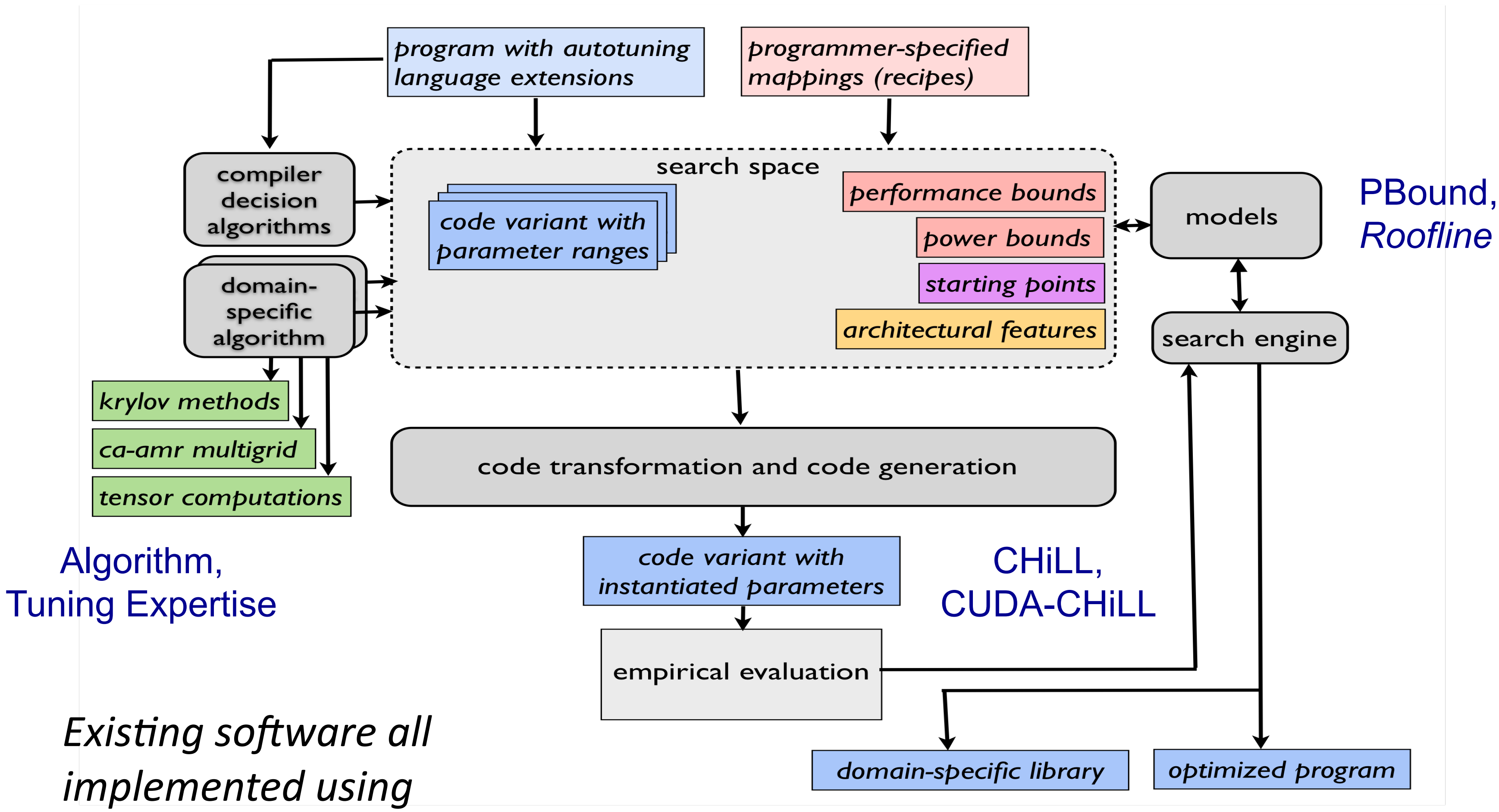
X-TUNE Vision



Existing software all implemented using ROSE AST.

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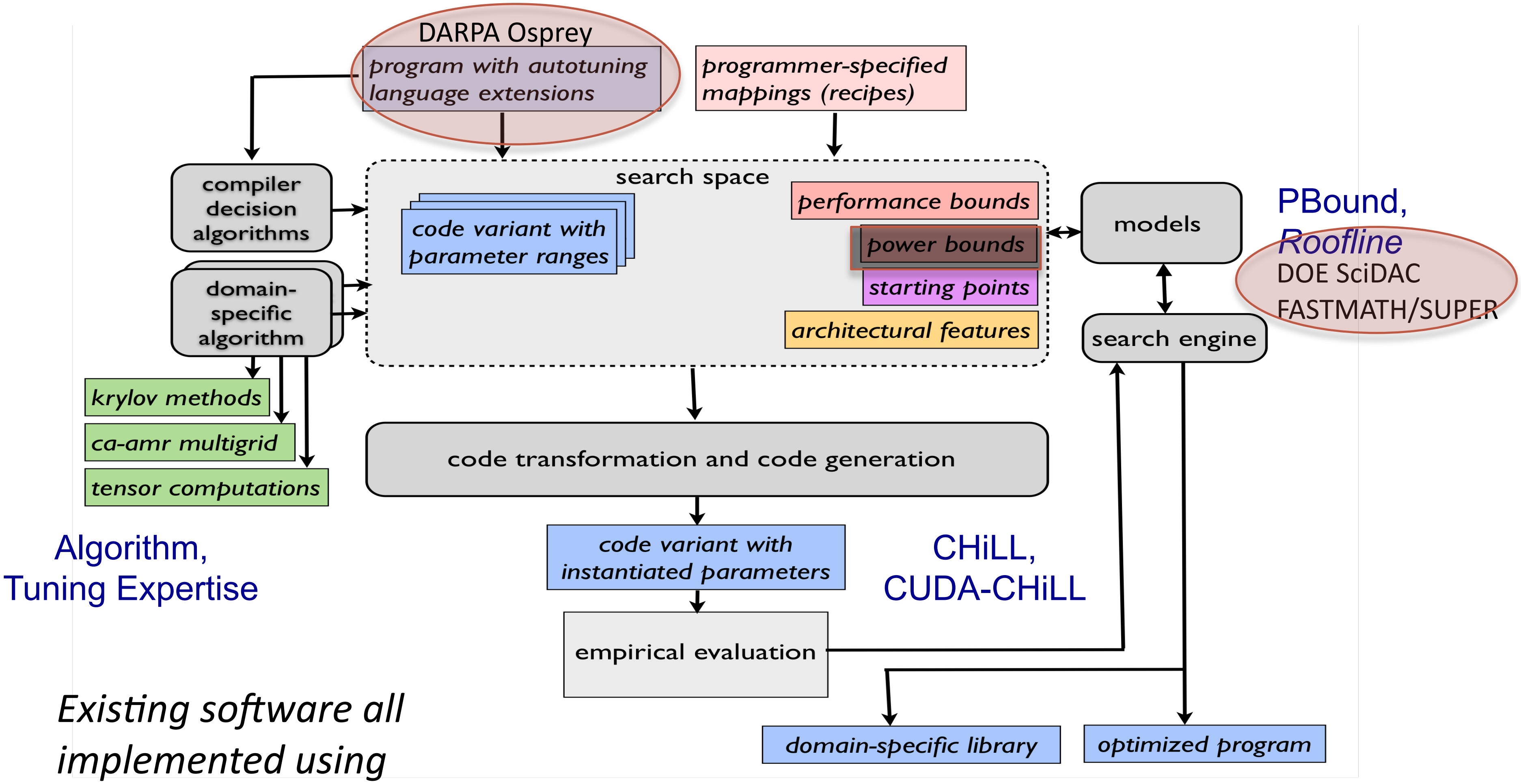
X-TUNE Vision and Status Overlay

Overlay for joint funding, power/energy not part of X-TUNE, remainder in progress



Existing software all implemented using ROSE AST.

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X-TUNE Approach at a Glance

- When available, start with manually-tuned code or work with developer of new code
  - What are the performance bottlenecks, inherent and on specific architectures?
  - What transformations are needed to target specific architectures?
  - What performance questions can be addressed by autotuning?
- Attempt to automate
  - Develop new transformations and required analysis and code generation support
  - Develop modeling and decision algorithms
- Collect application code from collaborators, Co-Design Centers and other DOE application teams
  - Generalize from experiments with manually-tuned code

Outline

- Technical Approach
  - Communication-Avoiding Geometric Multigrid (use case)
  - OCTOPI: Tensor Computations and Tensor Contraction (use case)
  - Modeling and Decision Algorithms
- Summary of Interactions
- Remainder
  - Comparison with state-of-the-art

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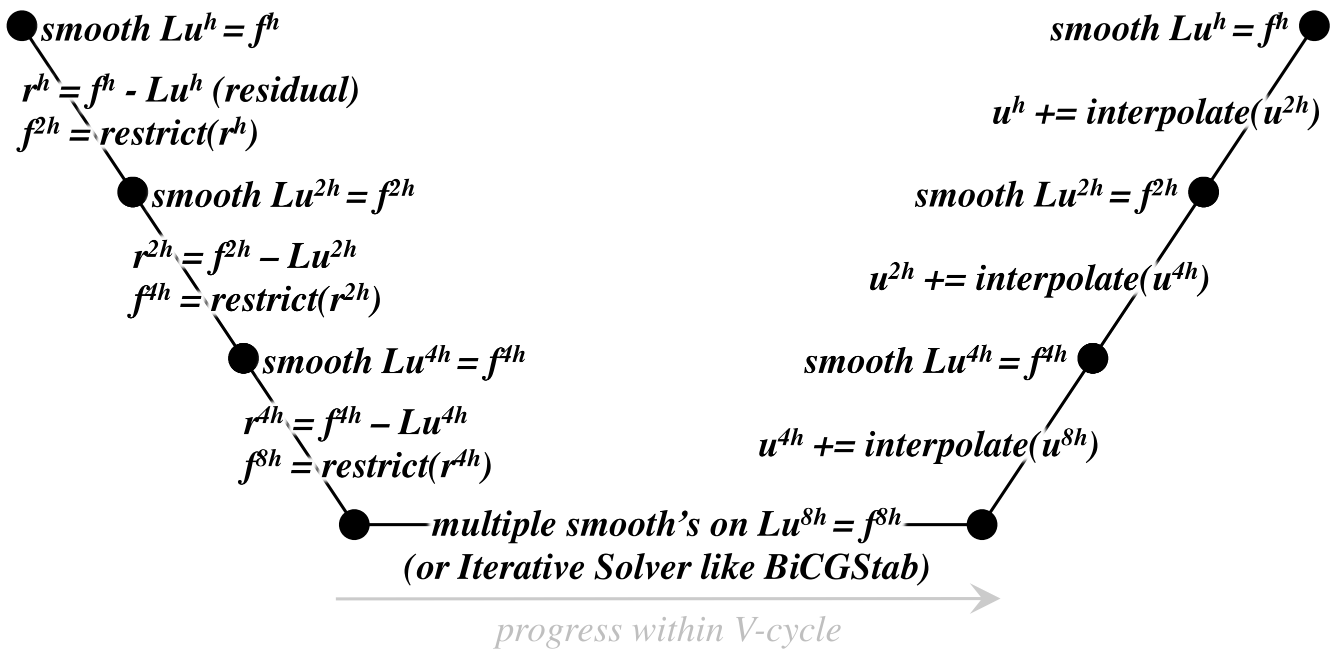
Geometric Multigrid

- Multigrid solves elliptic PDEs in O(N) computational complexity by using a hierarchical approach.



❖ As a result, the degree of Parallelism **decreases exponentially**…
- N-way parallelism, N/8, N/64, … 1-way parallelism across the entire machine … N/64, N/8, N
- This is major worry for exascale machines 1000's of cores per node

❖ Geometric Multigrid (**GMG**) is specialization in which the operator (A) is simply a stencil on a structured grid (i.e. *matrix-free*)

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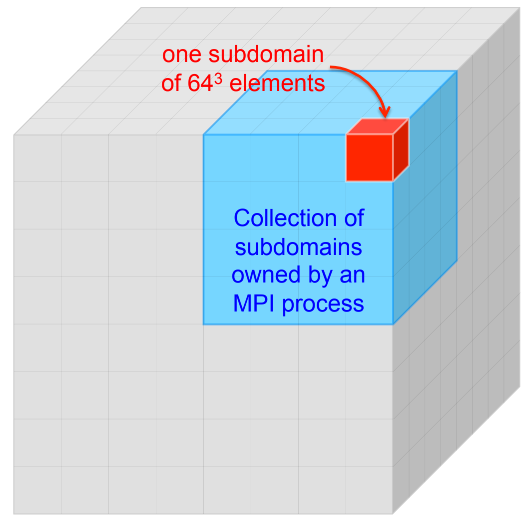
miniGMG Benchmark

- **miniGMG proxies the MG solves in BoxLib/Chombo codes**
- Cubical domain decomposed among processes into **boxes**.
- Fine-grid box dimension is configurable.
  - **smaller boxes mimic AMR MG challenges**
  - fewer boxes per process can be used to mimic combustion code constraints.
- **operator** is configurable
  - 7pt variable coefficient **proxies LMC**
  - 7pt constant coefficient is simpler
  - 27pt/13pt high-order stencils are available.
- **smoother** in the v-cycle is configurable
  - Gauss Seidel, Red-Black ("GSRB") = **proxies LMC**
  - Jacobi (mathematically weaker)
- **bottom solver** is configurable
  - multiple GSRB's
  - Krylov solver like **BiCGStab**, CG, CA-BiCGStab, CA-CG, etc…



Compiler Optimization of miniGMG (Smooth)

Optimization Using Known Transformations

- Loop skew, permute and tiling to create a parallel wavefront

New Domain-Specific Transformations

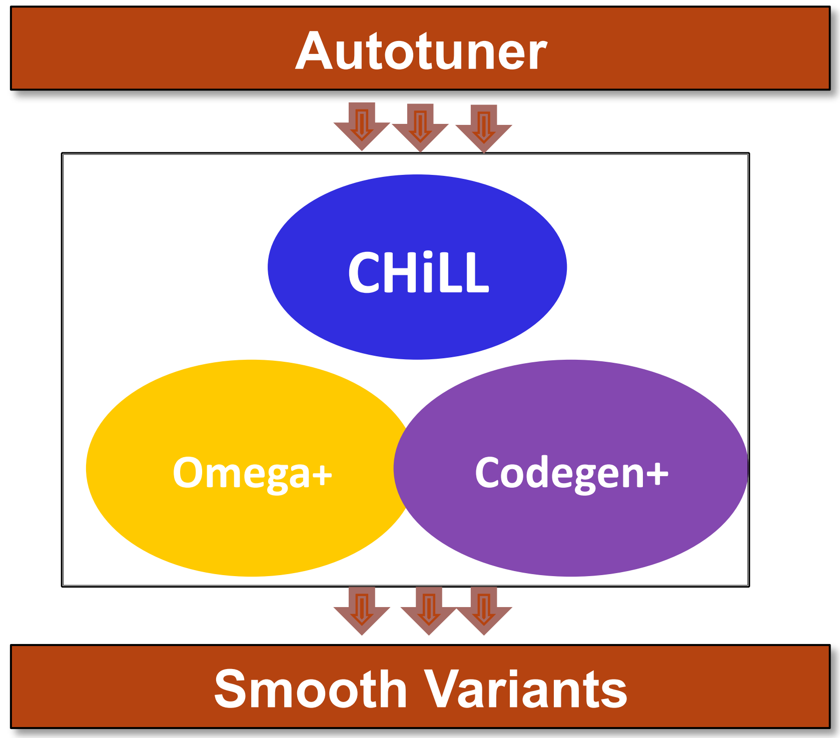
- Loop fusion in presence of fusion-preventing dependences
- Eliminating temporaries
- Adding ghost zones (comm. avoiding) to Multigrid operators

High-Performance OpenMP Code Generation

- Vary parallelism (intra-box) for different box sizes.

Optimizations Built into CHiLL

- CHiLL = loop transformations and code generation



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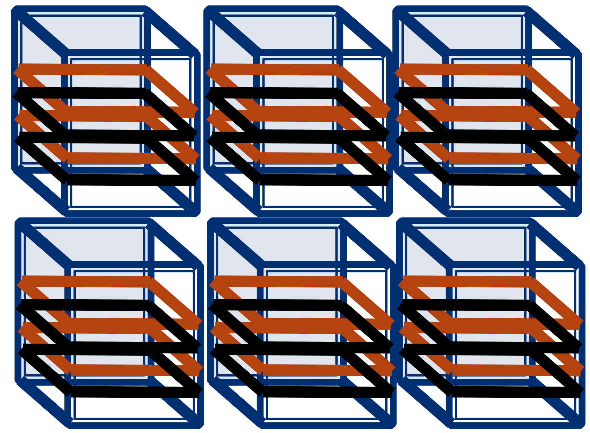
Inter-Box Parallelism
Thread Configuration
<6,1>



Best parallel code generation strategy depends on box size and machine!

Parallel Decomposition

Nested Parallelism
Thread Configuration
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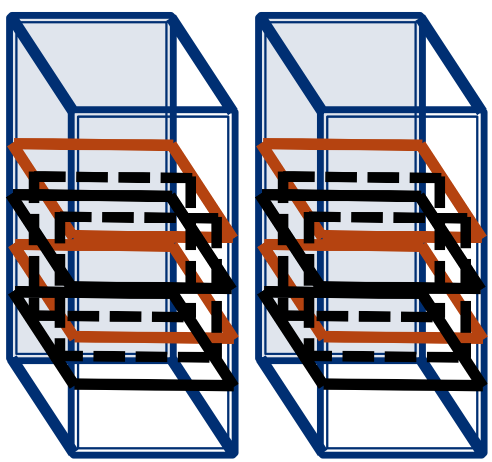

Intra-Box Parallelism
Thread Configuration
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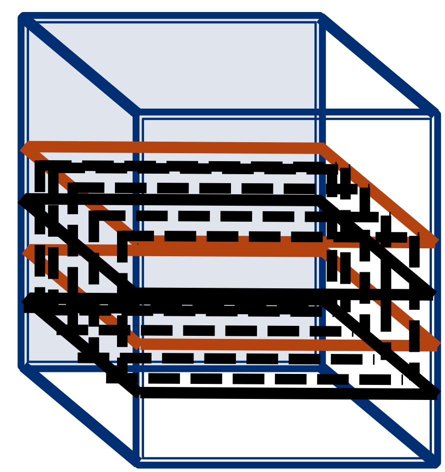

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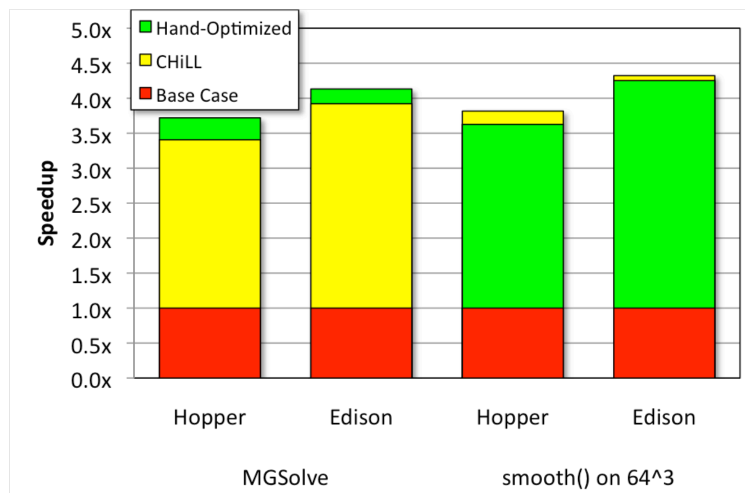
Highlight – April 2014

Compiler Autotuning for Geometric Multigrid

- Problem
  - Geometric multi-grid (GMG), is one of the most popular methods for solving partial differential equations, but is very difficult to optimize on evolving CPU architectures
- Solution
  - Leverage communication-avoiding optimizations which reduce communication overhead
  - Apply CHiLL compiler technology, using a set of novel transformations to derive performance comparable to hand-written optimizations
  - Make the approach portable, via autotuning system that explores tradeoffs between reduced communication and increased computation, as well as tradeoffs in threading schemes
- Recent results
  - Improved overall multi-grid solve execution by over 4x on NERSC Edison vs. reference version *(Basu et al., HIPC 2013 & WOSC 2013)*
  - Improved smooth at finest level by over 4x - ***CHiLL-generated code outperforms hand-tuned***
  - Demonstrated comparable performance for low-level OpenMP threads & higher level ***Habanero C phasers***
- IMPACT
  - Achieves comparable performance to hand-tuned code without sacrificing programmer productivity
  - Demonstrates capability of compiler-directed autotuning, with broad impact on important numerical methods for the DOE Office of Science



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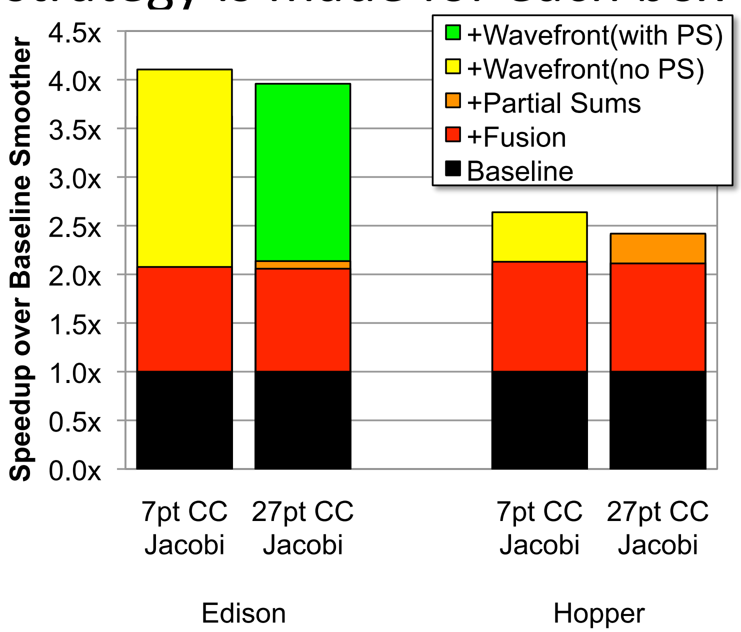
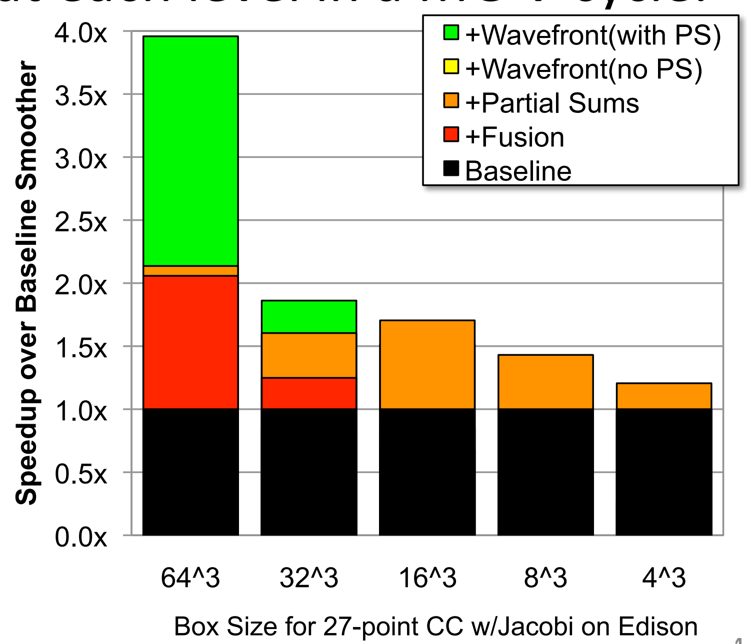
Recent Work: Compiler Optimization of miniGMG (Smooth+Residual+Restrict)

- CHiLL can tune and generate the best implementation for a given combination of operator (7pt or 27pt) and smoother (Jacobi).
  - Fusion may include smooth+residual+restriction
  - Partial sums optimization reduces computation, exposes reuse in cache and registers, improves SIMD code generation
- This choice of optimization, ghost zone depth, and threading strategy is made for each box size at each level in a MG V-cycle.





Tensor Products and Tensor Contractions

- Develop autotuning strategy for tensor computations such as Nekbone (CESAR) and NWCHEM (SciDAC)
  - Express tensors in mathematical notation (borrowing from Build-to-Order BLAS)
  - Decision algorithm maps to CHiLL recipes
  - Use Orio to explore autotuning search space
- Builds on prior work for small matrix-multiply kernels in Nek5000
- Leverages and integrates existing tools

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Example: Spectral Element Method from nek5000/nekbone (CESAR)

$$C = A \otimes B \underline{u}$$

- A and B are square matrices
- $\underline{u}$ is a component vector
- In 2-d, C can be computed:

$$c_{i,j} = \sum_{l} \sum_{k} a_{j,l} b_{i,k} u_{k,l}$$

Order O(n^4)

Optimize by rewriting to the following:

$$C = (A \otimes I)(I \otimes B)\underline{u}$$

Partial Results: $\underline{w} = (I \otimes B)\underline{u}$ → $w_{i,j} = \sum_{l} u_{i,l}\, b_{l,j}^{T}$

Final Results: $C = (A \otimes I)\underline{w}$ → $c_{i,j} = \sum_{k} a_{i,k} w_{k,j}$

Order O(n^3), Can use DGEMM

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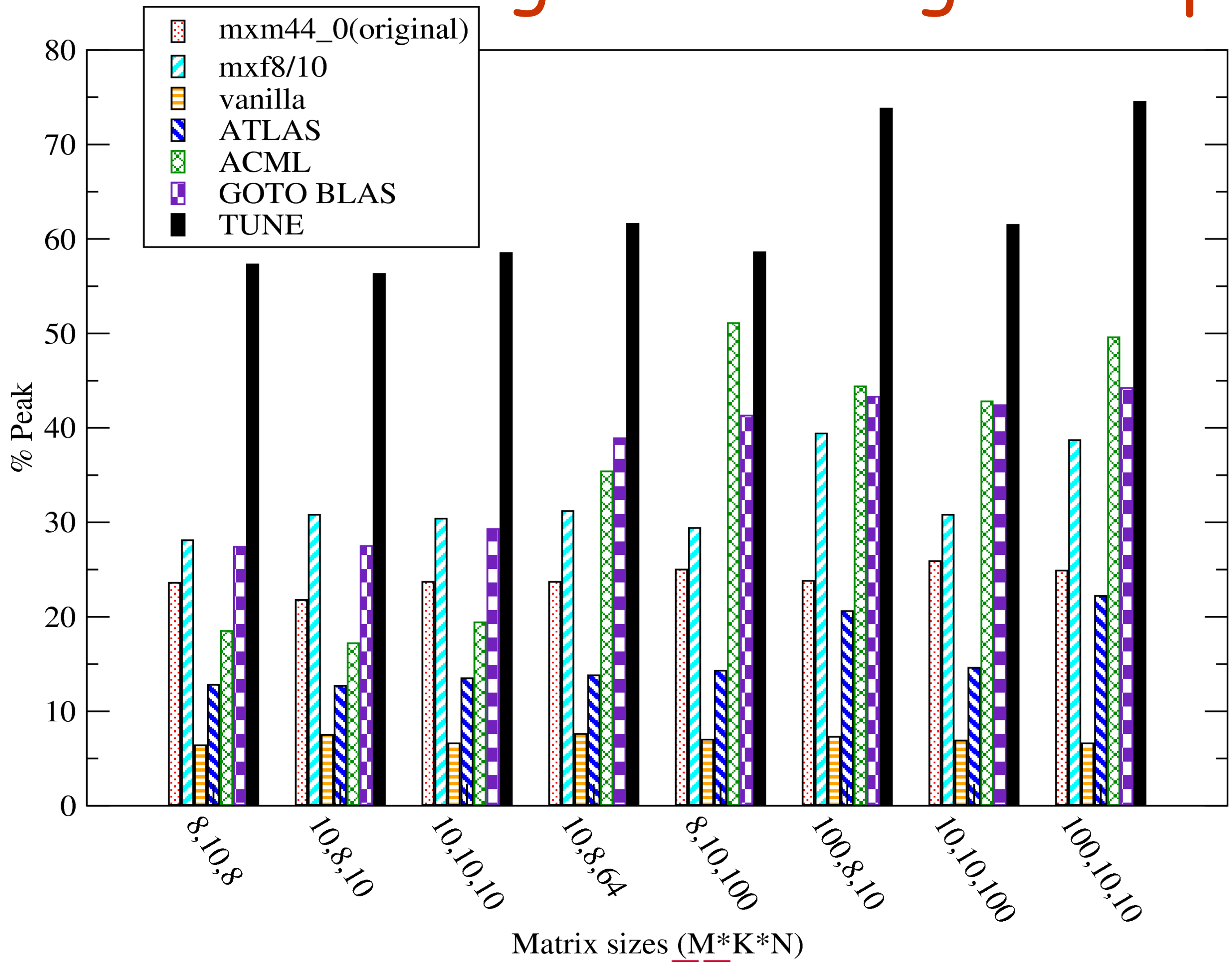
Prior Work (TUNE): Matrix Multiply for Small Matrices using Autotuning and Specialization



Net result:
1.36 speedup
in overall Nek5000
performance

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Toward a High-Level Representation

- Prior work ignored tensor structure

```
 subroutine local_grad3(ur,us,ut,u,n,D,Dt)
c      Output: ur,us,ut          Input:u,n,D,Dt
       real ur(0:n,0:n,0:n), us(0:n,0:n,0:n), ut(0:n,0:n,0:n)
       real u(0:n,0:n,0:n), D(0:n,0:n), Dt(0:n,0:n)
       integer e,i1,j1

       m1 = n+1
       m2 = m1*m1

       call mxm(D,m1,u,m1,ur,m2)
       do k=0,n
          call mxm(u(0,0,k),m1,Dt,m1,us(0,0,k),m1)
       enddo
       call mxm(u,m2,Dt,m1,ut,m1)

       return
       end
```

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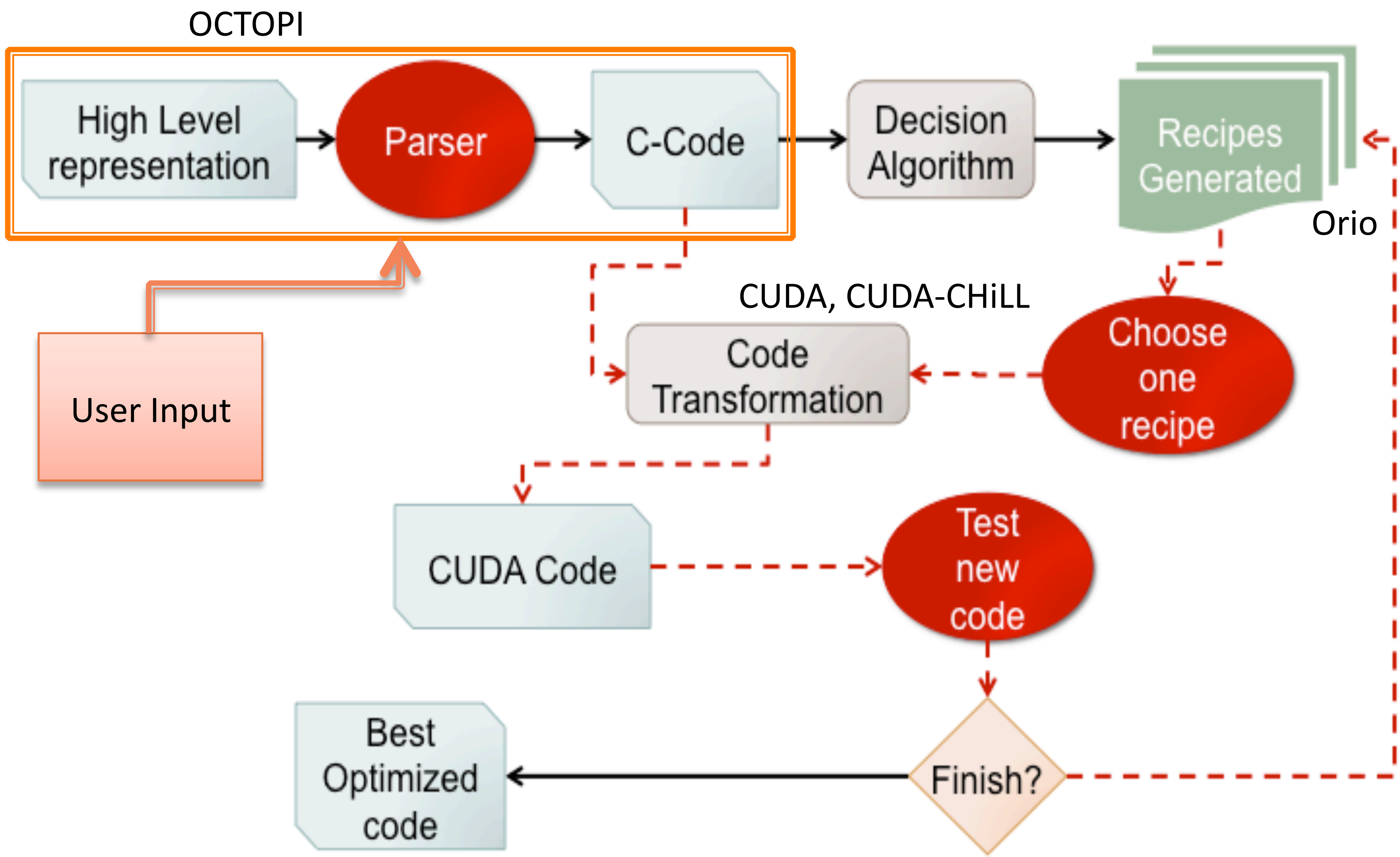
Goal

```
 subroutine local_grad3(ur,us,ut,u,n,D)
c      Output: ur,us,ut           Input:u,n,D
       real ur(0:n,0:n,0:n),us(0:n,0:n,0:n),ut(0:n,0:n,0:n)
       real u(0:n,0:n,0:n), D(0:n,0:n)
```

$$UR_{ijk} = D_{il}U_{ljk}$$
$$US_{ijk} = D_{il}U_{ilk}$$
$$UT_{ijk} = D_{il}U_{ijl}$$

```
       return
       end
```

Experimental Framework



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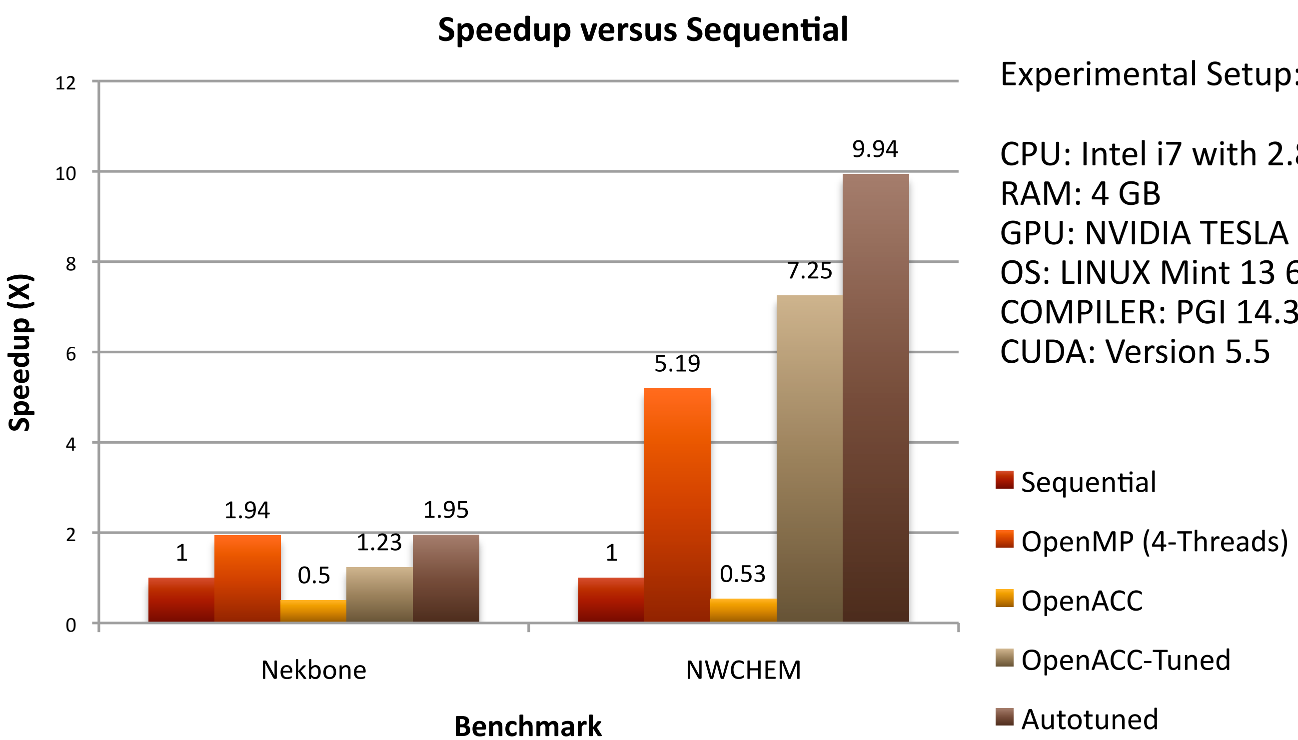
Preliminary Results



Experimental Setup:

CPU: Intel i7 with 2.8 GHz
RAM: 4 GB
GPU: NVIDIA TESLA C2050 (FERMI)
OS: LINUX Mint 13 64 bits
COMPILER: PGI 14.3 with OpenACC support
CUDA: Version 5.5

- Speedup on GPU: 1.95x Nekbone and 9.94x NWCHEM
- Speedup over OMP: 1.01x Nekbone and 1.95x NWCHEM
- Speedup tuning OpenACC: 2.45x Nekbone and 13.68x NWCHEM

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Model-Guided Compiler Decision Algorithms

- Goal: Automate the generation of code variants by compiler decision algorithms
- Models and analysis derive information about application
  - data dependences, data reuse, instruction counts, performance bounds
- Application and architecture information guide decisions
  - transformations, data placement

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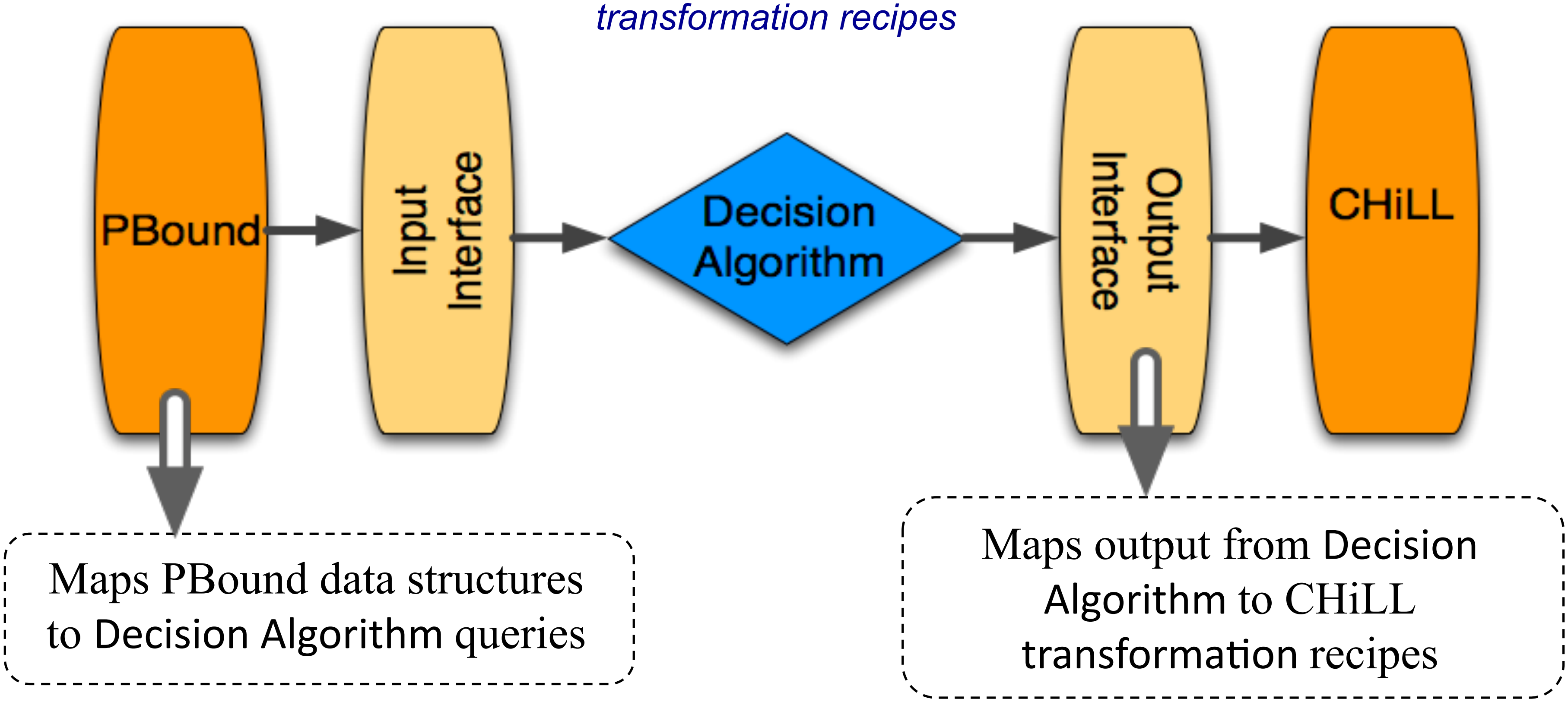
Modeling and Compiler Decision Algorithm

PBound analyzes code to derive reuse distance, and data footprint, integration with roofline

Decision Algorithm examines dependences and data reuse to generate a set of CHiLL transformation recipes

CHiLL performs transformations and code generation as specified by parameterized recipes



Modeling and Decision Algorithm Status

- A new data reuse algorithm with more precise identification of reuse types added to PBound.
- A new locality decision algorithm was implemented and integrated with PBound
- A new algorithm targeting GPUs was developed and integrated with PBound
- NWCHEM
  - locality algorithm generates scripts that are used by CHiLL to generate code variants

Interaction with X-Stack and Co-Design Projects

- Sam Williams - ExaCT and DEGAS
- Brian van Straalen – D-TEC
- Paul Hovland – CESAR
- Also interfacing with other X-Stack software
  - Orio/Active Harmony and OpenTuner planned
  - Habanero C
  - ROSE
- Additional code excerpts
  - TiDA (LBNL), S3D (LANL), HPGMG (LBNL)

Raising Run-Time Level of Abstraction with Habanero C for miniGMG

```
#pragma omp forall … (inter-box parallel loop)
…
for (k = -3; k <= 66; k++) {
  for (t = 0; t <= min(3,intFloor(t+3,2)); t++) {
   for (j = t-3; j <= -t+66; j++) {
     for (i=t-3+intMod(-k-color-j-(t-3),2); i<=-t+66; i+=2)   {
          S0(t,k-t,j,i); /* Laplacian */
          S1(t,k-t,j,i); /* Helhmoltz */
          S2(t,k-t,j,i); /* GSRB      */ }}}
     }
```

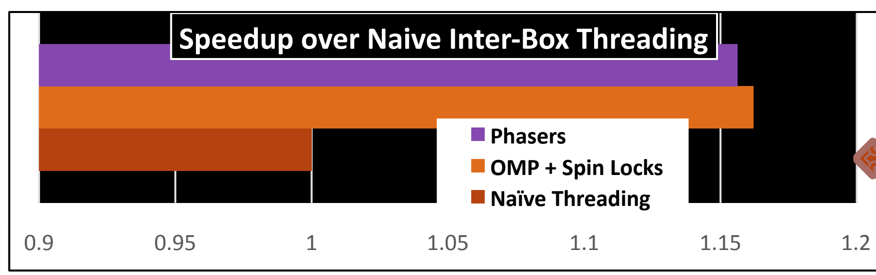
Naïve (Inter-Box) Threading

```
#pragma omp forall … (inter-box parallel loop)
…
#pragma omp parallel private (...) num_threads(y)
{
#pragma omp single
initPhasers();
tid=omp_get_thread_num();
for (k = -3; k <= 66; k++) {
  for (t = 0; t <= min(3,intFloor(t+3,2)); t++) {
   for (j = 6*tid-3; j <= min(6*tid+2,66); j++) {
     for (i= t-3+intMod(-k-color-j-(t-3),2); i<=-t+66; i+=2) {
        S0(t,k-t,j,i);  S1(t,k-t,j,i); S2(t,k-t,j,i); }}}
   doNext(omp_get_thread_num());
}}
```

Habanero Phasers

```
#pragma omp forall … (inter-box parallel loop)
…
#pragma omp parallel private (...) num_threads(y)
{
tid=omp_get_thread_num();
for (k = -3; k <= 66; k++) {
  for (t = 0; t <= min(3,intFloor(t+3,2)); t++) {
     for (j = 6*tid-3; j <= min(6*tid+2,66); j++) {
        for (i= t-3+intMod(-k-color-j-(t-3),2); i<=-t+66; i+=2) {
           S0(t,k-t,j,i);  S1(t,k-t,j,i); S2(t,k-t,j,i); }}}
      zplanes[tid] = t2;
      if (left != tid) {while(zplanes[left] < t2)
{ _mm_pause();}} else{}
      if (right != tid) {while(zplanes[right] < t2)
{_mm_pause();}} else{}}}
```

OMP Spin-locks



Edison Phase(II) , 12 cores per chip, 2 chips per node

Increasing number of threads inside a box
Widens gap between OMP Barrier and spin locks

Connection to State-of-the-Art (MPI+OpenMP)

- miniGMG uses MPI for domain decomposition and OpenMP for thread parallelism
- X-TUNE is agnostic about code outside its purview but introduces thread-level parallelism
  - Goal is to find right abstraction for compiler
  - Compatible with a variety of run-time systems
- Autotuning and communication-avoiding optimizations complementary to run-time and communication support

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Papers and Presentations

- Papers
  - P. Basu, M. Hall, M. Khan, S.Maindola, S.Muralidharan, S.Ramalingam, A.Rivera, M.Shantharam, A.Venkat. Towards Making Autotuning Mainstream. International Journal of High Performance Computing Applications, 27(4), November 2013.
  - P. Basu, S. Williams, A. Venkat, B. Van Straalen, M. Hall, and L. Oliker. Compiler generation and autotuning of communication-avoiding operators for geometric multigrid. In High Performance Computing Conference (HIPC), 2013.
  - P. Basu, S. Williams, A. Venkat, B. Van Straalen, M. Hall, and L. Oliker. Compiler generation and autotuning of communication-avoiding operators for geometric multigrid. In Workshop on Optimizing Stencil Computations (WOSC), 2013.
  - P. Basu, S. Williams, B. Van Straalen, L. Oliker, and M. Hall. Compiler-directed stencil reordering transformations for geometric multigrid. (submitted to) Supercomputing (SC), 2014.
  - S.H.K. Narayanan and P. Hovland. Calculating Reuse Distance from Source Code, (submitted to) Fifth International Workshop on Parallel Software Tools and Tool Infrastructures (PSTI 2014).
  - M.F. Adams, J. Brown, J. Shalf, B. van Straalen, E. Strohmaier and S. Williams, HPGMG 1.0: A Benchmark for Ranking High Performance Computing Systems, LBNL Technical Report LBNL-6630E, 2014.
- Presentations
  - Tiling Dense and Sparse Computations for Parallelism and the Memory Hierarchy of GPUs, Mary Hall, SIAM Parallel Processing Symposium, Feb. 2014.
  - Compiler-Automated Communication-Avoiding Optimization of Geometric Multigrid, Protonu Basu, SIAM Parallel Processing Symposium, Feb. 2014.
- Thesis and Dissertations
  - Axel Rivera. Using Autotuning for Accelerating Tensor-Contraction on GPUs, Masters thesis, University of Utah, July 2014.
  - Other (PhD) students: Thomas Nelson (Colorado), Protonu Basu (Utah)