Performance Optimization and Autotuning in the SUPER Project

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October 7, 2014

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Research Themes

Architectures and applications are evolving rapidly

- Exponential growth in cores, which are becoming heterogeneous
- Scientific questions spanning multiples scales and phenomena
- High performance is increasingly difficult to achieve and maintain

Energy consumption has emerged as a major concern

- Cost of power and cooling is constraining science

Resilience will be a challenge in the very near future

- Shrinking VLSI geometries and voltages will reduce device reliability

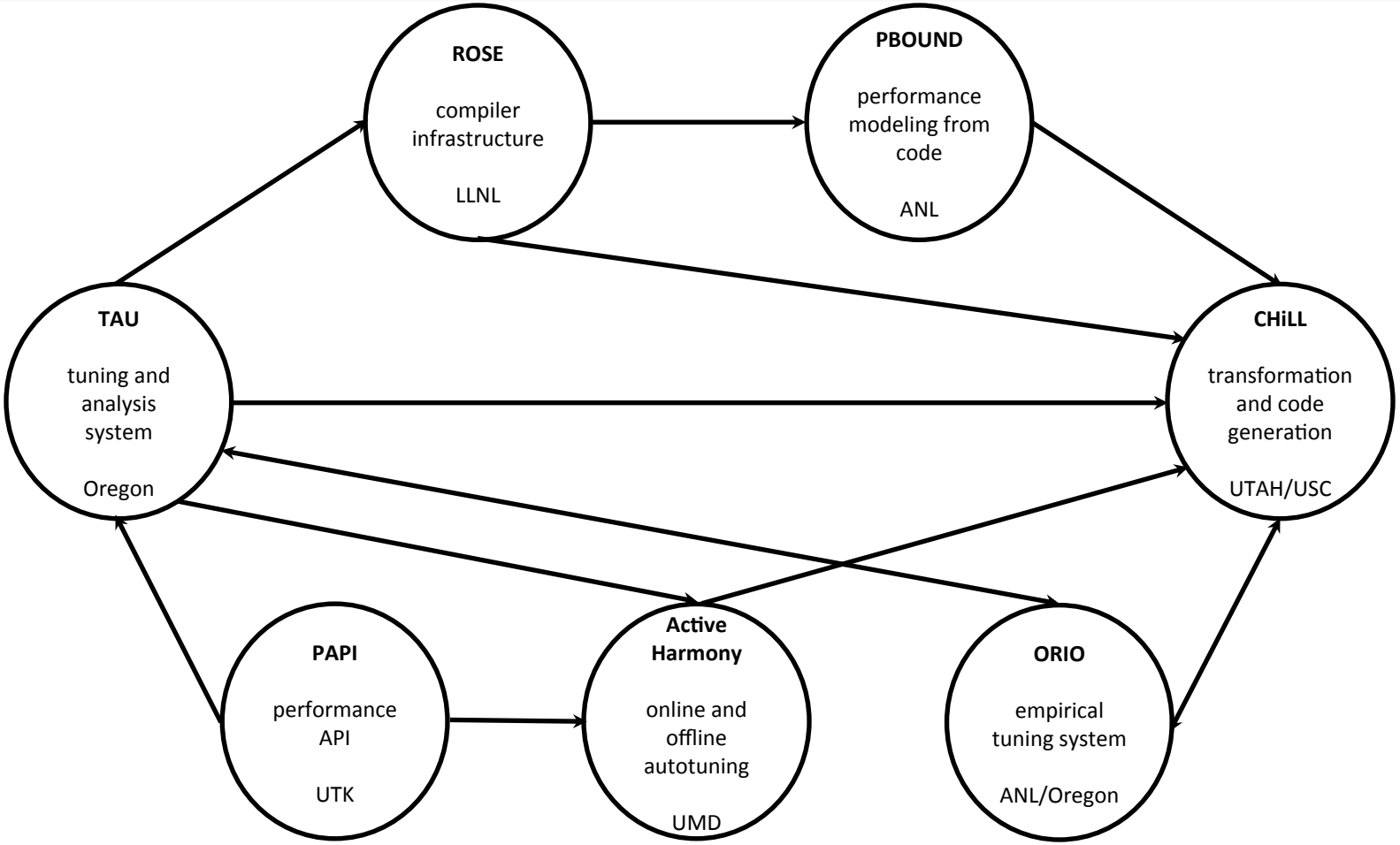
These can be traded off against each other

- Maximize scientific throughput per dollar or Watt

Presentation Focus

- Tool Integration and Development
- Optimization of MPAS-Ocean
- Summary of other Measurement/Analysis/ Optimization Efforts

SUPER Tool Integration

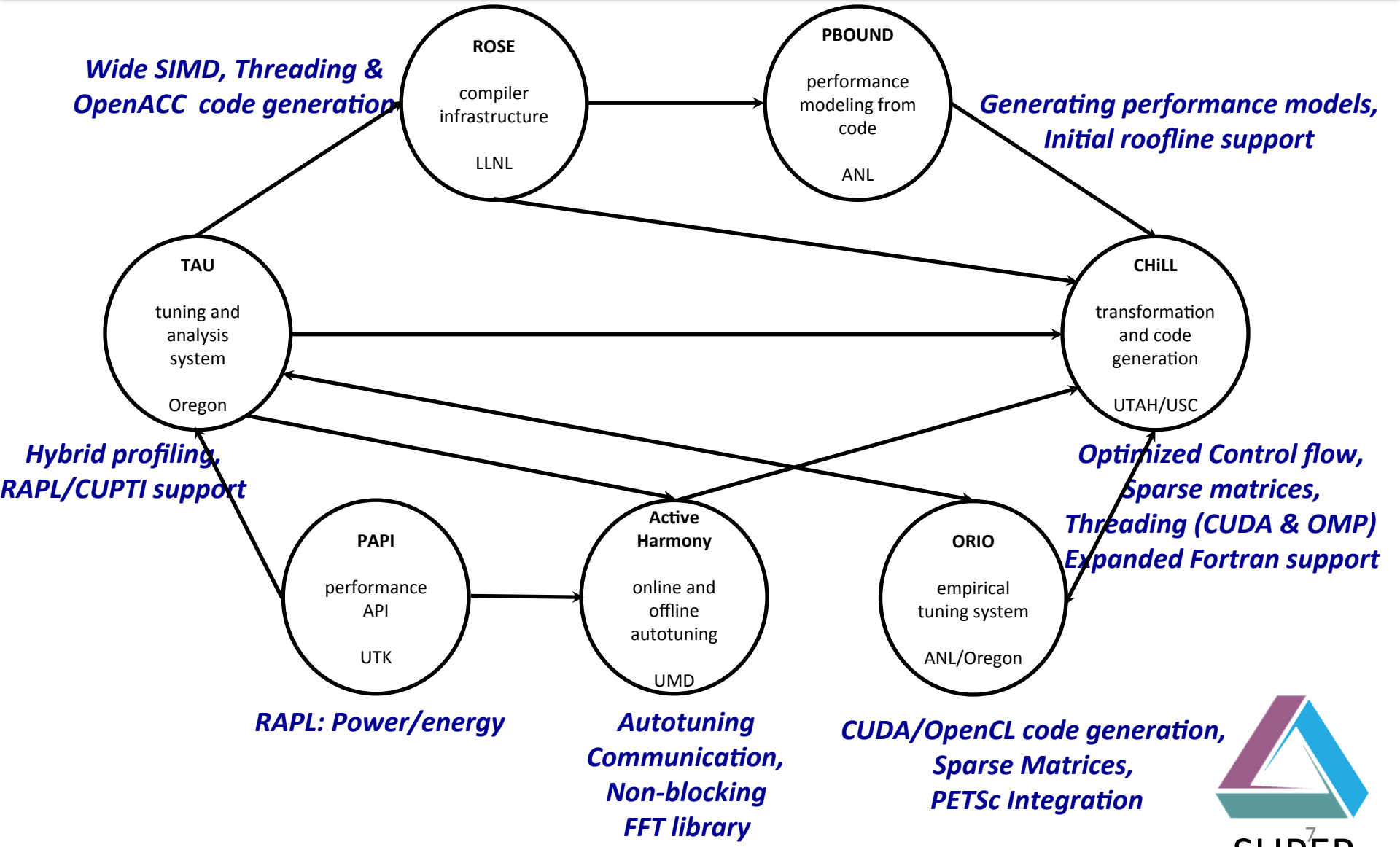


Focus of first year on tool integration.
Edges/arrows show SUPER tools that have been integrated.

SUPER Performance Focus

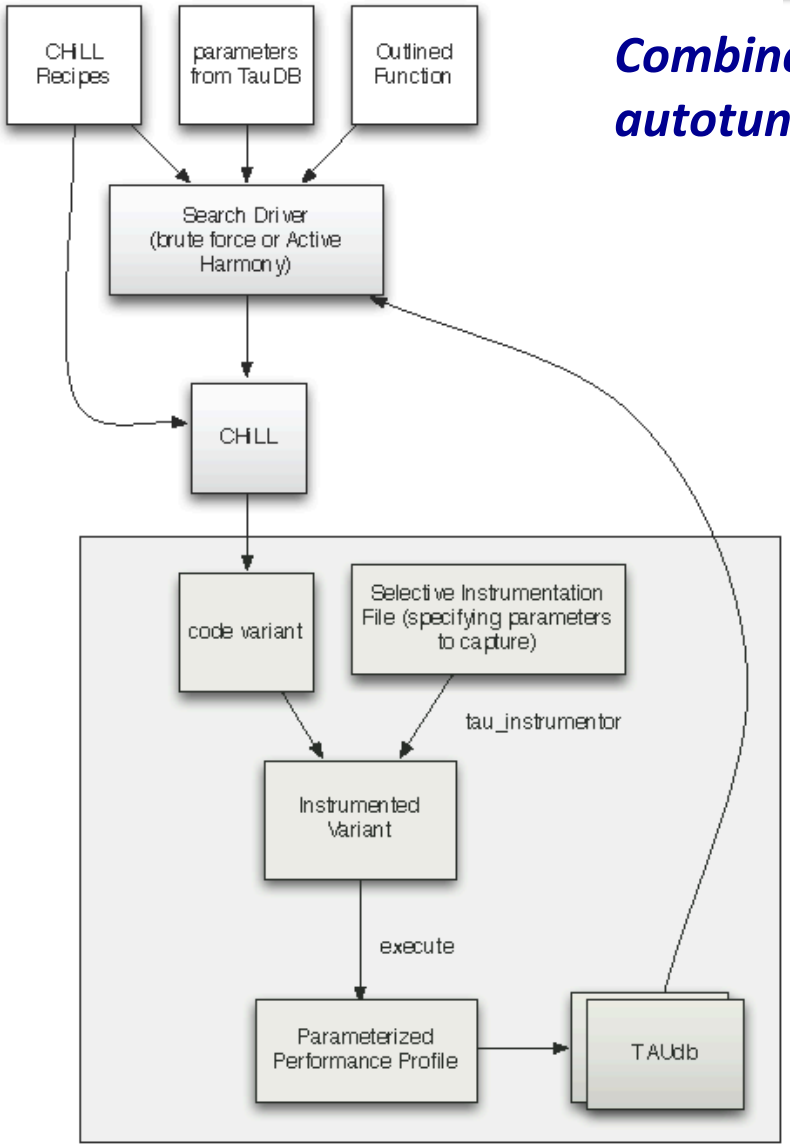
- Tools must support architectural changes…
  - Heterogeneous processing units
  - Hierarchical parallelism, mixed threads and processes
  - Wide SIMD
- … and application requirements
  - Scalability to many cores, processes
  - Dynamic parallelism
  - Batched linear algebra
  - Sparse matrices

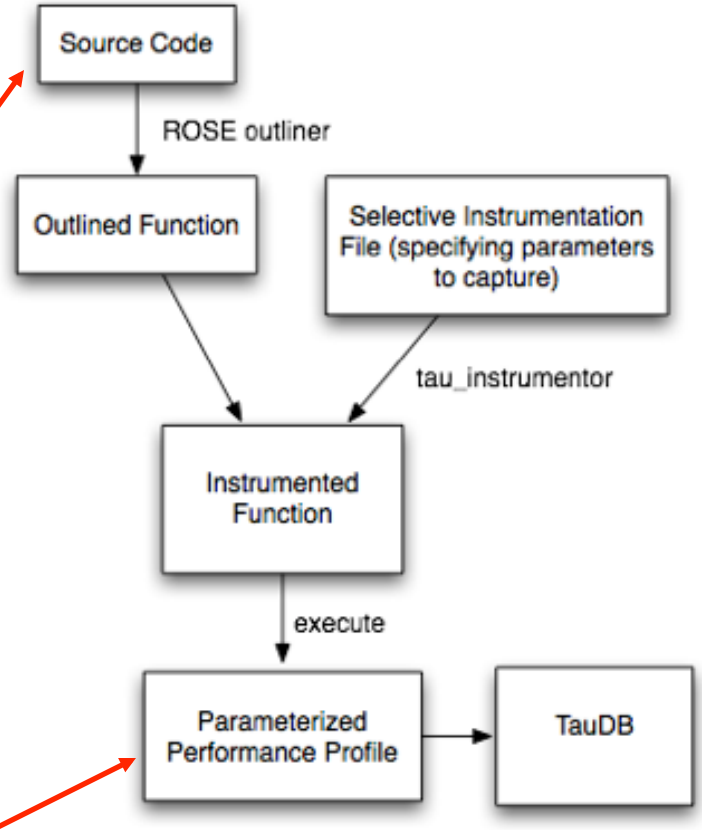
Progress on Tool Development



Example: TAU + ROSE + CHiLL + Active Harmony

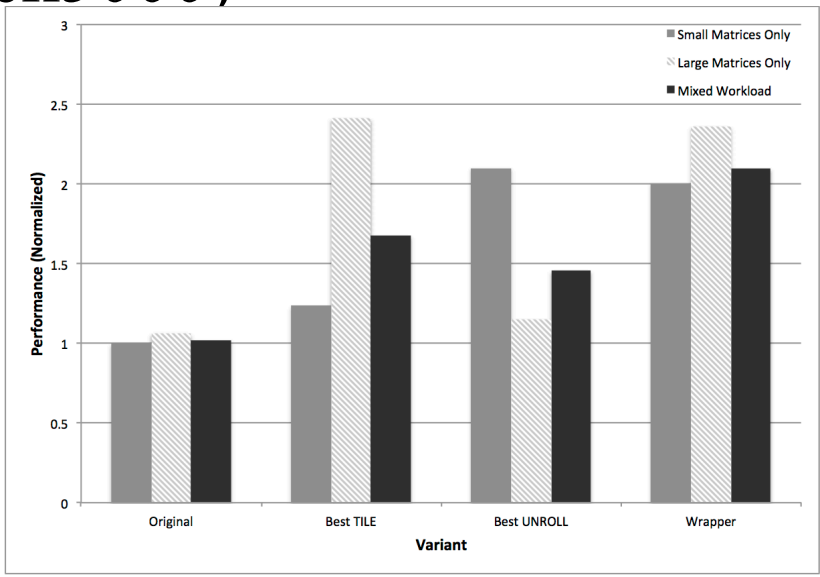
Combine tools to create, store and query results of autotuning experiments in TAUdb

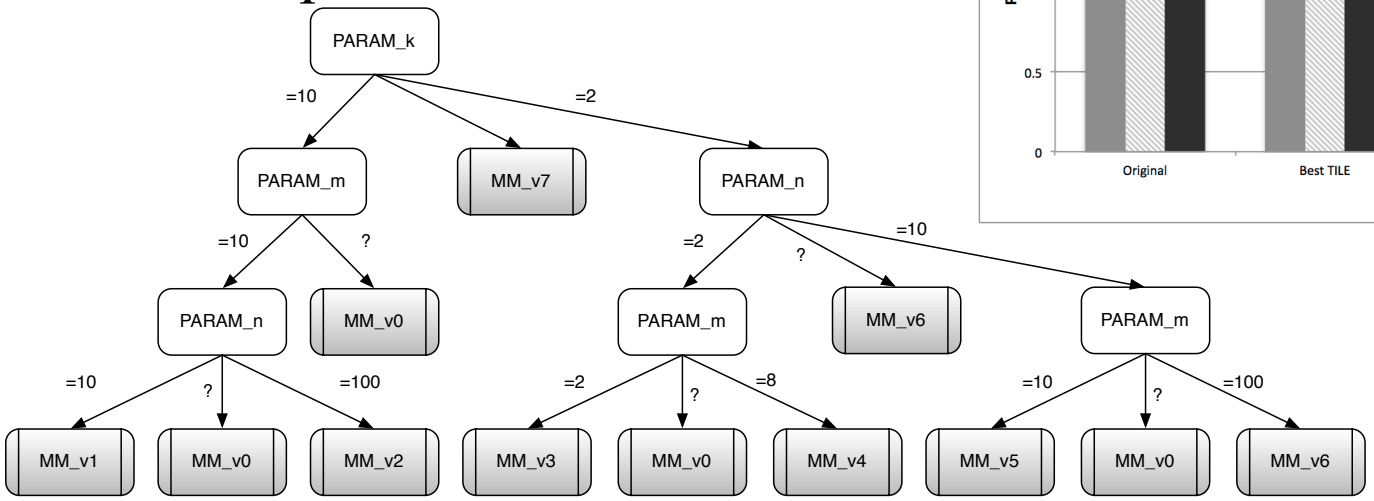




Example: TAU + ROSE + CHiLL + Active Harmony

- Apply machine learning to data stored in TAUdb
  - Generate decision trees based upon code features
- Consider matrix multiply (e.g., Nek5000)
  - Matrices of different sizes with different performance
  - Automatically generate function to select specialized variants





Applying Tools to SciDAC Codes

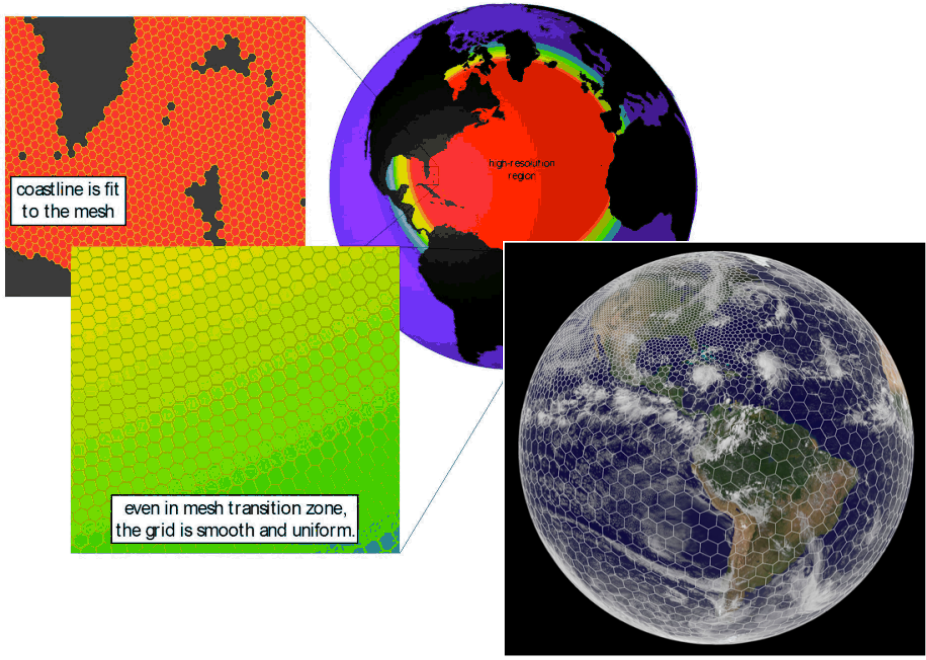
- SUPER interaction with SciDAC application teams
- Approach:
  - Collection of SUPER researchers examine application excerpt or full application to identify performance bottlenecks
  - Opportunities to improve code in different ways are explored.

MPAS-Ocean

- A new code ➔ an opportunity to have early impact
- Complex representation: variable resolution irregular mesh of hexagonal grid cells

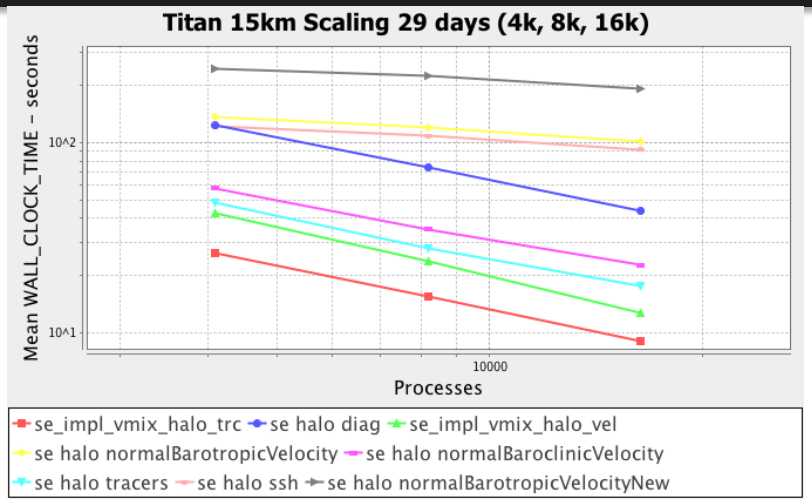
MPAS
Model for Prediction Across Scales

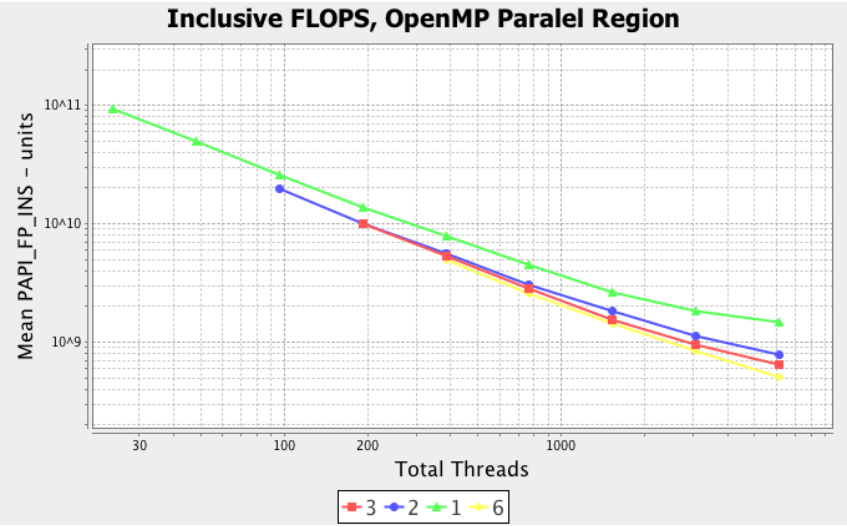
http://mpas-dev.github.io

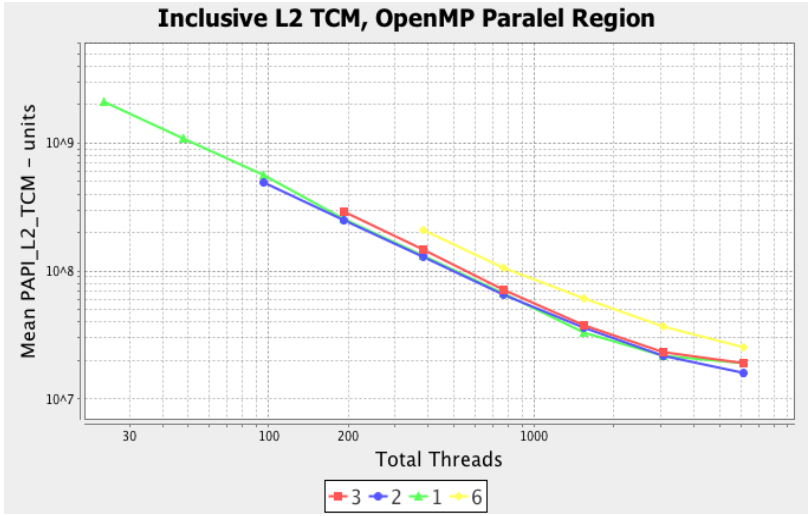


Issue 1: Limited Scalability

- MPI-only scaling leads to additional halo computation, communication
- OpenMP scaling promising, but reduction in FLOPs/core offset by increase in cache misses

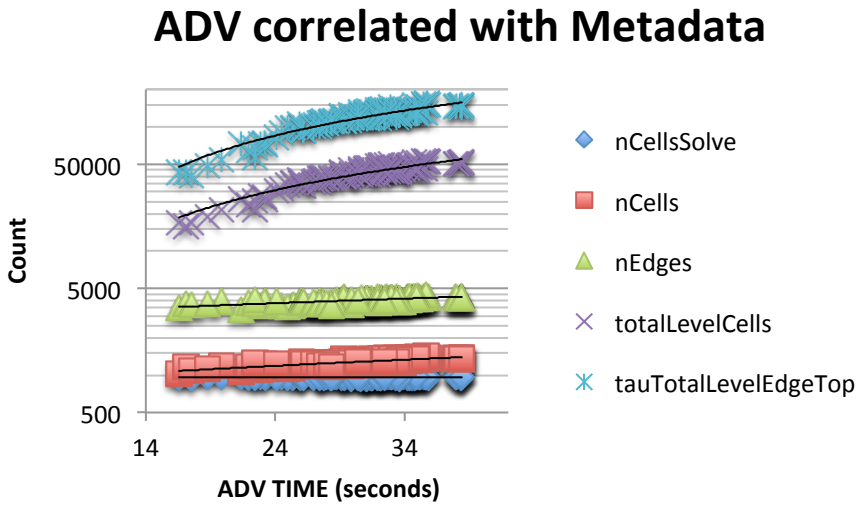


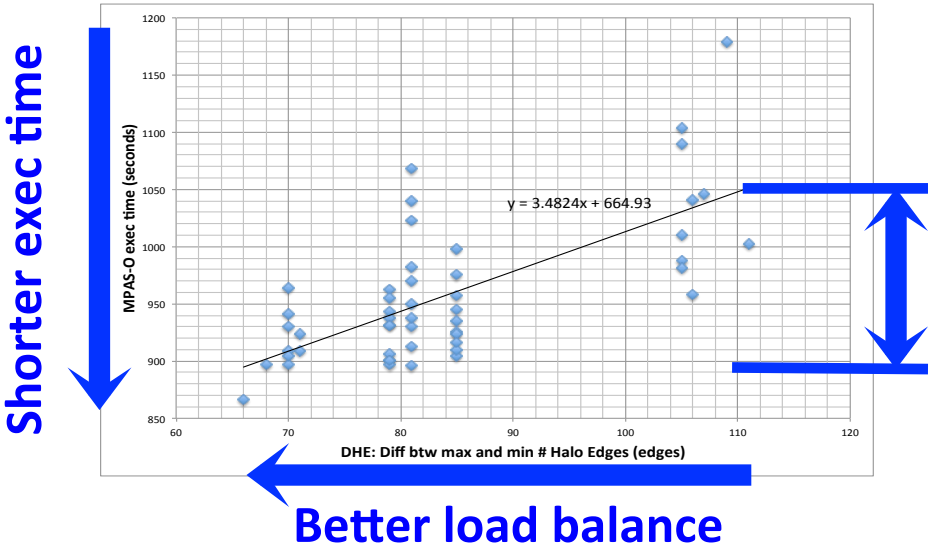




Issue 2: Load Imbalance Due to Partitioning

- Add TAU_METADATA calls to capture sizes of structures
  - Correlate computation balance with metadata fields
- Explore different partitions with METIS





- Conclusion:
  - Partition on nCellsSolve, but value unknown before partitioning

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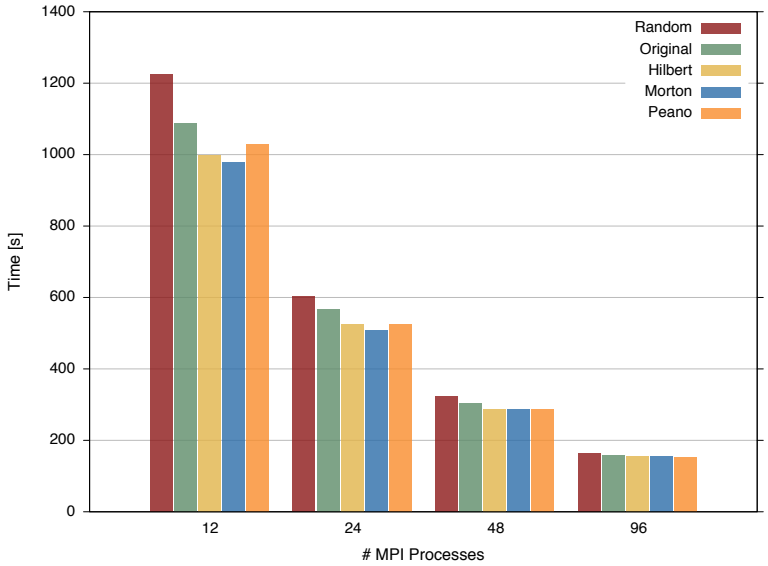
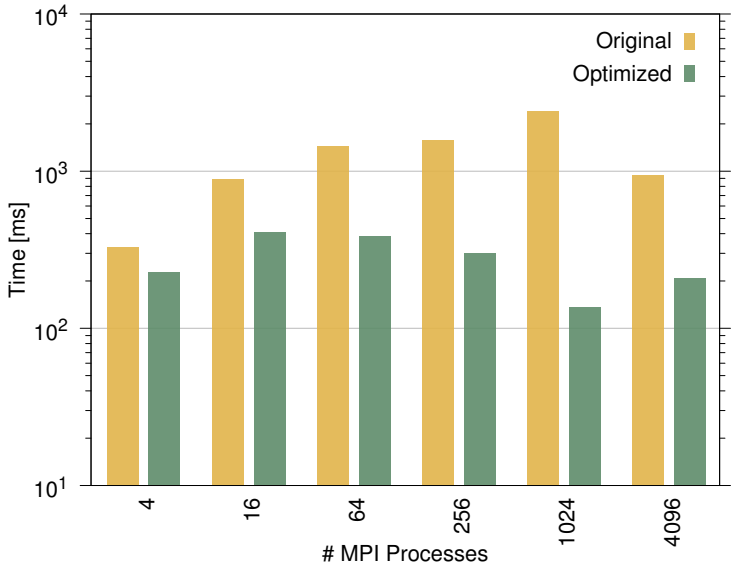
Issue 3: Communication Costs

Intra-Node:
Ordering of Cells Impacts Cache Behavior



Solution:
Use space-filling curves to explore different cell orderings

Inter-Node:
Communication Frequency Adds Overhead



Solution:
Aggregate communication, represented by benchmark

Issue 4: Indirection Increases Instruction Count

Performance Issue: Significant structure indirection inside loop nests

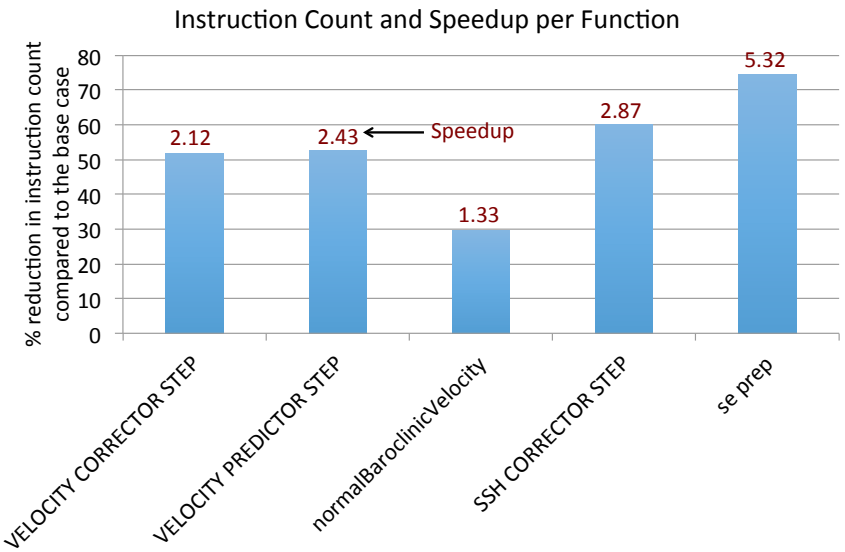
block%mesh%cellsOnEdge%array(1,iEdge) block%mesh%cellsOnEdge%array(2,iEdge)

Solution: Replace with pointer buffers that point directly to array

```
block => domain%blocklist
do while (associated(block))
  !...
    do iEdge=1,block%mesh%nEdges
      cell1 = block%mesh%cellsOnEdge%array(1,iEdge)
      cell2 = block%mesh%cellsOnEdge%array(2,iEdge)
      !...
  end do
  block => block % next
end do  ! block
```

Pointer buffer Auto-generator

```
! define Pointer buffers
real(kind=RKIND),dimension(:,:),pointer :: cellsOnEdge
block => domain%blocklist
do while (associated(block))
  ! associate pointer buffer to target variable
  cellsOnEdge => block%mesh%cellsOnEdge%array
  !...
    do iEdge=1,block%mesh%nEdges
      !Using pointer buffers to do calculation
      cell1 = cellsOnEdge(1,iEdge)
      cell2 = cellsOnEdge(2,iEdge)
      !...
  end do
  ! nullify the association when computation finished
  nullify(cellsOnEdge)
  ! deallocate buffers
  deallocate(cellsOnEdge)
  block => block % next
end do  ! block
```



Using pointer buffers in all functions: overall **1.16x** application speedup

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Applying Tools to SciDAC Codes, cont.

- Other code examples employing SUPER tools
  - XGC1
    - Performance measurement using TAU/CUPTI (also, HPC Toolkit and PerfExpert)
    - Conclusion: low IPC and high data accesses in PUSHE
    - Currently working on semi-automated generation of OpenACC directives
  - USQCD
    - Sub-optimal performance for quantum linear algebra
    - Rewrote to higher level and used CHiLL to regenerate low-level complex matrix-vector multiplies
    - Need to generalize to higher-dimensional lattices

NWChem TCE module

- Tensor Contraction Engine
  - implements approximations that converge toward exact solution of the **Schrödinger equation**
- libtensor
  - ***Key Challenge:*** Master-worker task parallelism of small BLAS calls, agnostic of NUMA and cache locality
  - Implementing NUMA measurement capability in PAPI to enable optimization of task scheduling

"Analysis and Tuning of Libtensor Library"
Khaled Ibrahim and Samuel Williams (Lawrence Berkeley National Lab)

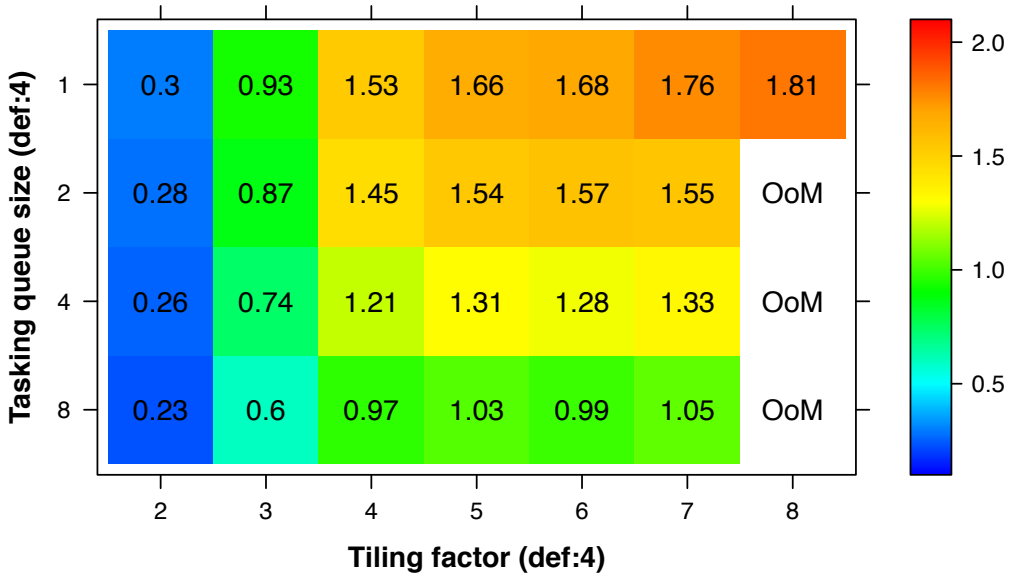
Objectives:

- Multicore architectures are imposing multiple challenges for scaling scientific applications.
- This work aims at identifying performance bottlenecks in multiple quantum chemistry chemistry frameworks.
- Expose challenges in quantum chemistry codes to computer scientist.

Impact:

- Tuning scientific codes leads to performance improvement and efficient execution.
- Make domain scientists focus efforts on the chemistry research rather than computational aspects.
- Allow computer scientists to explore efficient techniques to increase the productivity of developing codes for quantum chemistry computations.

Performance improvement on 24 core Intel Ivy-bridge (Edison)



Progress and Accomplishments:

- **More than 1.8X improvement in performance on 24-core Ivy-bridge system. More than 2X improvement on AMD Magny-Cours.**
- **Speedup improvement from 9.5x to 15.3x on 24 core Intel Ivy-bridge.**
- **Results and techniques to be published.**

Conclusion

- SUPER creates the opportunity for state-of-the-art performance tuning to be applied to SciDAC applications (e.g., MPAS-Ocean).
- SUPER fosters a community of performance tuning researchers, informed by the needs of application programmers.
- SUPER performance tools have been integrated, and are continuously extended to meet these needs.