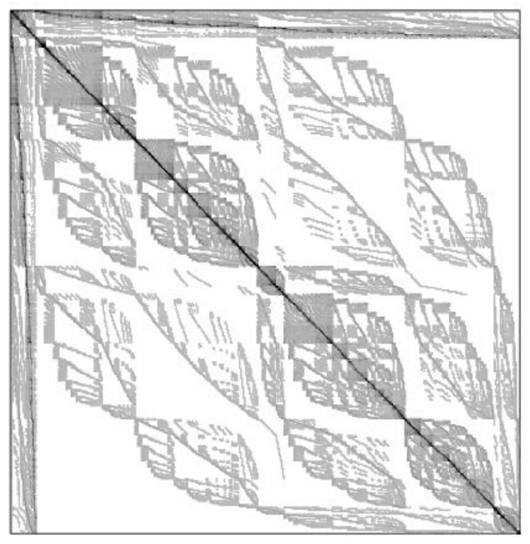
SUPER Performance Auto-Tuning and MPAS-Ocean Optimization

SUPER INSTITUTE FOR SUSTAINED PERFORMANCE, ENERGY, AND RESILIENCE

U.S. DEPARTMENT OF ENERGY | Office of Science

MFDn Application (NUCLEI)



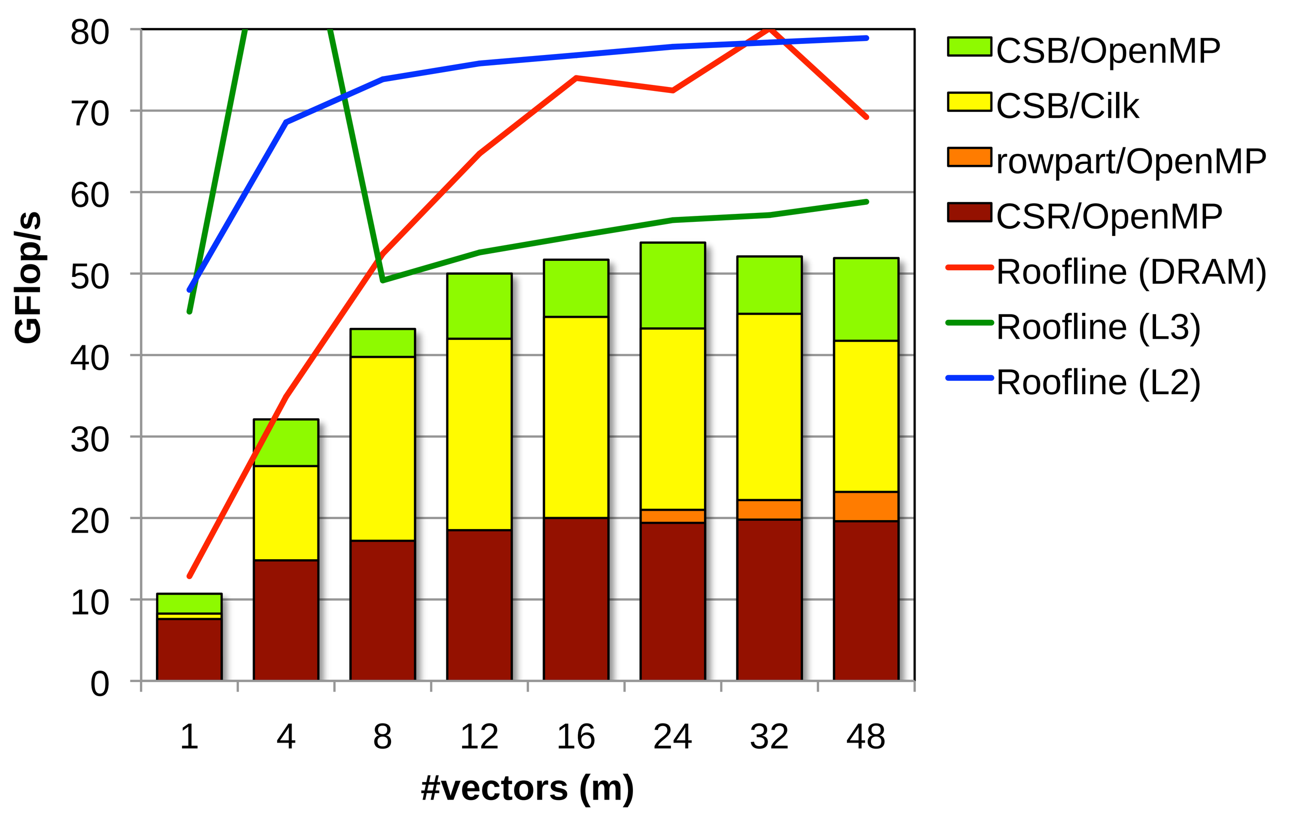
- Many Fermion Dynamics: Nuclear (**MFDn**) is used to calculate the properties of light atomic nuclei.
- Nominally, this requires an eigensolver like **Lanczos** which requires applying the operator repeatedly.
- MFDn forms the very large (**half a billion nonzeros per process**) symmetric configuration interaction matrix explicitly.
- As such, repeated application of the operator is particularly **bandwidth-intensive** and time-consuming.
- Symmetry further complicates this as it necessitates high performance SpMV and SpMV_T (transpose)

LOBPCG

- **LOBPCG is a block eigensolver** that restructures computation into a series of Sparse Matrix-Dense Matrix Multiplications (**SpMM**) where the dense matrix is tall and skinny (500,000 x 16 per process).
- Once again, symmetric necessitates SpMM_T (transpose)
- The advantage (assuming comparable convergence) is that one can reduce the number of times the matrix must be read by a factor of m (the number of vectors in block). **Ideally, this should result in a m-fold increase in performance.**
- Unfortunately, naïve implementations of SpMM and SpMM_T **failed to deliver the expected performance**.
- **SUPER collaborated with FastMath to model, analyze, and optimize these operations.**

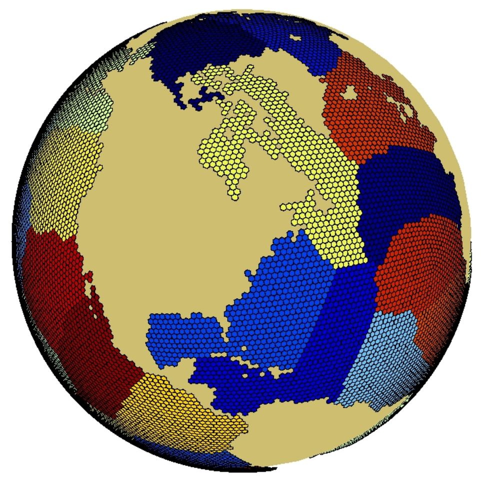
Compressed Sparse Blocks (CSB)

- Using the CSB data format, we tiled each local matrix into βxβ tiles.
- Through the use of CSB and tuning of β, we were able to improve performance by **1.5x for SpMM and 3x for SpMM_T**.
- Unfortunately, **performance seemed to saturate at m~12**
- We constructed a series of **Roofline Models** to capture the effects of limited L2 and L3 locality on finite L2, L3, and DRAM bandwidth.
- The result clearly shows when one can no longer maintain a working set of vector data in the L2 a transition from DRAM-limited to L3-limited performance

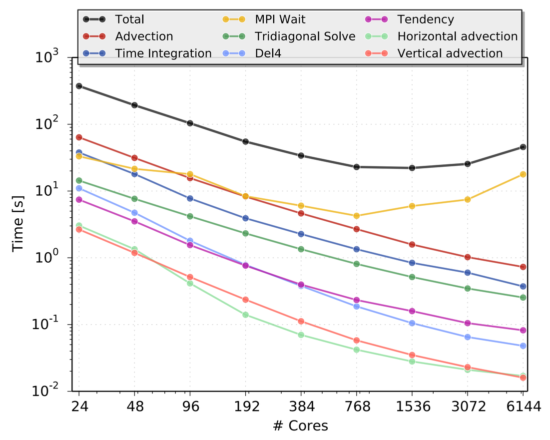


H. M. Aktulga, A. Buluc, S. Williams, C. Yang, **"Optimizing Sparse Matrix-Multiple Vector Multiplication for Nuclear Configuration Interaction Calculations"**, *2014 International Parallel and Distributed Processing Symposium (IPDPS 2014), May 2014*

MPAS-Ocean Application

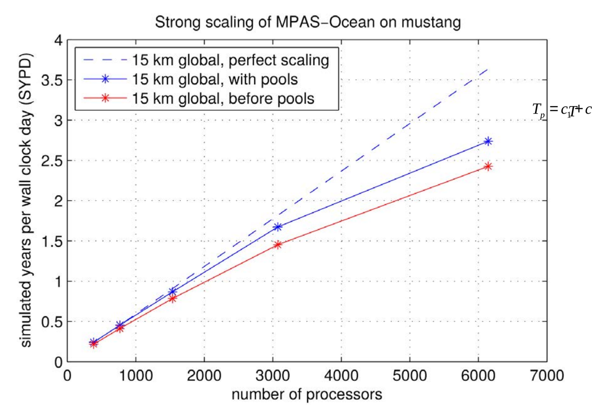


- The Model for Prediction Across Scales (MPAS) is a modeling framework for climate simulations.
- MPAS utilizes a fully unstructured mesh, which allows more flexibility in the description of the mesh locations.
- But it also has negative impact on performance due to multiple factors such as unordered data elements, irregular memory access patterns, mesh partitioning and communication imbalance.
- Regression analysis of scaling experiments shows scalability bottlenecks with runtime functions of the form $T_p = c_1 + c_2 * (T_1/p)$, where c_1 is a large constant, thus limiting scalability; investigating the reasons for this behavior.

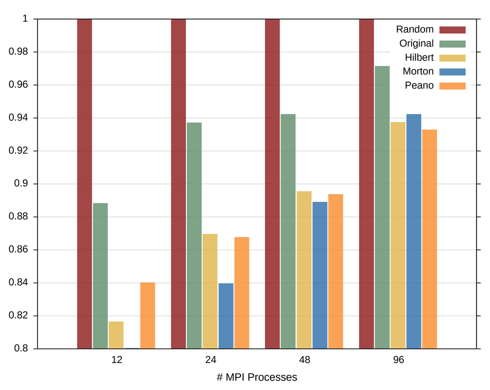


MPAS-Ocean Optimizations

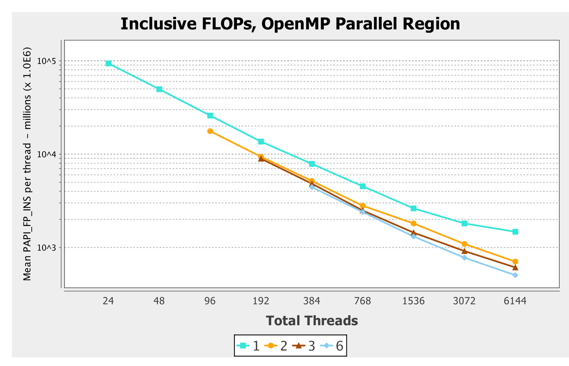
① To improve compiler-based vectorization of MPAS-Ocean, the data structures were rewritten utilizing hash tables. 10-15% performance improvement was achieved.



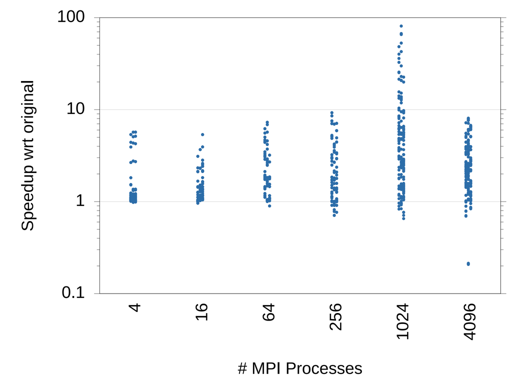
② Data element reordering based on Space Filling Curves was done to improve on-node cache performance. Up to 20% reduction in overall application runtime was observed.



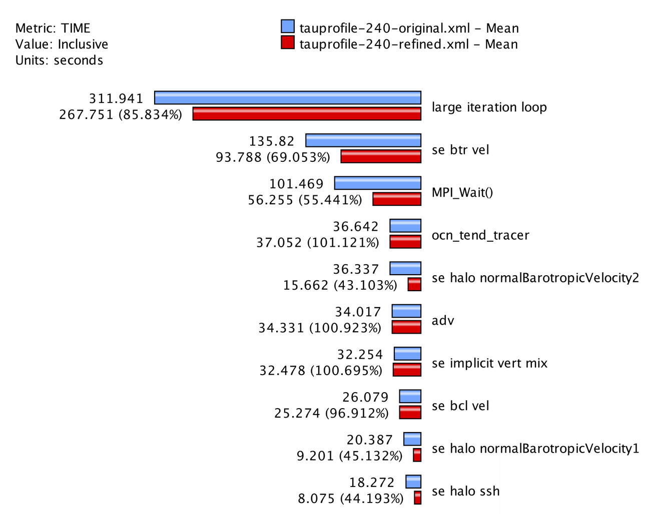
③ On-node threading using OpenMP was explored showing significant reduction in number of FLOP per core.



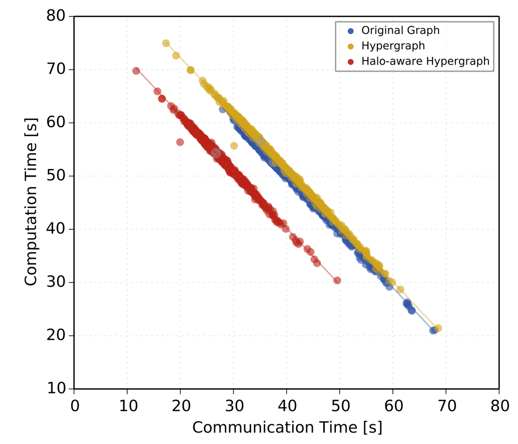
④ A benchmark for reorganization of halo-exchanges through data aggregation was written. Benchmark shows significant potential in communication performance improvement.



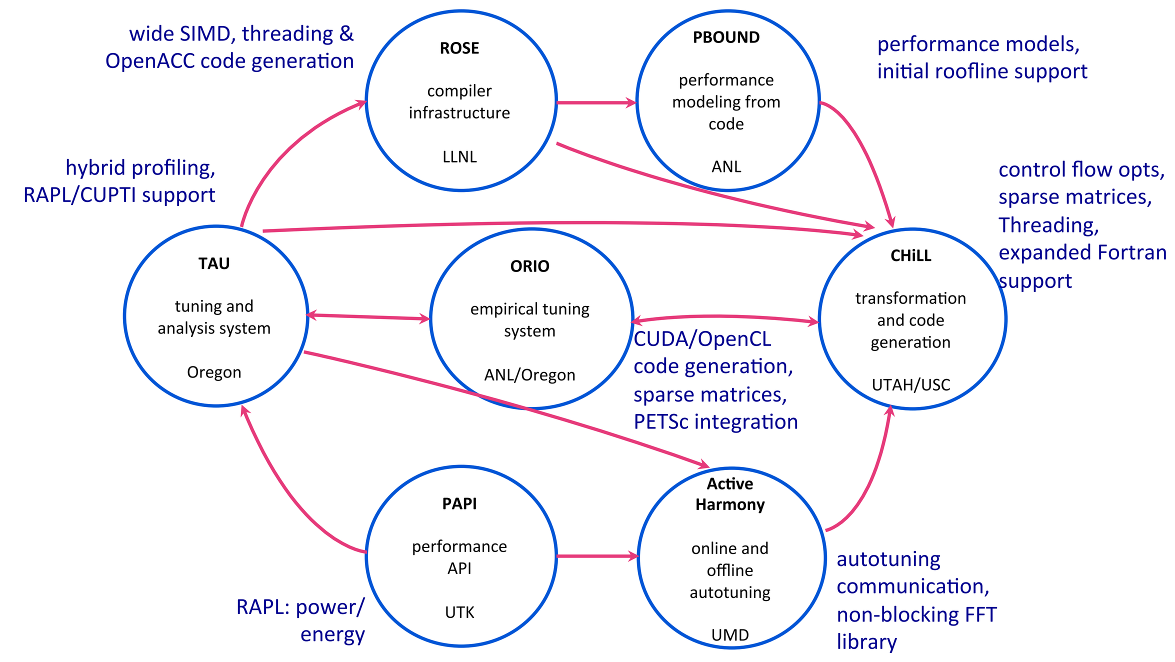
⑤ A new weighted graph partitioning scheme "Hindsight" was developed. About 10-15% reduction in overall runtime was observed.



⑥ A new weighted hypergraph-based and halo-aware partitioning scheme was developed. About 20% reduction in overall runtime was observed.



Autotuning Tool Integration

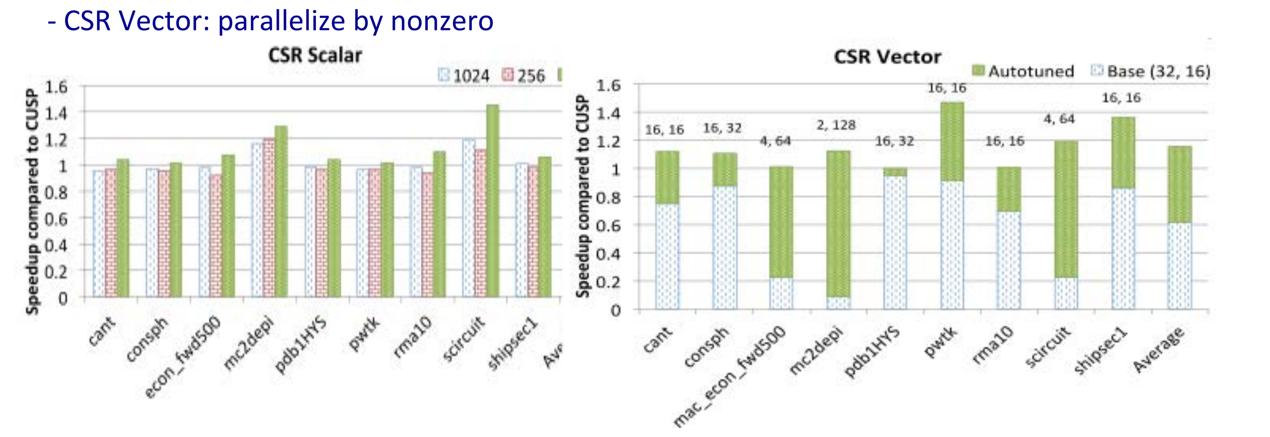


- Tools must support architectural changes and application requirements.
- Tools are extended in response to application tuning.

Example Extension: Sparse Matrices

GOAL: Extend compiler transformations and code generation to non-affine bounds and subscripts with index array. Compose with other transformations.

Performance comparison with manually-written CUSP library
- Using autotuning, outperforms CUSP
- CSR Scalar: parallelize by row
- CSR Vector: parallelize by nonzero



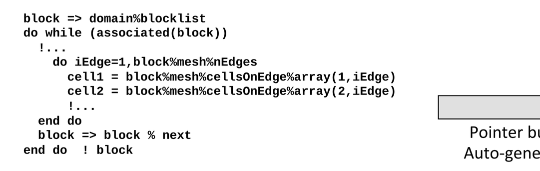
Supporting NUCLEI SpMM requires block sparse column representation and using OpenMP threading. These extensions are underway in CHiLL.

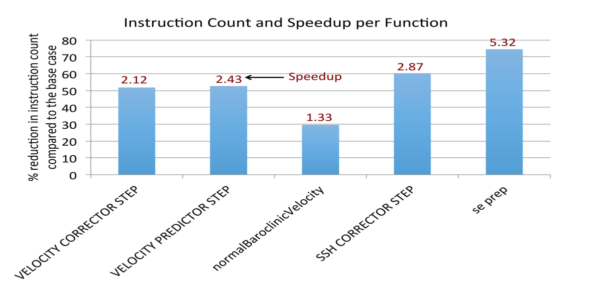
Example Tool for MPAS

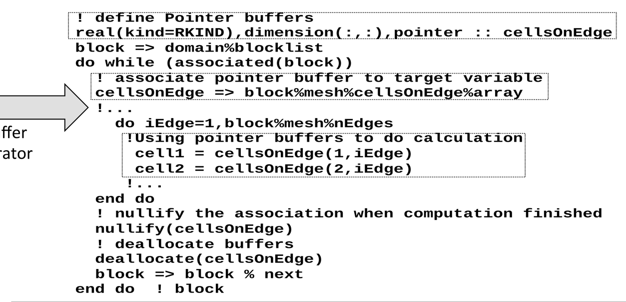
Performance Issue: Significant structure indirection inside loop nests

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

Solution: Replace with pointer buffers that point directly to array



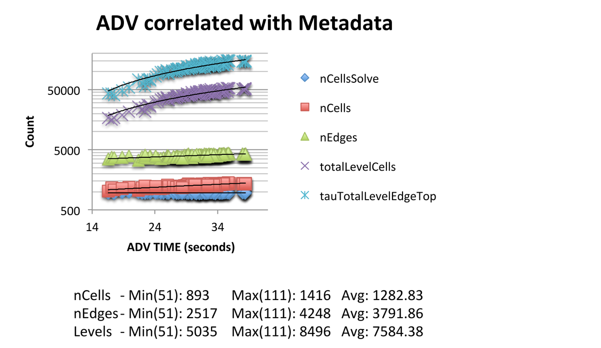


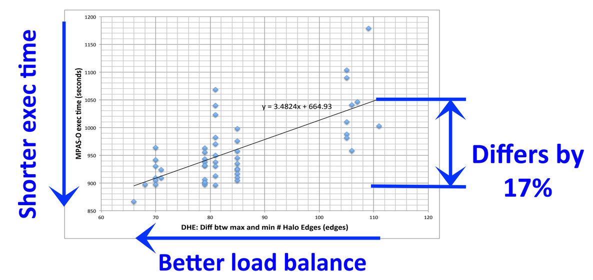


Using pointer buffers in all functions: overall **1.16x** application speedup

Autotuning Experiments for MPAS

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





- Conclusion:
  - Partition on nCell, but value unknown before partitioniing

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