OpenMP®

SC24 Booth Talk Series

AI/ML-Guided Auto-tuning for OpenMP

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Motivating Example Code: MPI-only

Needs: 1. Scientific Discovery 2. Engineering Innovation 3. service for Industry, AI/ML

stencil.cpp

```
#include <mpi.h>
int main(int argc, char* argv[])
{
  MPI_Init(&argc, &argv); // assume a weak scaling where each process gets n+2 elements
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  double* u = malloc(sizeof(double)*n+2);
  double* unew = malloc(sizeof(double)*n+2);
   int tstep = 0;
  while(tstep < 1000){
    if(myrank != 0) { MPI_Irecv(leftBoundary, …); MPI_Isend(leftBoundary, …);}
    if (myrank != (numprocs - 1)){ MPI_Irecv(rightBoundary); MPI_Isend(rightBoundary);}
    MPI_Waitall(...);  u[0] = leftBoundary;  u[n+1] = rightBoundary;


    for (i = 0; i < n+2; i++)
      unew[i] = (u[i-1] + u[i] + u[i+1])/3.0;

      MPI_Allreduce(err, MAX);
      tstep++;
  }

  MPI_Finalize();
}
```

Computational operation

Local operation

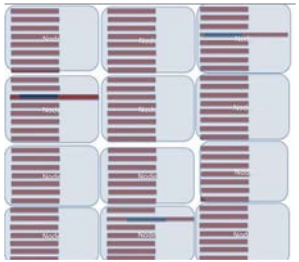
MPI communication operation

CC stencil.cpp -lmpich; mpirun -n 4 ./a.out 100 1000;

Platform: supercomputer, cloud

Slow OpenMP Prohibits MPI Scalability!

Time



Noise delays every timestep on some node[1,2]

Performance improves if we can perfectly redistribute work within each node[3]

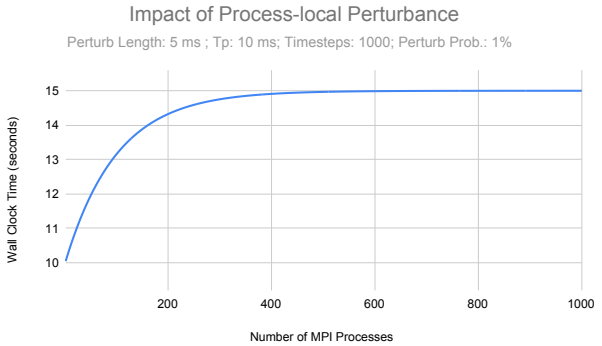
Example: 10 ms timestep, 10 of 1000 timesteps delayed by 5 ms

1 node

- Noise delay: 50 ms
- *Time with noise*: 10.05 seconds → 0.5% slower.

1000 nodes

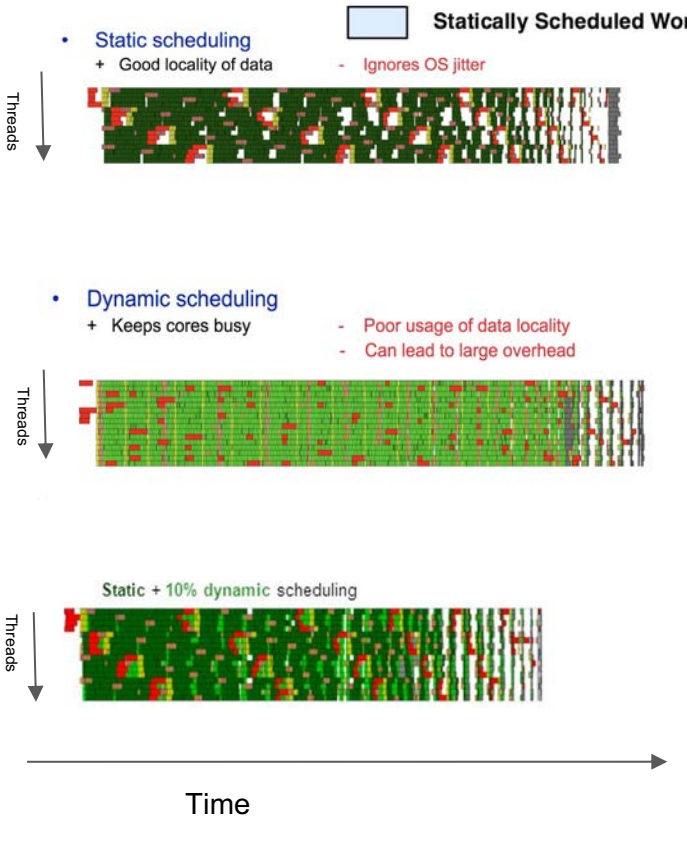
- Noise delay: 1000 x (1 - (1-.01^{1000})) x 5 ms = 4449 ms
- *Time with noise*: 14.449 seconds → 50% slower!

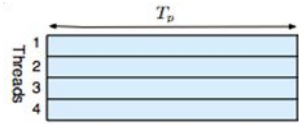


- Noise Amplification problem → Open CS problem: Wait-free consensus

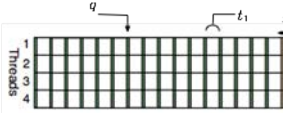
[1] Torsten Hoefler and Timo Schneider and Andrew Lumsdaine. Characterizing the Influence of System Noise on Large-Scale Applications by Simulation. International Conference for High Performance Computing, Networking, Storage and Analysis (SC'10). November 2010.
[2] Vivek Kale. Low-overhead Scheduling to Improve Performance of Scientific Applications. Dissertation. May 2015. University of Illinois at Urbana-Champaign.

AI/ML to Find Right OpenMP Strategy

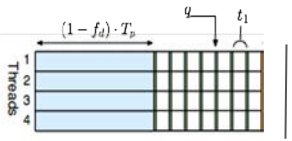





```
#pragma omp parallel for schedule(static)
     for(int i=0; i<n; i++)
               loop_body(i);
```




```
#pragma omp parallel for schedule(dynamic)
     for(int i=0; i<n; i++)
               loop_body(i);
```




```
double fd = predict_dynamic_fraction();
#pragma omp parallel for nowait
     for(int i=0; i< ceil((1.0-fd)*n); i++)
               loop_body(i);
#pragma omp parallel for schedule(dynamic)
     for(int i= ceil((1.0-fd)*n); i<n; i++)
               loop_body(i);
```

$$f_s \leq 1 - \frac{\delta_{total}}{T_P}$$

- More nodes means higher average delta

→ More nodes means best-performing f_s lower.

[3] Vivek Kale and Simplice Donfack. Lightweight OpenMP Static/Dynamic Scheduling for Scalable Numerical Linear Algebra. Arxiv. September 2020.

AI/ML guided OpenMP Performance Tuning

1. **Generate:** Identify new OpenMP algorithmic strategy's via defining control points
2. **Tune:** Tune each new strategy's control points
3. **Search**: find best-performing algorithmic strategy with best-performing parameters

→ *Token Generation Problems*[1]

→ Bayesian Statistical Models[2]

For the above to work, need:

1: Prototyping and experimentation

2: OpenMP features

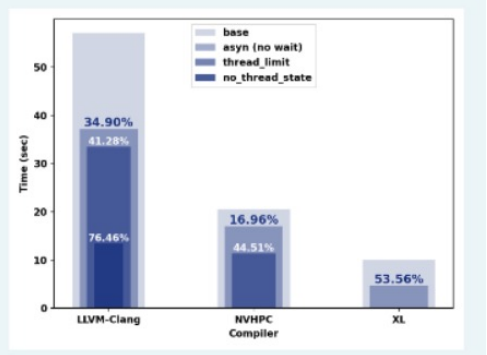
3: Software tools

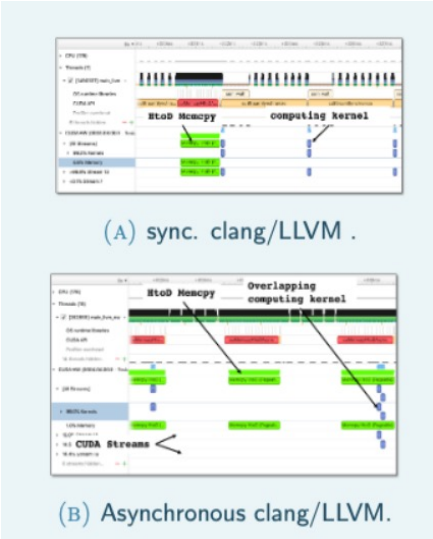
[4] Daejin Jo and Taehwan Kwon and Eun-Sol Kim. **Token Manipulation Generative Adversarial Network for Text Generation.** https://arxiv.org/abs/2005.02794
[5] X. Wu, M. Kruse, P. Balaprakash, H. Finkel, P. Hovland, V. Taylor, and M. Hall, "Autotuning PolyBench benchmarks with LLVM Clang/Polly loop optimization pragmas using Bayesian optimization (extended version)," Concurrency and Computation. Practice and Experience, Volume 34, Issue 20, 2022. ISSN 1532-0626 DOI: 10.1002/cpe.6683

1: Control Points for OpenMP Tuning

CPU-GPU Multi-parameter Tuning

- **Different Programming Models**
- **Tune**: {host-device coordination}

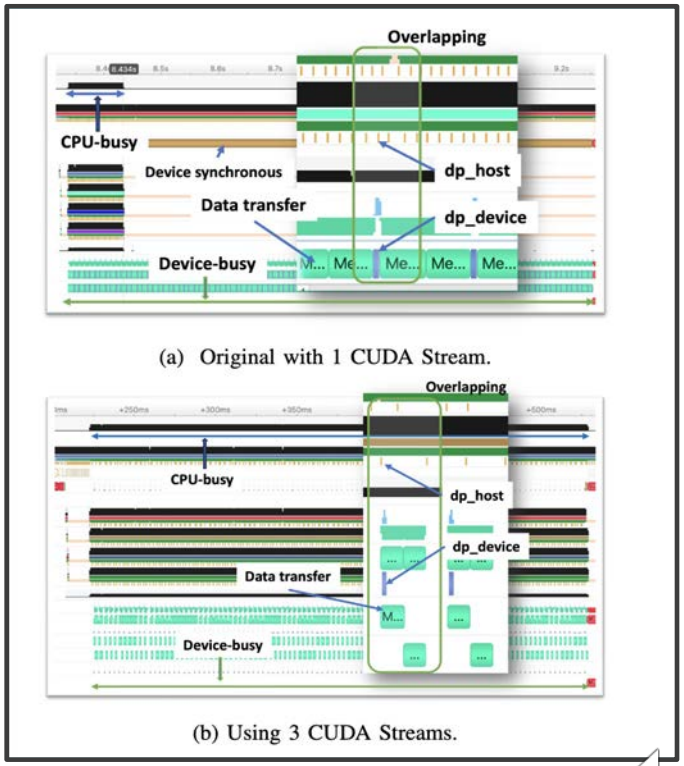




Stepwise tuning of asynchronous version of OpenMP offload program

[6] Mathialakan Thavappiragasam and Vivek Kale. **OpenMP's Asynchronous Offloading for All-pairs Shortest Path Graph Algorithms on GPUs**. IEEE/ACM HiPar 22 at SC '22. November 17, 2022. Dallas, Texas, USA.

- **OpenMP+CUDA**
- **Tune**: {intra-CPU and Intra-GPU} x {host-device coordination} x {host-device load balancing}

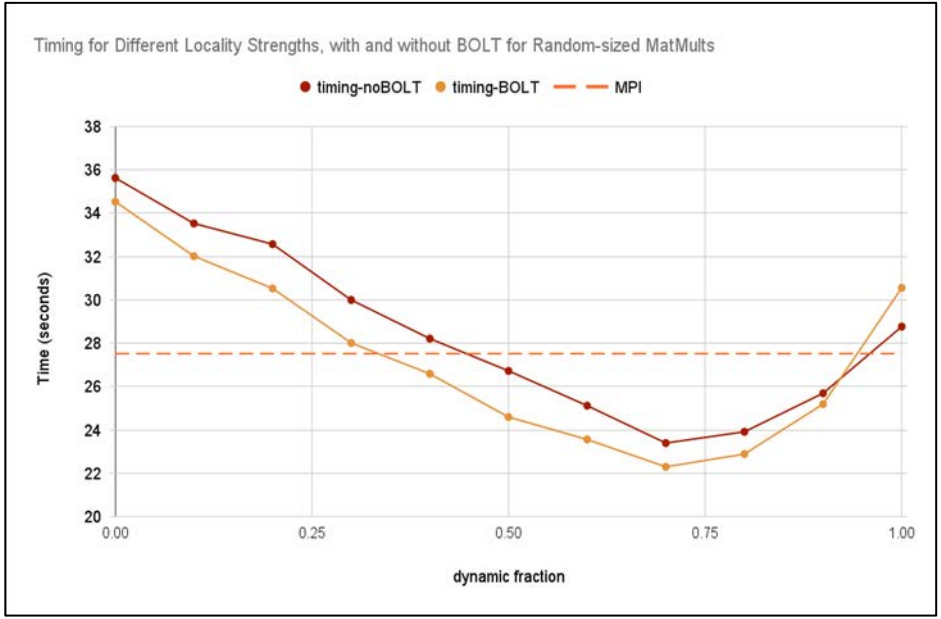


[7] Mathialakan Thavappiragasasm and Vivek Kale. ***CPU-GPU Performance Tuning for Impr... Performance of Modern Scientific Applications on Exascale Supercomputers.*** IEEE ...ational Conference on High-Performance Computing (HiPC) 2023. Goa, India. December 18-21, ...

National Nuclear Security Administration

Full Node Multi-Objective Multi-Parameter Tuning

- Randomized Mat Mul Summit
- GitHub for task-to-GPU scheduling prototype: github.com/SOLLVE/openmp-rts
- Experiments are done on node of Summit using clang15

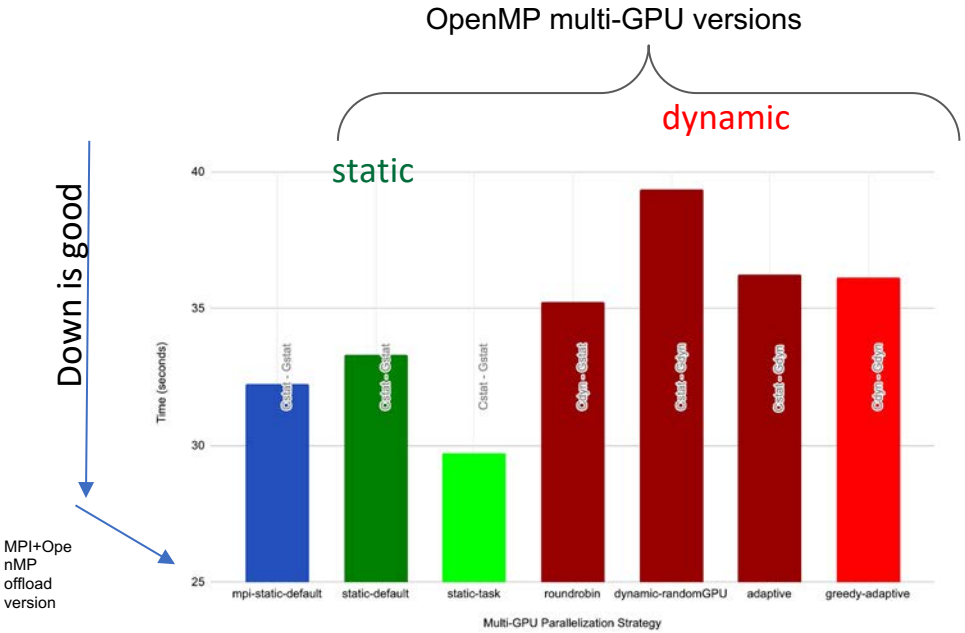


→ Prototype library for the LLVM OpenMP runtime that supports OpenMP task-to-multiGPU scheduling improves performance over OpenMP static by 43.6% and MPI version by 16.8% when affinity scheduling through low-overhead static/dynamic scheduling.

[8] Vivek Kale, Wenbin Lu, Anthony Curtis, Abid Malik, Barbara Chapman and Oscar Hernandez. ***Toward Supporting MultiGPU targets via taskloop and User-defined Schedules*** Proceedings of the 2020 International Workshop of OpenMP. September 23-25, 2020. Austin, USA.

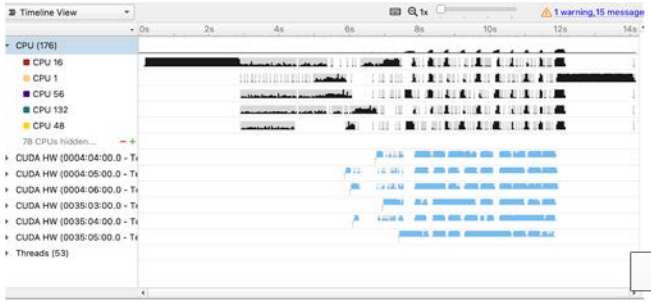
Multi-objective Multi-parameter Tuning: Heat2D

- **Application:** Stencil heat2D with problem size 32768 x 32768, 100 timesteps, Grain size 4
- **Platform:** Spectrum MPI, LLVM OpenMP , use '#pragma omp requires unified_shared_memory' , Perlmutter
- **Runtime params:** 1 OpenMP thread per core. For OpenMP multi-GPU versions, used 2 MPI processes per node. cpu to gpu binding.



Static-task

RandomGPU



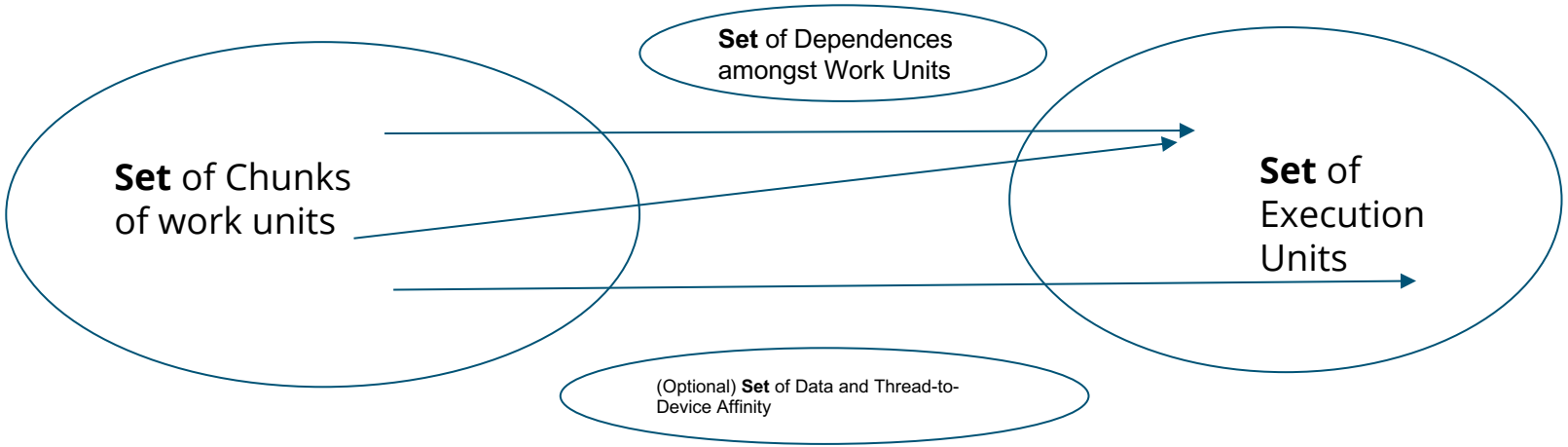
[9] Mathialakan Thavappiragasam, Vivek Kale, Oscar Hernandez and Ada Sedova. ***Addressing Load Imbalance in Bioinformatics and Biomedical Applications: Efficient Scheduling across Multiple GPUs.*** In Proceedings of 12th International Workshop on High Performance Bioinformatics and Biomedicine. December 9th, 2021. Houston, Texas

2: OpenMP Features for Enabling AI/ML Guided Tuning

OpenMP Set Object: A Way to More Easily Use AI/ML for OpenMP

- Augment OpenMP to be higher-level and consider node-level heterogeneity
- Can consider literature on parallel algorithm design[10]
- Define sets of entities to describe parallelization of computation in OpenMP:
  1. A **set** of (OpenMP) work units is distributed across
  2. a **set** of (OpenMP) devices/threads in way that is
     - constrained by a **set** of dependencies amongst work units and
     - aims to satisfy a **set** of OpenMP associations between work units and/or devices/threads. [11]

```
#pragma omp set(setName) [omp_list_t_kind: {listelemlist_id_1, listelemlist_id_2, listelemlist_id_n}]
```




```
#pragma omp set(myChunkSet) [chunk: {{0, 3}, {4, 7}, {8, 11}, {12, 15}}]
```

```
#pragma omp set(myThreadSet) [thread: {1, 5, 2, 3}]
```


[10] https://relate.cs.illinois.edu/course/cs554-f23/f/slides/slides_02.pdf
[11] Vivek Kale and Thomas R. W. Scogland. OpenMP Sets for Sustainable HPC Software Technology. Arxiv. Technical Report. September 8, 2023.

Putting it Together: Using Sets in OpenMP for Heterogeneous Programs

```
#pragma omp parallel num_threads()
#pragma omp single
{
 #pragma omp target spread(levelNum) teams distribute parallel for \
   set(devices:<[device_list]>,  <levelNum>)  set(chunks:  <chunk_list>)  spread_schedule(<levelNum>,
   <strategy>)
   map(close: to: A[omp_spread_start:omp_spread_size] ) \
   map(from:  B[omp_spread_start:omp_spread_size])
    depend(in:A[omp_spread_start:omp_spread_size]) nowait
    for (i = 0; i < n; i++)
      doWork(i);
  }
}
```

- Parallelism
- Work Sharing
- Loop Scheduling / Tasking
- Data dependences
- Communication
- Affinity

- **`spread_schedule:`** sets distribution `strategy` and `chunk size`; has all schedules from OpenMP in `schedule` clause of `parallel for` and can also take in set of chunk-to-device assignments, which is a user-defined schedule.

[12]Vivek Kale, Christian Iwainsky, Michael Klemm, Jonas H. Muller Kondorfer and Florina Ciorba. ***Toward a Standard Interface for User-defined Scheduling in OpenMP.*** Fifteenth International Workshop on OpenMP. September 2019. Auckland, New Zealand.

[13] Raul Torres, Vivek Kale, Abid Malik, Tom Scogland, Roger Ferrer and Barbara M. Chapman. ***Support in OpenMP for Multi-GPU Parallelism.*** The International Conference for High Performance Computing Networking, Storage, and Analysis. Extended Abstract and Poster. November 19, 2021. St. Louis, Missouri, USA.

3: Automation Tools for AI/ML Guided OpenMP Performance Tuning

From Manual to Automated Performance Improvement

1 Kokkos User Code

```
Kokkos::View<double> u(102);
Kokkos::View<double>::HostMirror host_u =
create_mirror_view(u);
Kokkos::parallel_for(0, 102, KOKKOS_LAMBDA(int i) {
unew[i] += (u[i] + u[i-1] + u[i+i])/3.0;}
);
swap(u,unew);
Kokkos::deep_copy(host_u, u);
```

Kokkos Library backends supporting user-defined hints

github.com/vlkale/kokkos

2 Manual, Rose-based clangASTRewriter, ORIO

3 Source-to-source code transformation
- based on user-defined hints
- contiains any transformation-specific runtime callbacks

4 Kokkosp_.. Callbacks Connector for parameter tuning and measurements

github.com/vlkale/kokkos-tools

4 Auto-tuning engine

5 Binary instrumented Code
- contains Kokkos Tools Callback invocations, which in turn call auto-tuning engine [8]

6 ./a.out 10000 1000;

6 Performance Optimization Report

[14] David Boehme, Kevin Huck, Shravan Kale, Vanessa Surjadidjaja, Vivek Kale. Sophisticated Tool Support to Aid Performance Portable Programming. SC 23. Extended Abstract and Poster. November 14, 2023. Denver, Colorado, USA.

Conclusion

- **Challenge**: large search space for OpenMP optimization for MPI+OpenMP
- **Opportunity**: AI/ML can prune large search space significantly
- **Approach**:
  - Training via experimentation of OpenMP strategies, identifying control points
  - Easier machine generation and tuning via OpenMP Set interface.
  - Search for best-performing OpenMP strategies via Kokkos Tools auto-tuning
- **Outcomes**:
  - 8.3x speedup via software tools appropriate control point transformations and tuning on single GPU; 1.7x speedup on multi-GPU experimentation
  - New OpenMP features and software tools for use.

Ongoing and Future Work

- More investigation of Kokkos Tools auto-tuning with OpenMP+CUDA
  - See new MDRange Tuning feature in APEX TPL at github.com/kokkos/kokkos-tools/ added July 2024
- Experiment with HPX + Kokkos and/or Charm++ + Kokkos → in progress with Kokkos-comm subproject of Kokkos
- Consider full-fledged applications for protein folding and weather simulation.
  - Early work in August 2024 on Kokkos-E3SM Scream to tune OpenMP team size parameter at runtime

Thanks!

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