**Activities and Impacts**

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### Xolotl/Paraspace Performance Comparison

**Phillip C. Roth**  
Oak Ridge National Lab

**Background**
- Developing Electron-Correlated Methods for Excited State Structure and Dynamics in the NWChem Software Suite  
- SDSC Supercomputer Partnership (PI: Christopher J. Cramer)
- Examined two important NWChem modules: Coupled Cluster Triples
- Performance of triples part of CCSD(T) improved 65x
- SUPER Institute collaboration to integrate OpenMP parallelism
  - Flat MPI only
  - Open source, publicly available via SourceForge

**Objective**
- Xolotl plasma surface interactions simulator
  - New code being developed as part of Plasma Interaction Surfaces FES SDSC Partnership (PI: Brian With)
  - Continuum model for solving cluster dynamics
  - Reaction-diffusion-reaction equation with incident flux
  - Support for 1D, 2D, and 3D problems
  - Uses PETSc solver
  - MPI only

**Activities and Impacts**
- Recently compared Xolotl performance and scalability against that of Paraspace
  - Paraspace: ParaSail SPAdes-dependent Cluster Evolution
    - Implements parallel cluster dynamics
    - reaction-diffusion-reaction equation with incident flux
    - Mature code, but limited to 1D and OpenMP only
  - Used both programs to simulate same problem simulation
    - Xolotl retention in Tungsten divertor wall with incident He flux of 4x10^15 H/atom/s for 1x10^6 seconds
    - Used several 1D code parallelizations (mainly nx=256, dx=0.25)
  - Ran on Eos, a Cray XC30 within the Oak Ridge Leadership Computing Facility
    - Two eight-core Intel E5-2670 processors at 2.6GHz per node, Hyper-Threading supported
    - 64 GB SDRAM per node
  - Xolotl outperformed Paraspace on full problem, scaled well when increasing problem size
  - Paraspace computes more time steps at higher accuracy (hypothesized)
  - Xolotl predicted Paraspace solver tolerances that reduce number of time steps but may also reduce accuracy
  - Working on threading/GPU optimizations for Xolotl
    - Targeting 1D and 3D problems
    - Little improvement expected for 1D problems including the one used in this performance comparison

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### NWChem OpenMP Threading

**Honghoong Shin, Bert de Jong, Lorenz Ceder, Samuel Williams**  
Lawrence Berkeley National Lab

**Background**
- Developing Electron-Correlated Methods for Excited State Structure and Dynamics in the NWChem Software Suite  
- SDSC Supercomputer Partnership (PI: Christopher J. Cramer)
- Examined two important NWChem modules: Coupled Cluster Triples
- Performance of triples part of CCSD(T) improved 65x
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**Objective**
- NWChem OpenMP Threading
- NWChem CCSD Data-flow Implementation
- MPAS-Ocean Performance Data

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### NWChem CCSD Data-flow Implementation

**Anthony Davais, Heike McGehee, George Bosilca**  
University of Tennessee

**Background**
- NWChem's CCSD has been converted to a data-flow representation

**Objective**
- Increase scalability and performance by porting CCSD of NWChem to a data-flow representation

**Activities and Impacts**
- Performance improvement of dataflow version (executing over PaRSEC) in comparison to original code for CCSD.
- The modified code yields 2x higher performance and keeps scaling until all 16 cores of all 64 nodes have been utilized in contrast with original code.

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### MPAS-Ocean Performance Data

**Kevin Hsu, (SUPER), Hank Childs (SDSC), Allen Malony (SUPER)**  
University of Oregon

**Background**
- MPAS-Ocean core uses Voronoi tessellation based unstructured grids.
- It has the benefits of providing multi-resolution and quasi-uniform grid properties at the same time to facilitate better simulations.
- Structured grids have a negative impact on performance due to factors such as non-obvious domain decomposition, parallel load imbalance, unbalanced load and irregular memory access patterns.
- MPAS-Ocean utilizes deep halo regions on the grid. These magnify the load imbalance factor significantly.
- MPAS-Ocean performance was analyzed on DOE supercomputer, Edison, a Cray XC30 at NERSC.

**Objective**
- Developed a weighted halo-aware grid partitioning scheme based on iterative refinement of the partitions using halo information. Using hence generated grid partitioning resulted in improved scaling at high concurrencies.

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### Analysis and Visualization of MPAS-Ocean Performance Data

**Kevin Hsu, (SUPER), Hank Childs (SDSC), Allen Malony (SUPER)**  
University of Oregon

**Background**
- SUPER and SDSC collaboration.
- Objective was to Map TAU performance measurements to the MPAS-Ocean spatial domain to assist in optimization of partition strategies

**Activities and Impacts**
- Demonstrated that the load imbalance problem is correlated with variability among partition block size due to relatively large halo regions
- Visualizations also show that vertical depth, coastlines and number of neighbors affect performance, communication times

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