First OpenMP Users Monthly Telecom of 2021

Oscar Hernandez & Dossay Oryspayev
Friday, February 26, 2021
Who's attending today

- OpenMP ARB (openmp.org)
  - Michael Klemm (CEO), Matthijs van Waveren (Marketing Coordinator)

- Compiler vendor reps
  - AMD - Ron Lieberman, Ethan Stewart
  - ARM - Graham Hunter
  - HPE/Cray - Deepak Eachempati, Jeffrey Sandoval
  - IBM - Wang Chen
  - Intel - Xinmin Tian, Alejandro Duran
  - Mentor Graphics - Catherine Moore
  - NVIDIA - Graham Lopez

- Exascale Computing Project (ECP) SOLLVE/OpenMP Team
Who's attending today (cont.)

- ECP Application teams
  - Application development (AD)
- Application teams from OpenMP hackathons
  - August 2020 and January 2021
- Some DOE Facilities application teams were invited
- CORAL-2 Application Readiness Teams (CAAR)
- Organizations: Ames Laboratory, ANL, BNL, Boeing, University of Bristol, University of Colorado Boulder, Iowa State University, Indian Institute of Technology Hyderabad, LANL, LBL, Linaro, LLNL, NASA Ames Research Center, NAG Ltd., ORNL, PNNL, PPPL, and University of Delaware.
Application Engagement, Training, and Outreach

- Training activities part-funded by ECP Broader Engagement
  - Disseminate best practices of latest OpenMP features
  - In-depth interactions between SOLLVE and apps
  - Tutorials at ECP, ISC, IWOMP, SC
  - Webinars on latest features
  - OpenMP Performance Portability P3HPC breakout sessions/user-engagement
  - Hackathons
    - August 2020 and January 2021
  - 5 ECP SC’20 OpenMP Booth talks (YouTube OpenMP Channel)
    1. SLATE: https://www.youtube.com/watch?v=bmz-NqihvVg&feature=youtu.be
    2. GAMESS: https://www.youtube.com/watch?v=9_nYCijgrn4&feature=youtu.be
    3. GESTS: https://www.youtube.com/watch?v=qHIRjFBhsY&feature=youtu.be
    4. GenASiS: https://www.youtube.com/watch?v=VhHlIN_z-nLA&feature=youtu.be
    5. QMCPACK: https://www.youtube.com/watch?v=iPGMYVViQzI&feature=youtu.be
  - ECP OpenMP Redmine Issue Tracking System:
    - openmp-ecp.ornl.gov/redmine
OpenMP Applications, Mini-apps, Frameworks, and Scientific Libraries

- Applications
  - QMCPACK Quantum Monte Carlo
  - QCD Molecular Dynamics
  - GAMESS Electronic Structure
  - ExaStar Astrophysics
  - XGC Particle Physics
  - GESTS CFD Turbulence
  - LSMS Materials Science
  - GenASIS Astrophysics

- Mini-apps
  - MiniQMC Quantum Monte Carlo
  - Grid Mini QCD
  - miniVite Graph Algorithm
  - MiniSweep Radiation Transport
  - SU3 Lattice QCD
  - AutoDock mini-app

- Parallel Programming Models, Frameworks, Co-Design, & Scientific Libraries
  - Kokkos C++
  - RAJA C++
  - AMReX AMR
  - CEED Particle
  - SLATE QCD

- ECP apps: SLATE, RAJA, QMCPACK, GAMESS, Grid, XGC
- ECP Parco 2020 Journal paper “OpenMP Application Experiences: Porting to Accelerated Nodes”
OpenMP Application Experiences

- Significant restructuring before applying any offload model
  - e.g., hoist conditionals, inlining functions, enough work to offload (like batching, fusion, etc.)
- High-level abstractions for data structures help the porting process
  - e.g., using container-like classes in C++ or Fortran storage classes
- Implementations are improving at a very fast rate
- There is a degree of tuning for specific accelerators
- Orchestration between CPU, GPU, and asynchronous libraries is done via tasking
- Need more tools to understand better mappings, code listings, etc.
  - requires unified_memory directive will help ease these challenges/debug
Topics

- Any OpenMP questions - no NDA discussions
- OpenMP gaps
  - In the context of directives, implementations, examples, and documentation
- Performance portability issues
  - Across systems, devices, and compilers
- Topics of interest to be discussed in Webinars
  - OpenMP 5.1 new features
  - Application experiences with OpenMP 5.1
- OpenMP.org user website - outreach
  - Agenda for upcoming telecons
  - Blog stories to share with the community
  - Highlights and outcomes
Topics (cont.)

- What is really needed to improve the adoption of OpenMP in applications
- Example of OpenMP specific topics:
  - Memory Management APIs
    - Dynamic allocators for GPU shared memory
    - Pinned memory to optimize data movement to an accelerator
  - Loop construct
  - Detach
  - Combining tasking with target
    - How to create pipelines
  - Fortran best practices to program devices
  - Interop - Interoperability with CUDA/HIP/SYCL
  - How to implicitly deal with GPU Streams and GPU shared memory
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Upcoming Events of interest (2021)

- ECP annual meeting, April 12 - 16 (https://ecpannualmeeting.com/agenda.php)
  - Vendor session - update on their roadmaps
  - User session - summary on their applications
  - OpenMP tutorial - focused on offload
  - Validation & Verification suite for OpenMP session
- ISC HPC, June 24 - July 2
- OpenMPCon, September 13 - 15
- IWOMP, September 15 - 17
- European OpenMP Users Conference, September
- Supercomputing, November 14 - 19
  - BoF (?), OpenMP Tutorials (?)