First OpenMP Users Monthly Telecon of 2021

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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
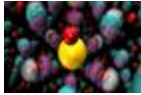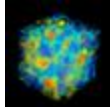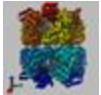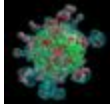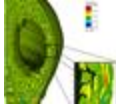
Who's attending today (cont.)

- 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
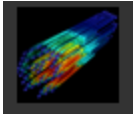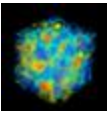
▶ **Training activities part-funded by ECP Broader Engagement**

▶ Disseminate best practices of latest OpenMP features
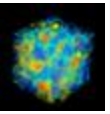
▶ In-depth interactions between SOLLVE and apps

▶ 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=qHIRjGFBhsY&feature=youtu.be
4. GenASiS: https://www.youtube.com/watch?v=VhHIN_z-nLA&feature=youtu.be
5. QMCPACK: https://www.youtube.com/watch?v=iPGMYVViQzM&feature=youtu.be

▶ http://phys.org/news/2019-06-scientific-applications-exascale.html

▶ ECP OpenMP Redmine Issue Tracking System:

    ▶ openmp-ecp.ornl.gov/redmine

OpenMP Applications, Mini-apps, Frameworks, and Scientific Libraries

▶ Applications

QMCPACK	QCD	GAMESS	ExaStar	XGC
Quantum Monte Carlo	Molecular Dynamics	Electronic Structure	Astrophysics	Particle Physics

GESTS	LSMS	GenASiS
CFD Turbulence	Materials Science	Astrophysics

▶ Mini-apps

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

▶ Parallel Programming Models, Frameworks, Co-Design, & Scientific Libraries

Kokkos	Raja	AMRex	CEED	SLATE
C++	C++	AMR	Particle	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 – <u>no NDA discussions</u>
- 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

General format

Date	Topics	Presenter
March 26, 2021	General Format: • Application experiences • OpenMP topics • Q&A	TBA
April 30, 2021	…	…
May 28, 2021	…	…
June 25, 2021	…	…
July 30, 2021	…	…
August 27, 2021	…	…
September 24, 2021	…	…

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 (?)