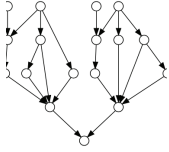
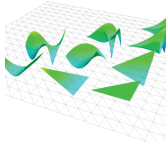
NUWEST: NNSA-University Workshop on Exascale Simulation Technologies



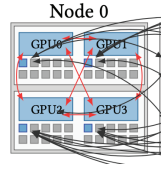


```
comm = comm1.COMM_WORLD
bufs = ...
requests = [comm.Irecv(
            for i, n in
            ]
# do other work
...

for i, r in enumerate(r
    r.wait()
    processFn(bufs[i])
```

$$\partial_r \mathbf{f} \approx \sum_{\ell=1}^{n} D_{i\ell} f_{\ell j}$$

$$\partial_s \mathbf{f} \approx \sum_{\ell=1}^{n} D_{j\ell} f_{i\ell}$$



Bill Gropp (CS/NCSA)
Luke Olson (CS)
Andreas Klöckner (CS)
Daniel S. Katz (NCSA)
Jonathan Freund (AE)

NUWEST's Goal

To share ideas on tools for facilitating exascale predictive science

- Showcase and characterize available technologies
- Identify challenges and limitations
- Provide opportunities to initiate collaboration

- Focus on sharing specific examples
- Invite PSAAP CS leads and small teams and similar # of lab personnel
- Focus on hands-on experience
  - we have tools to look at in detail
  - we have trans-petascale and soon exascale hardware models
- Participants in dual roles
  - Tool developer
  - Prospective tool user
  - *Not a rigid separation*

Guiding questions

- What ideas are working for actual simulations?
- Which pivots should be made?
- How are others thinking?
- What are lab needs?
- What are the tools like in detail?
- What are barriers for adoption of hardware-flexible tools?
- How do tools work with end-to-end simulation workflows?

What WEST Was

- WEST—Workshop on Exascale Software Technologies
  - Albuquerque, NM, January 27–28 (2016)
- An opportunity for PSAAPII Centers and DOE laboratories to interact

Participants:

- 19 LANL
- 15 SNL
- 12 LLNL
- 3 NNSA/Leidos/ASC
- 14 non-Illinois PSAAPII
- 6 Illinois/XPACC

Workshop on Exascale Technologies 2016
AGENDA

Speaker	Institution	Title	Time
Wednesday	**January 27**		
		Breakfast	**7:45 AM**
William Gropp	Illinois	Welcome and Charter	8:30 AM
Dave Richards	LLNL	Perspectives on Research and Production Tool Use from an Application Developer	8:45 AM
Gabe Rockefeller	LANL	Present Use and Future Needs for Tools in Integrated Code Development	9:00 AM
Mike Glass and Robert Hoekstra	SNL	Experience with Tools for Next Generation Platforms	9:15 AM
Martin Schulz	LLNL	Production and Research Development Tools for Current and Future Platforms	9:30 AM
Sam Gutierrez	LANL	Gladius: A Framework for Online Distributed Heap Analysis	9:45 AM
		BREAK	10:00 AM
Scott Pakin	LANL	Optimizing Applications for Future Hardware with Byfl	10:30 AM
David Boehme	LLNL	Caliper: Enabling Performance Annotations for Context_Aware Performance Analysis	10:45 AM
Sanjay Ranka	Florida	Autotuning and Multiobjective optimization for CMT NEK	11:00 AM
Carter Edwards	SNL	Kokkos: Performance portability for next generation HPC	11:15 AM
Alex Aiken	Stanford	Legion: Mapping and Analysis Tools	11:30 AM
Andreas Kloekner	Illinois	Loopy	11:45 AM
		Lunch	12:00 PM
Andrew Lumsdaine	Indiana	The Matrix Template Library: A generic programming approach to scalable linear algebra libraries	1:00 PM
James Sutherland	Utah	Spatial Ops/Nebo: A Domain-Specific Language for Portable Solution of PDEs on Structured Meshes	1:15 PM
Lawrence Rauchwerger	Texas A&M	TBA	1:30 PM
William Gropp		Description of breakout charge	1:45 PM
		Breakouts (5 rooms available)	2:00 PM
		BREAK	3:00 PM
		Breakouts continute	3:30 PM
		Breakout report	4:30 PM
		Adjourn for the day	5:00 PM
Thursday	**28-Jan**		
		Breakfast	**7:45 AM**
Arun Rodrigues	SNL	Performance Analysis and HPC System Simulation Tools	8:30 AM
Abhinav Bhatele	LLNL	Analyzing HPC Interconnects using Network Simulators	8:45 AM
Todd Gamblin	LLNL	Tools for Monitoring Entire HPC Centers: the Sonar Project at LLNL	9:00 AM
Sam White	Illinois	Charm++ & Adaptive MPI	9:15 AM
Jeremy Wilke	SNL	DHARMA: Distributed asyncHronous Adaptive and Resilient Models for Applications	9:30 AM
Abhishek Kulkarni	Indiana	HPX-5: An experimental platform for exascale runtime system research	9:45 AM
		BREAK	10:00 AM
Tarun Prabhu	Illinois	Moya: A JIT compiler for HPC	10:30 AM
Kathryn Mohror	LLNL	Scalable Checkpoint / Restart Library (SCR)	10:45 AM
Sam Gutierrez	LANL	QUO: Accommodating Thread-Level Heterogeneity in Coupled MPI Applications	11:00 AM
Stephen Olivier	SNL	Qthreads: A library for lightweight threading	11:15 AM
Dong Ahn	LLNL	HPC Debugging Made Easy: LLNL's Debugging Tools Strategy	11:30 AM
Todd Gamblin	LLNL	Spack: A Tool for Managing Exascale Software	11:45 AM
		Lunch	12:00 PM
		Breakouts (5 rooms available)	1:00 PM
		BREAK	3:00 PM
		Breakout report	3:30 PM
		Adjourn	4:30 PM

Agenda Proposal

- Keynote 1 [Bill Gropp, Illinois]
- Keynote 2 [NNSA Labs]
- Code-to-know-each-other
  - 2 min/1 slide per participant, prospective users and tool folks
  - Show a code snippet *representative of a difficulty* from day-to-day work
- Practical flash tool showcases (5 min each)
  - 1D Finite differences with MIRGE
  - (For example) Cholesky with Parla
  - (For example) Circuit simulation with Legion
  - UQ run orchestration with Parsl
- Parallel tool workshops: MIRGE/Parla/Legion/Parsl/... (e.g.)

Sample Tool Workshop Outline: MIRGE

- Conceptual Overview (2× 20 min, morning/afternoon)
  - *Idea:* Tensorflow for HPC/immutable arrays for everything
  - *Scientist interface:* arrays, array contexts, array containers
  - *Intermediate Representations:* Array data flow graph, loop IR
  - *Transform path:* metadata, metadata propagation, writing transforms
- Jupyter notebook code-along: 2D GPU finite differences using MIRGE (40 min)
  - Some Python, laptop and web browser suffice to participate
- Small group interactions: Bring your own code (3h drop-in window)
  - Facilitated by CEESD staff in the room

Sample Tool Workshop Outline: Parsl

- Conceptual Overview (2× 20 min, morning/afternoon)
  - *Idea:* Workflows as asynchronous Python code
  - *Predictive Science Applications:* Remote runs, pre-/postprocessing, UQ sampling
  - *Implementation:* 'Macro' graph of dependencies, scheduling, funcX, Globus
- Jupyter notebook code-along: run a model problem
  - Some Python, laptop and web browser suffice to participate
- Small group interactions: Bring your own code (3h drop-in window)
  - Facilitated by CEESD staff in the room

Staying Humble

No plan survives its first contact with ~~the enemy~~ code.

- Few if any (especially new) tools will ‘work’ smoothly/‘out of the box’ for new users!
- Two-way information flow is key:
  - Users meet tool developers, learn about possibilities
  - Tool developers meet users, learn about needs, obstacles, mismatches
- The point is to provide a space for those conversations to happen

NUWEST: Planning Plan

- CEESD lead organizers: Gropp, Olson, Klöckner, Katz, Freund
- Main supporting staff: M. Campbell, M. Smith, M. Diener, D. Friedel, plus CS students
- Develop and roadtest the CEESD part of NUWEST for NCSA
  - revise detailed plans based on that (especially for hands-on components)
- Summer 2023: pick final date/location (ABQ Jan 2024?)
- Do NUWEST!

Next steps

- PSAAP Centers:
  - Hopefully plan to present a tool and/or send user(s)
  - Someone from CEESD will be in touch with PIs
- NNSA Labs:
  - Keynote
  - Tool presenters
  - Users
  - Determine point-of-contact for each lab

Questions?

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