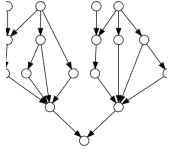
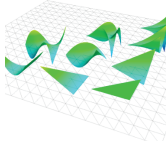
NUWEST: NNSA-University Workshop on Exascale Simulation Technologies

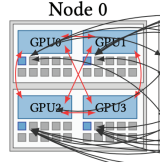




```
comm = comm1.COMM_WORLD
bufs = ...
requests = [comm.Irecv(
            for i, n in
            ]
# do other work
...
for i, r in enumerate(r
    r.wait()
    processFn(bufs[i])
```

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

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



January 18, 2024

Luke Olson
University of Illinois Urbana-Champaign

NUWEST's Goal

To share ideas on tools for exascale predictive science

- Showcase and characterize available technologies
- Identify challenges and limitations
- Provide opportunities to initiate collaboration
- Focus on hands-on experience — technologies to look at in detail

Schedule

https://illinois-ceesd.github.io/nuwest/

- Keynote 1 [Christian Trott, Sandia]
- Keynote 2 [Bill Gropp, Illinois]
- Conceptual Overview (4× 10–12 min, morning/afternoon) Ballroom
- Small group interactions: hands-on (2h window) In parallel

  Morning:
  - Scalable and portable HPC in Python using Parla and PyKokkos George Biros, University of Texas at Austin
  - Parsl - Python based workflow management Daniel S. Katz, Doug Friedel, University of Illinois Urbana-Champaign
  - Pragmatic performance-portable solids and fluids with Ratel, libCEED, and PETSc Jed Brown, University of Colorado Boulder
  - CUnumeric and Legion Charlelie Laurent, Stanford University
- View as 1 hour + 1 hour: try another session at the 1 hour mark!

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  Afternoon:
  - OpenCilk: A Modular and Extensible Software Infrastructure for Fast Task-Parallel Code Tao Schardl, Massachusetts Institute of Technology
  - MIRGE – A lazy evaluation framework in Python Andreas Kloeckner, University of Illinois Urbana-Champaign
  - MPI Advance - Optimizations and Extensions to MPI Purushotham V. Bangalore, University of Alabama
  - Acceleration and Abstraction of Python based Monte Carlo Compute Kernels for Heterogeneous machines via Numba Joanna Piper Morgan, Oregon State University
- View as 1 hour + 1 hour: try another session at the 1 hour mark!

Logistics

- https://illinois-ceesd.github.io/nuwest
- Contact Luke Olson (lukeo@illinois.edu) or
  Courtney McLearin (cmcleari@illinois.edu).
- See Slack for announcements
- 0800–0900 Keynotes
- 0900–1200 Morning session
- 1200–1300 Lunch (on site)
- 1300–1600 Afternoon session
- 1600–1700 Closing + collaboration time
- 1700–1900 Optional social @ Bow & Arrow Brewing Co.

Some questions to think about:

- What ideas are working for actual simulations?
- Any pivots needed?
- What are lab needs?
- What are barriers for adoption on conceivable hardware?
- How do tools improve with end-to-end simulation workflows?

Questions?

This material is based in part upon work supported by the Department of Energy, National Nuclear Security Administration, under Award Number DE-NA0003963.

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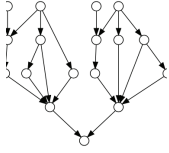

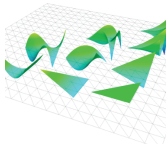

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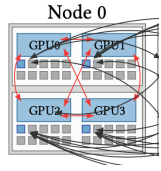

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Feedback:

`https://surveys.illinois.edu/sec/401981848`

- In the context of real, predictive simulation, what do you anticipate will be one or two pivots needed for new technology adoption. i.e., what will it take to effectively use technology XYZ?
- List barriers you see for adoption on conceivable hardware.
- List one or two lab needs not necessary covered or addressed by the suite of presented technologies.
- How do you foresee end-to-end simulation workflows impacting exacscale technologies? List one or two observations.

Take 3 minutes. . .

Thanks!

- Thank you for attending!
- Special Thanks to the speakers:
  - Christian Trott, Sandia
  - Bill Gropp, University of Illinois Urbana-Champaign
  - Charlelie Laurent, Stanford University
  - Daniel S. Katz, Doug Friedel, University of Illinois Urbana-Champaign
  - George Biros, Milos Gligoric, and Will Ruys, University of Texas at Austin
  - Jed Brown, University of Colorado Boulder
  - Joanna Piper Morgan, Oregon State University
  - Andreas Klöckner, University of Illinois Urbana-Champaign
  - Tao Schardl, Massachusetts Institute of Technology
  - Purushotham V. Bangalore, University of Alabama
- Thanks to the organizing team: Bill Gropp, Jon Freund, Andreas Klöckner, Dan Katz at Illinois
- Thanks Courtney McLearin at Illinois!
- Thanks to the PSAAP program and to the AST team for supporting this!