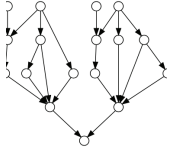
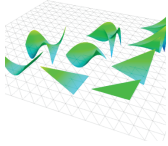
NUWEST: NNSA-University Workshop on Exascale Simulation Technologies

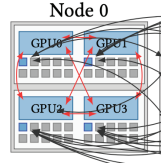




```
comm = comm1.COMM_WORLD
bufs = ...
requests = [comm.Irecv(
            for i, n in
            ]
# do other work
...
for i, r in enumerate(r
    r.wait()
    processFn(bufs[i])
```

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

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



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.

Feedback:

TODO

- In the context of real, predictive simulation, for the technologies you observed list one or two pivots needed for adoption. i.e., what would it take to effectively use technology XYZ?
- List any barriers 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.