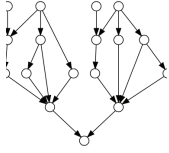
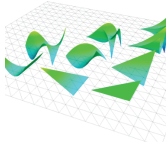
NCSA-WEST: NCSA-Workshop on Exascale Simulation Technologies



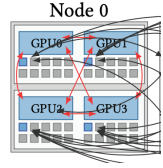


```
comm = comm1.COMM_WORLD
bufs = ...
requests = [comm.Irecv(
            for i, n in
            ]
# do other work
...

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

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

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



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What is this workshop about?

Goal: To highlight key technologies for facilitating exascale predictive science

- Showcase and characterize technologies in CEESD
- Identify challenges and limitations
- Provide opportunities to initiate collaboration at NCSA and beyond

Predictive Science Academic Alliance Program (PSAAP)

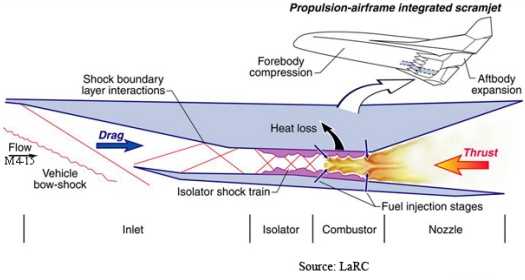
psaap.llnl.gov

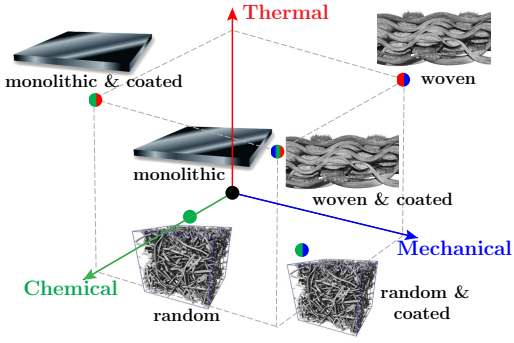
- . . . to further predictive science enabled by effective Exascale computing technologies;
- . . . technologies to support effective exascale computing in science/engineering; and
- Predictive science . . . for large-scale simulations

University of Colorado at Boulder	Center for Micromorphic Multiphysics Porous and Particulate Materials Simulations with Exascale Computing Workflows
University of Illinois	Center for Exascale-Enabled Scramjet Design
University of Texas at Austin	Exascale Predictive Simulation of Inductively Coupled Plasma Torches
Stanford University	Integrated Simulations using Exascale Multiphysics Ensembles
University at Buffalo	Center for Exascale Simulation of Hybrid Rocket Motors
Massachusetts Institute of Technology	Center for the Exascale Simulation of Material Interfaces in Extreme Environments
University of Maryland	Solution-Verification, Grid-Adaption and Uncertainty Quantification for Chaotic Turbulent Flow Problems
University of New Mexico	Center for Understandable, Performant Exascale Communication
Oregon State University	Center for Exascale Monte Carlo Neutron Transport

CEESD: The Center for Exascale-enabled Scramjet Design

- SCRAMJET — the technology for air-breathing hypersonics propulsion
- Employ light-weight, high-T composite materials to advance designs





- Predictive confidence: avoid costly/prohibitive testing, accelerate design and innovation

CEESD simulations

- Usability:
  Python-based simulation (performance with MIRGE)
  Python-based workflows (ease of execution with Parsl)

- Portability: Runs "out of the box" on most systems: performance with MIRGE, execution and job submission enhanced by Parsl

Mac/Linux
laptop/workstn.
AMD, Intel, M1, M2

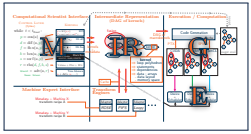
LLNL–Quartz
multi-core/node

LLNL-Lassen
4GPU/node

NCSA-Delta
4GPU/node

...

Exascale Technologies



Parsl

funcX

Center has utilized on and accelerated two key exascale tools:

- MIRGE: **M**ath · **I**ntermediate **R**epresentation · **G**eneration · **E**xecution
  - *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
- Parsl:
  - *Idea:* Workflows as asynchronous Python code
  - *Predictive Science Applications:* Remote runs, pre-/postprocessing, UQ sampling
  - *Implementation:* 'Macro' graph of dependencies, scheduling, funcX, Globus

Format

- Short (short!) overview on the MIRGE/Parsl vision
- Hands-on demos.

We want your feedback! What went well, what can be improved.

Questions?

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