PESO Workshop

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Challenges and opportunities for increasing the impact of DOE libraries and tools in collaboration with industry.

Challenges:

- Licensing – Not all licenses are created equal

- Benchmarking
  - Frequently comes in bursts around RFPs, difficult to *engage*
  - Meaningful benchmarks (right metrics, right software)
  - Addition of workflows, not just apps.

- Sustained collaboration
  - Frequently motivated by RFPs or other specific events
  - More regular cadence makes efforts less bursty and more sustained

Challenges and opportunities for increasing the impact of DOE libraries and tools in collaboration with industry.

Opportunities:

- Standardization – raises all boats, reduces support matrix, improves interoperability

- Semi-standards – Many math libraries serve as de-facto standards
  - Sparse Linear Algebra currently ripe

- Testing – DOE has an opportunity to lead
  - Composable software stacks (including vendor SW)
  - Mixed/reduced precision, letting go of the assumption FP64 is required

- Tools
  - Vendors often provide tools designed for their platform
  - DOE & community develop tools that support multiple platforms (multi-node, for instance)
  - These tools must work together

- Software distribution & Integration – Spack & Containers
  - Enables integration and testing of vendor & DOE software.
  - Simplifies user experience
  - Increasing important of Python ecosystem

- Resource management in complex workflows

- Emergent technologies
  - HPC + AI
  - LLMs
  - Quantum
  - …

NVIDIA.