

Building effective multidisciplinary teams: A Lab experience



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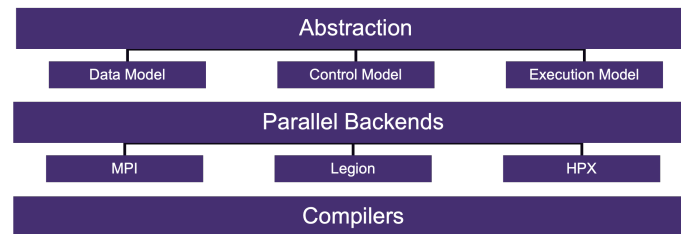
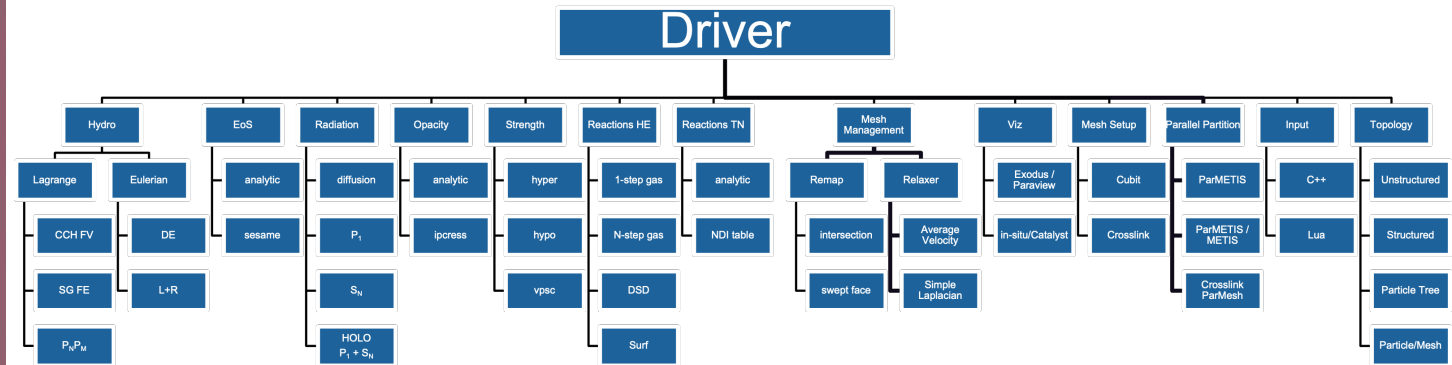
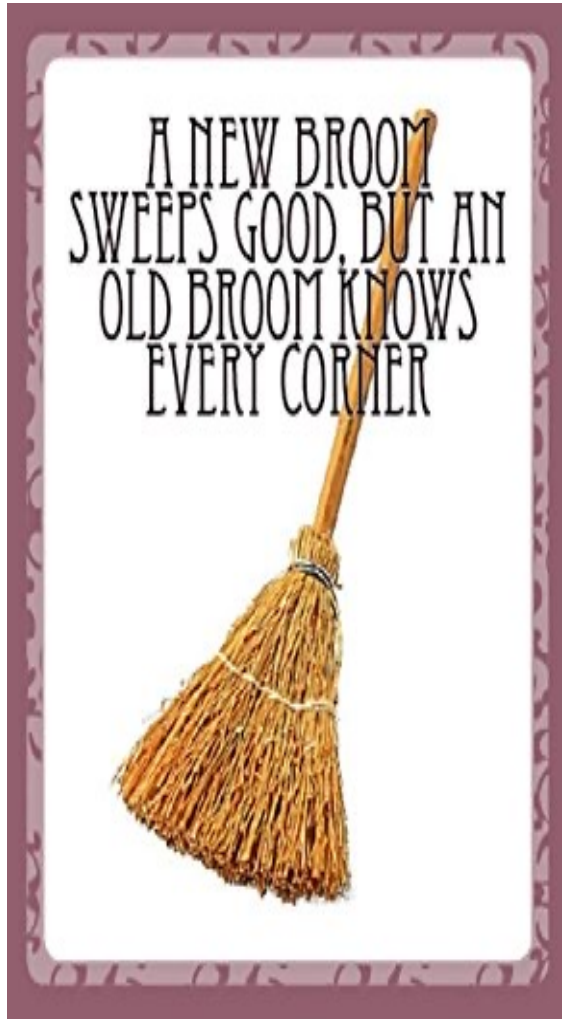


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Multiphysics code development teams face inherent tension

- New codes/alg's/env's to anticipate future physics, future computers
- Leveraging existing software to retain experience base



The reality is that both are done simultaneously:
adding new folks to existing efforts and combining existing efforts in new ways

Post-exascale challenges for future code capability

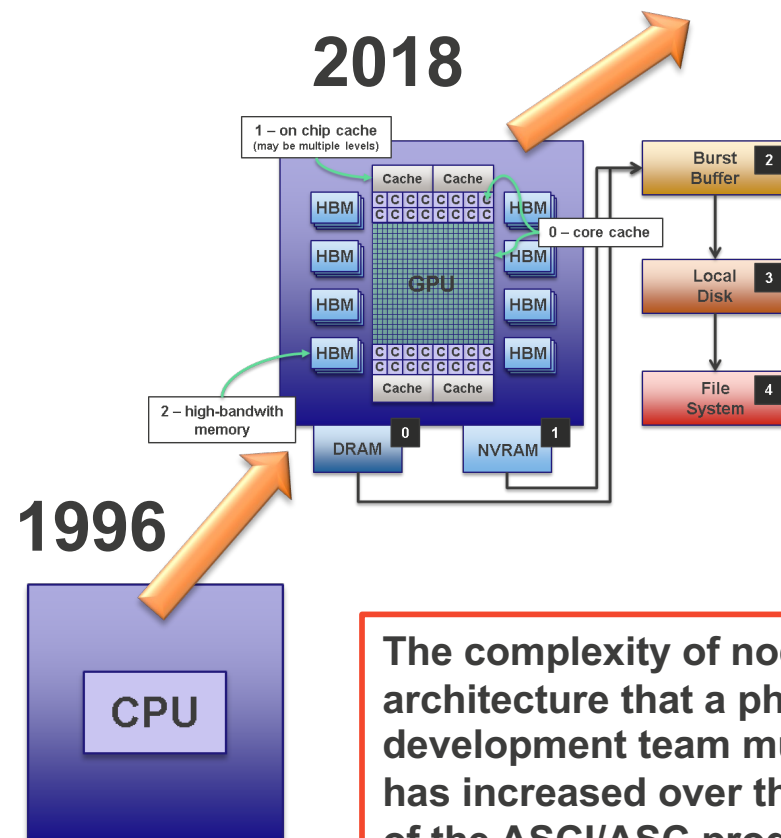
- Performance and productivity at extreme-scale
- Agile response to new scientific questions; integrating new physics

Change is driven by computing technology evolution: growth in scale, and node complexity

- **Massive parallelism of many-core/GPU nodes**
 - Leads to a push away from bulk synchrony
 - Task- and data-parallel programming models
- **Deep memory hierarchies (on node)**
 - Cache and scratchpad management
 - Challenge of spatial complexity in codes
 - *Need to get granularity of the tasks right*
- **Extreme scales**
 - Power, load balance, and performance variability
 - Reliability and resilience
 - Data management, and data analysis

Common theme: methods that can tolerate latency variability within a node and across an extreme-scale system

2028
?

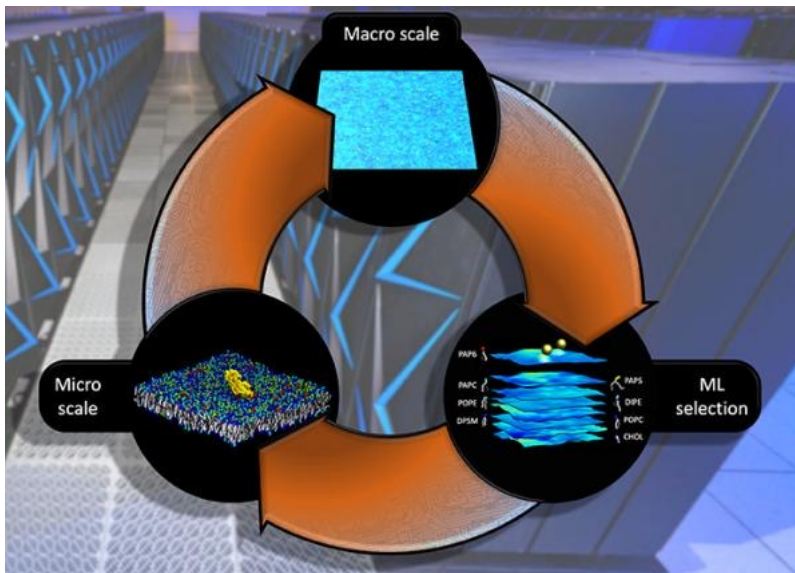


Multi-physics simulation has progressed beyond early stages

– Multi-scale methods as a path to higher fidelity physics

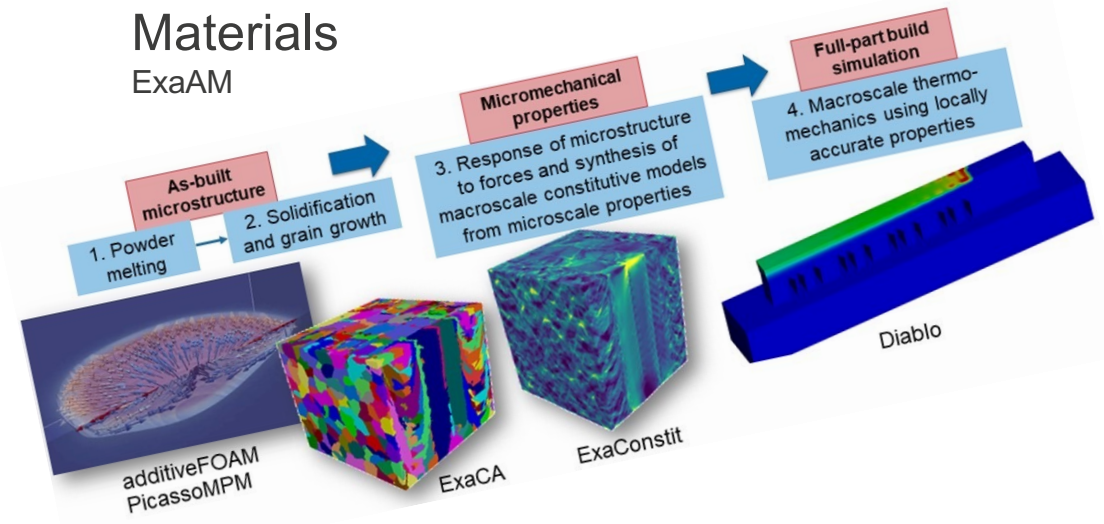
Biology

NCI-DOE Collaboration



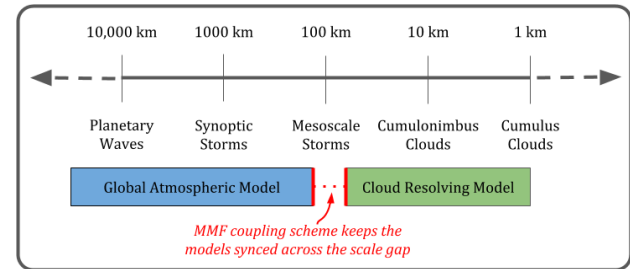
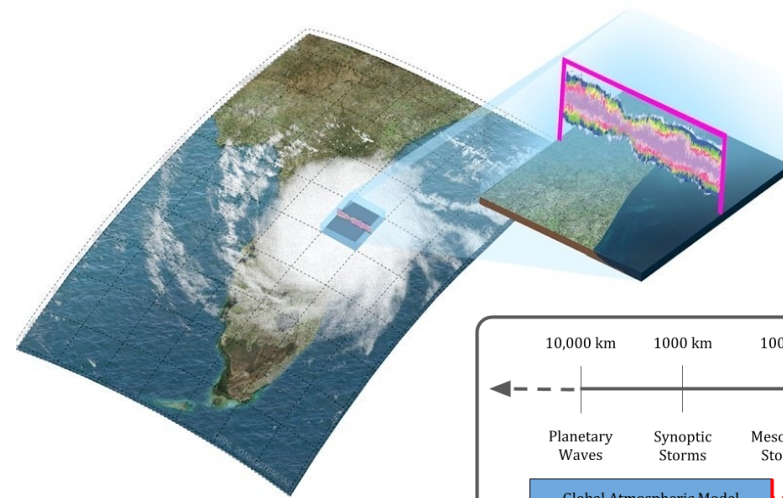
Materials

ExaAM



Climate

E3SM-MMF



Multi-physics simulation has progressed beyond early stages

– AI advances: fast surrogates, data driven workflows, in-line optimization



AI based surrogates for HPC

Climate Ensembles
Effective Zettascale on Exa

AI and robotics for autonomous discovery

Materials, Chemistry, Biology
Light-Sources, Neutrons

AI for software engineering and programming

Code Translation, Optimization
Quantum Compilation, QALgs

AI for prediction and control of complex engineered systems

Accelerators, Buildings, Cities,
Power Grid, Networks

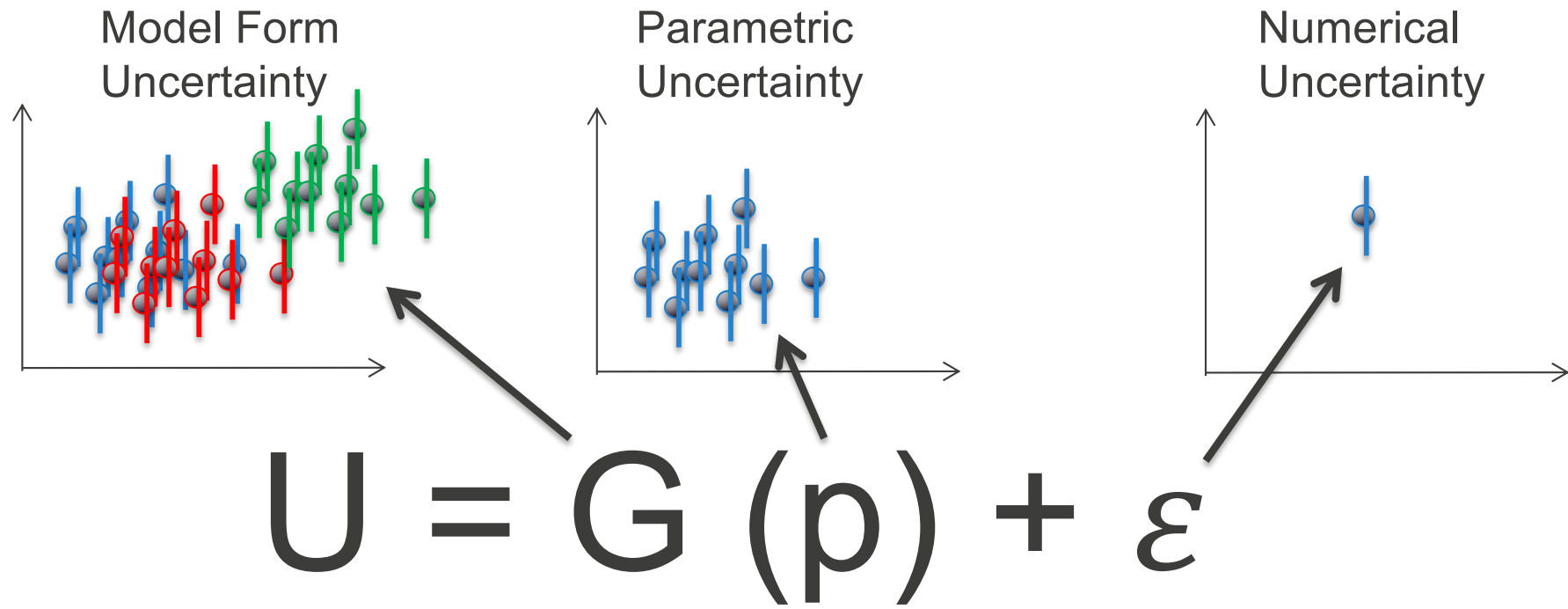
AI for advanced properties inference and inverse design

Energy Storage
Proteins, Polymers

Foundation AI for scientific knowledge

Multi-physics simulation has progressed beyond early stages

– *Model-form uncertainty studies benefit from a disciplined code modularity*



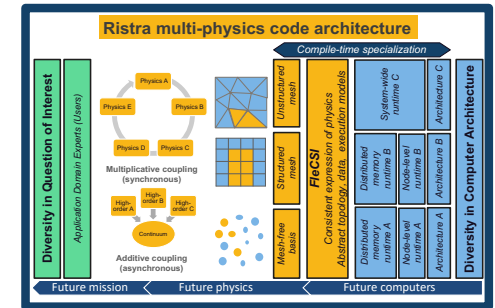
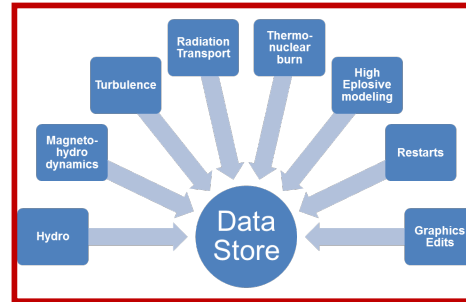
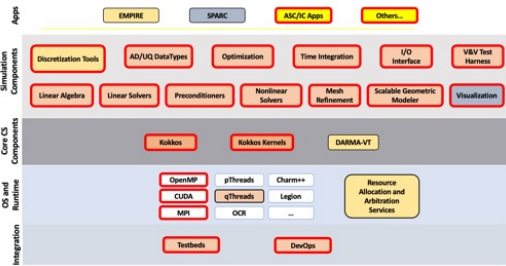
- **Experimental comparisons are a necessary ingredient for predictive science**
 - Experiments must quantify the errors
 - Simulations must quantify the uncertainty
- **Codes should be designed to enable straightforward fielding of a diverse set of physics algorithms**
 - Numerical and parametric uncertainty studies tend to be easier to accommodate
 - Model form uncertainty studies tend to be more invasive

ASC's Exascale Approach: NNSA ATDM Program

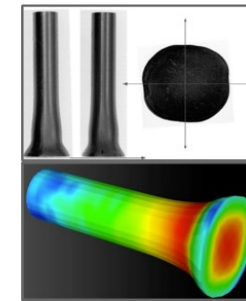
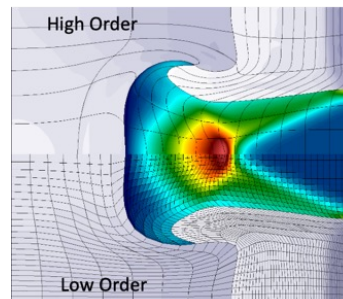
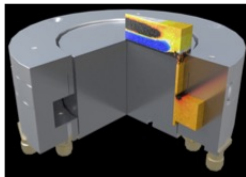
- Abstractions



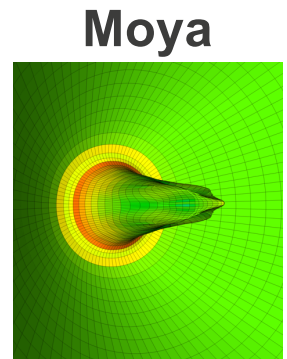
- Modularity



- Algorithms and Applications

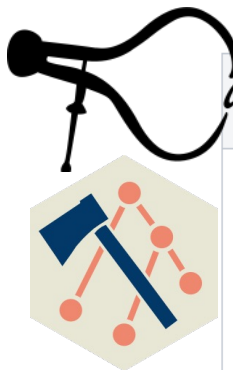
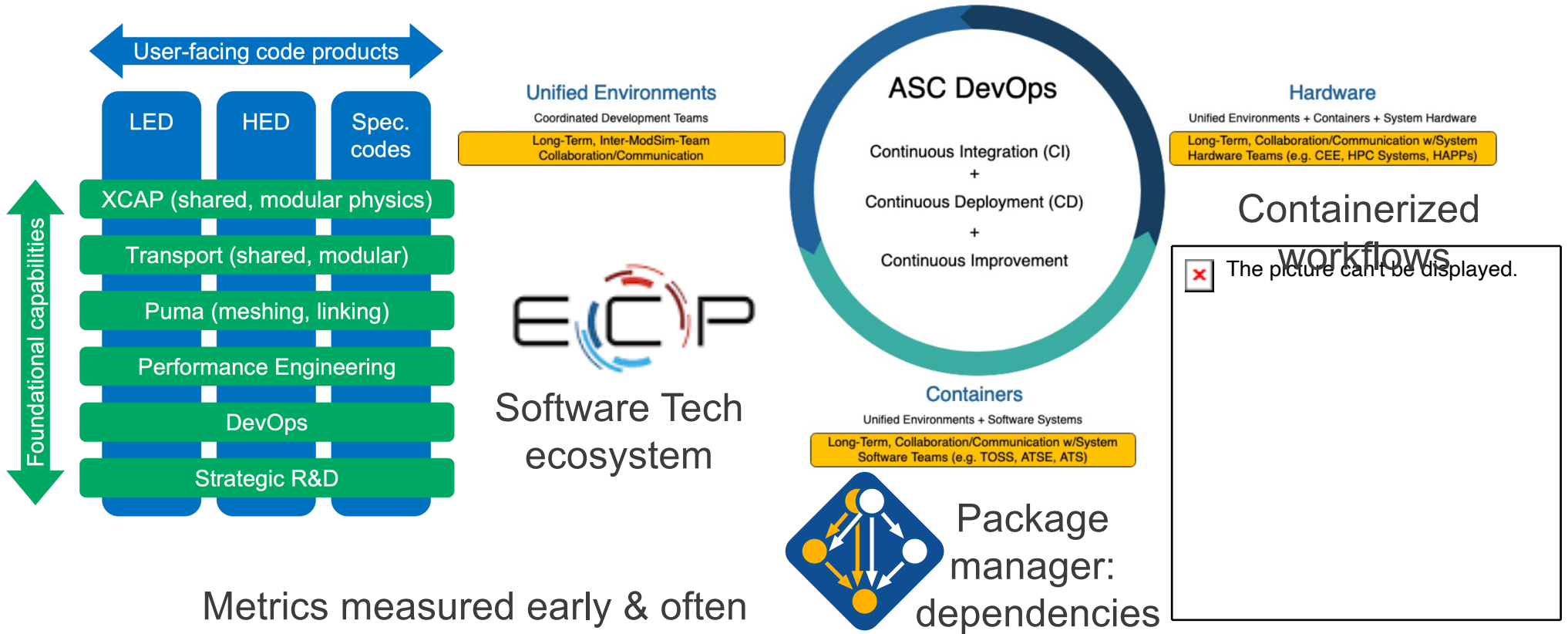


Symphony

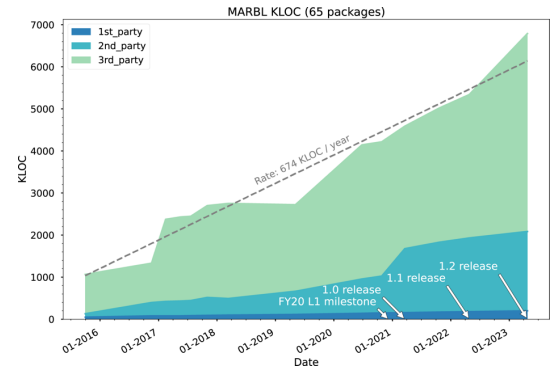


Moya

Technology for teams: tangibles



<i>aliper</i> 8 V100s	MI250X GCD Speedup (V100/MI250X)	8 MI250X GCDs
481.797 main 230.930 initialize 250.018 timeStepLoop 248.173 blast 83.388 Lagrange 84.638 Remesh 74.567 Remap	1.217 main 1.539 initialize 1.021 timeStepLoop 1.027 blast 0.922 Lagrange 1.285 Remesh 0.917 Remap	395.794 main 150.052 initialize 244.818 timeStepLoop 241.743 blast 90.464 Lagrange 65.850 Remesh 81.294 Remap

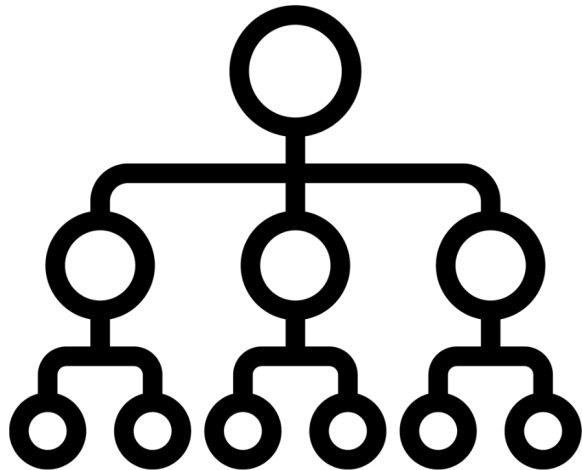


Defined software hierarchies:

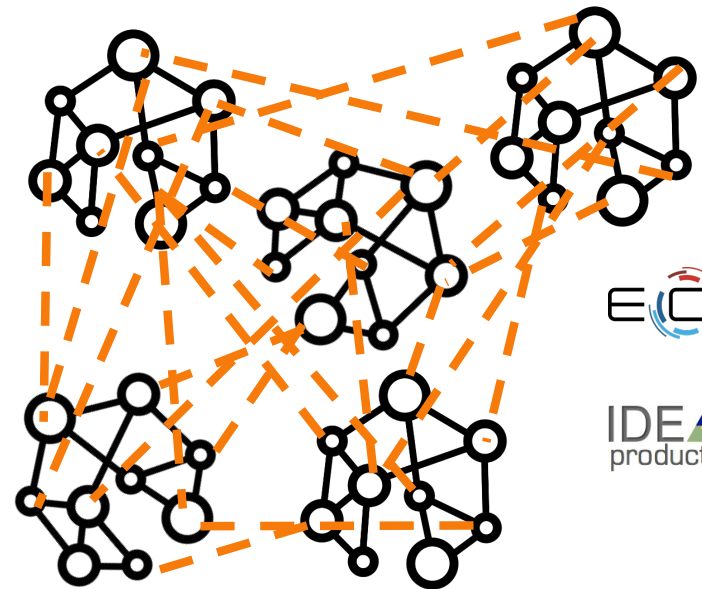
- 1st party
- 2nd party
- 3rd party

Leadership and culture of teams: intangible & invaluable

- **When the team is big enough to warrant software for coordinating parallel human effort → also big enough for culture clash!**
 - **Coding styles**
 - **Vocabulary / Jargon**
 - **Definition of “done”?**
 - research → productized
 - **Reporting requirements**
 - publications → informal conversations with Project Lead
 - **Communication avenues**
 - in person → social media
 - **Software development environments**
 - tar file → git repository



HIERARCHY



Bottom Line

- **Building multidisciplinary teams is one way to fill up a life**
 - Technically challenging
 - Socially challenging
 - Not just a challenge for the project lead, but every member
 - Make sure they know that
- **NNSA National Labs have tools and tricks (and traumas)**
 - We are the old brooms that know where all the dirt is!
 - Our origin story is that of team building

 - We are seeking new brooms!
 - ECP and PSAAP teams are also great resources