Introduction to Numerical Software

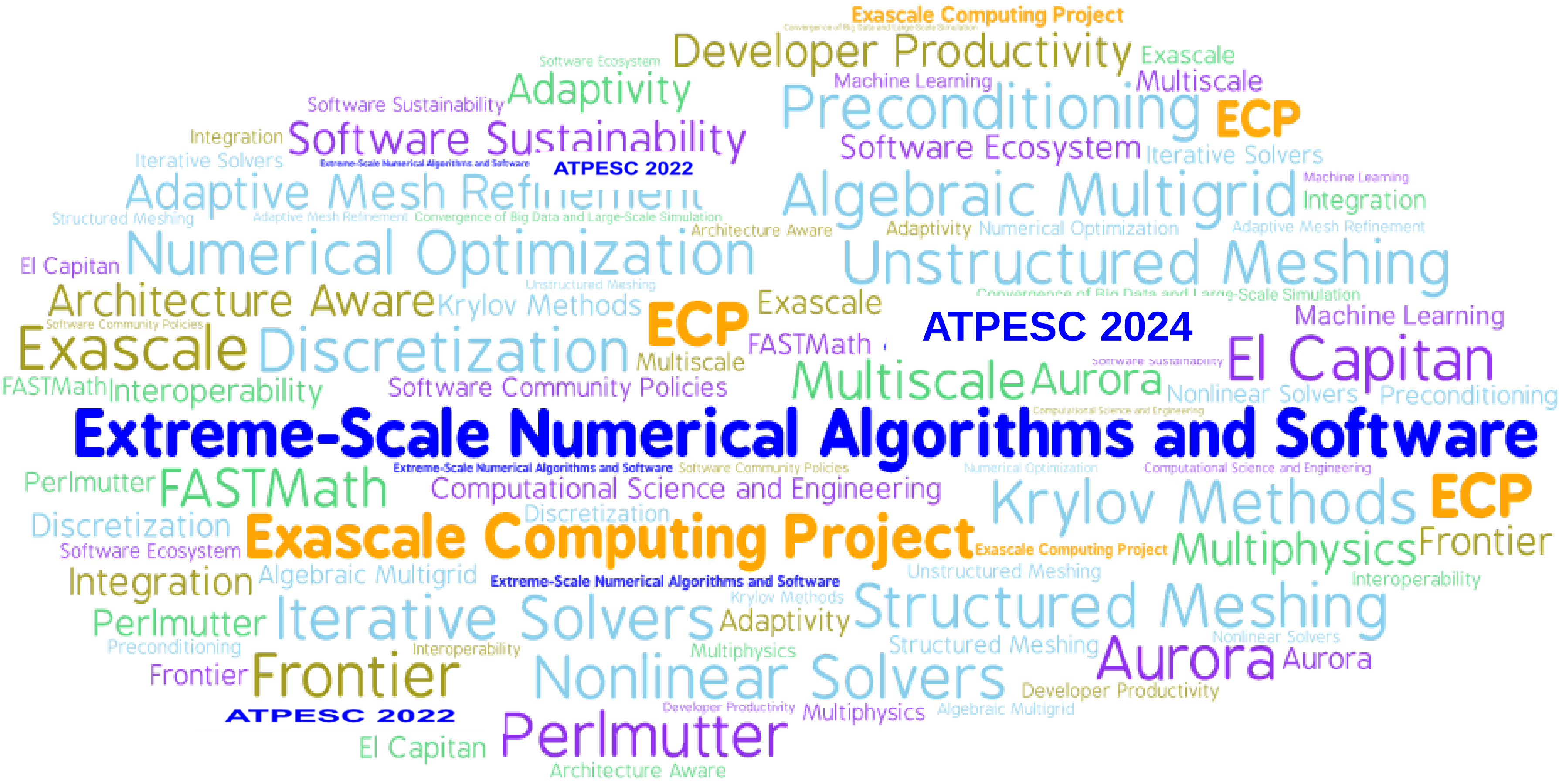
Presented to
ATPESC 2024 Participants

Ulrike Meier Yang
Lawrence Livermore National Laboratory

Date 08/06/2024

Outline

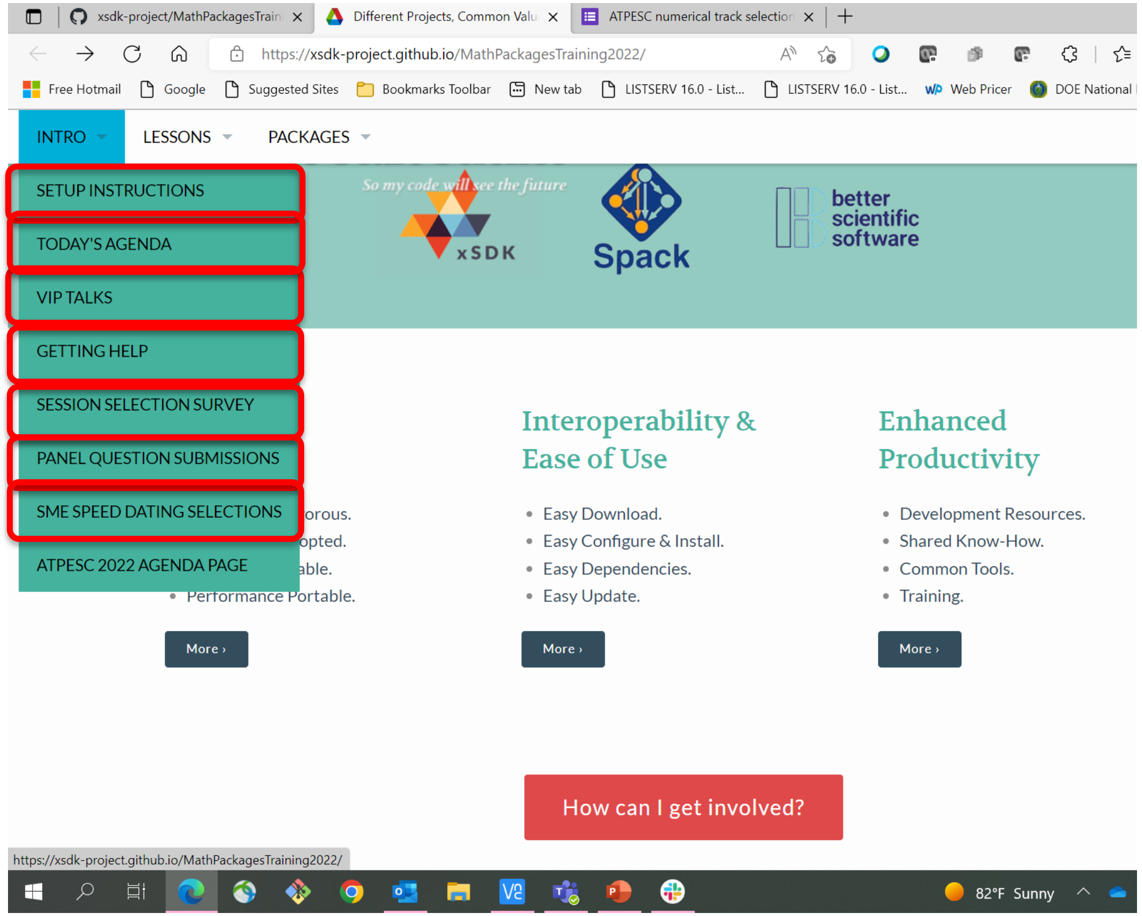
- Logistics for the day
- Intro to numerical algorithms and software for extreme-scale science



Your home bases for the day: ATPESC Track 5
Numerical Algorithms and Software for Extreme-Scale Science

- Main ATPESC Agenda
  - **https://extremecomputingtraining.anl.gov/agenda-2024/#Track-5**
  - slides (pdf) and presenter bios
- Math Packages Training Site
  - session abstracts, links to parallel breakout rooms, hands-on lessons, more
  - **https://xsdk-project.github.io/MathPackagesTraining2024/agenda/**

https://xsdk-project.github.io/MathPackagesTraining2024/


xsdk-project/MathPackagesTrain
Different Projects, Common Valu
ATPESC numerical track selection
https://xsdk-project.github.io/MathPackagesTraining2022/
Free Hotmail
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INTRO
LESSONS
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SETUP INSTRUCTIONS
TODAY'S AGENDA
VIP TALKS
GETTING HELP
SESSION SELECTION SURVEY
PANEL QUESTION SUBMISSIONS
SME SPEED DATING SELECTIONS
ATPESC 2022 AGENDA PAGE
So my code will see the future
xSDK
Spack
better scientific software
More ›
More ›
More ›
How can I get involved?
https://xsdk-project.github.io/MathPackagesTraining2022/
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- able.
- Performance Portable.

Interoperability & Ease of Use

- Easy Download.
- Easy Configure & Install.
- Easy Dependencies.
- Easy Update.

Enhanced Productivity

- Development Resources.
- Shared Know-How.
- Common Tools.
- Training.

- Setup instructions
- Today’s agenda
- VIP talks
- Getting help
- Session Selection Survey
- Panel question submission
- SME speed dating selections

Agenda

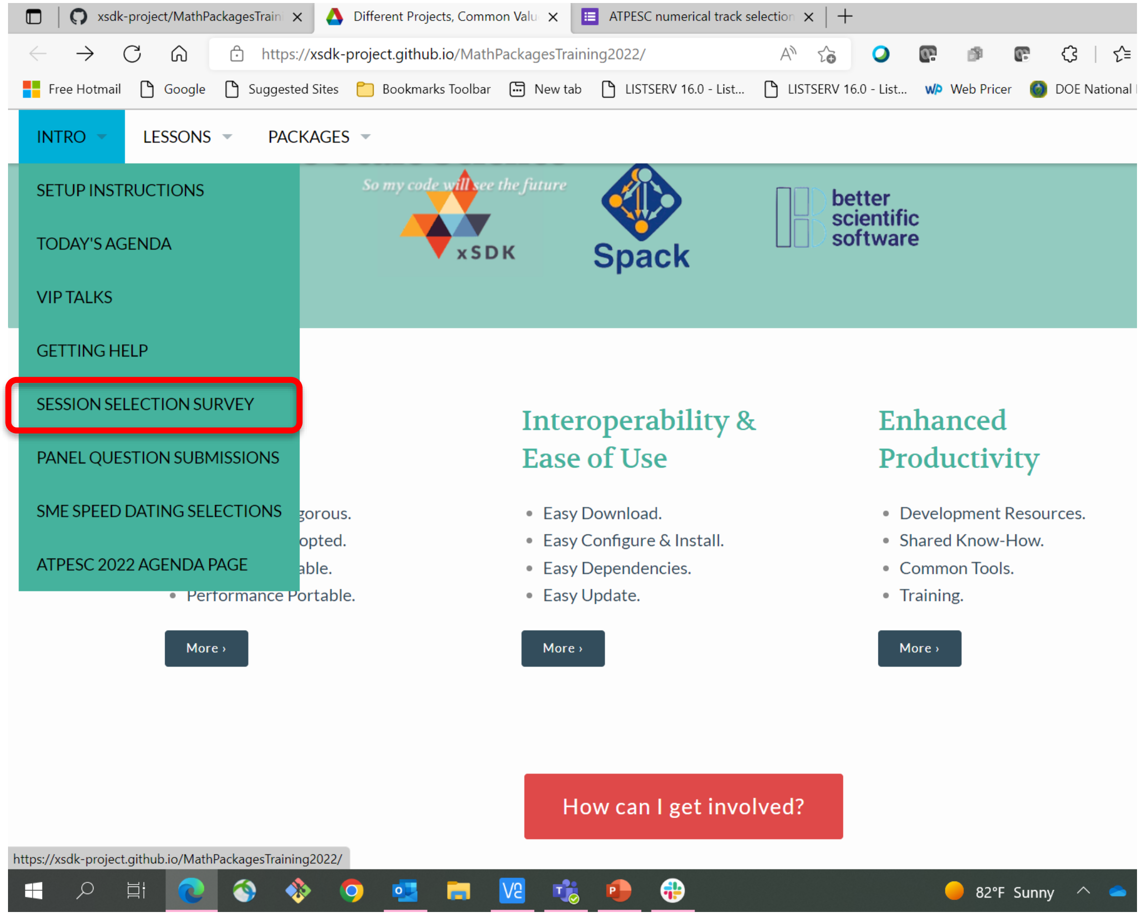
https://extremecomputingtraining.anl.gov/agenda-2024/#Track-5

Time	Room?	Room?
8:30 – 9:30	Introduction to Numerical Software – Ulrike Yang	
9:30 – 10:45	Structured Discretization (AMReX) – Andrew Myers, Weiqun Zhang	Unstructured Discretization (MFEM/PUMI) – Mark Shephard, Cameron Smith, Vladimir Tomov
10:45 – 11:15	Break, Subject Matter Expert (SME) Selections, Panel Questions	
11:15 – 12:30	Iterative Solvers & Algebraic Multigrid (hypre) – Daniel Osei-Kuffuor, Ulrike Yang	Direct Solvers (SuperLU, STRUMPACK) – Sherry Li, Pieter Ghysels
12:30 – 1:30	Lunch, SME Selections, Panel Questions	
1:30 – 2:45	Nonlinear Solvers (PETSc) – Toby Isaac	Time Integration (SUNDIALS) – David Gardner
2:45 – 3:15	Break, SME Selections, **Panel Questions Due**	
3:15 – 4:30	Optimization (TAO) – Todd Munson	Iterative Solvers & Algebraic Multigrid (Trilinos/ Belos/MueLU) – Christian Glusa, Graham Harper
4:30 – 5:30	Wrap-up (Ann Almgren) / Panel: Extreme-Scale Numerical Algorithms and Software	
5:30 – 6:30	Unstructured Time: **SME Selections Due**, Informal Discussion, Continue Hands-on	
6:30 – 7:30	Dinner	
7:30 – 9:30	Optional Activity: SME Speed-dating	

Choose which lecture you want to attend!

Access:https://docs.google.com/forms/d/e/1FAIpQLScuy_Y7pYhY0hqLt5NjVxs_tEHeYMO0QmgvRzGtbcMhQBQ6nA/viewform

https://xsdk-project.github.io/MathPackagesTraining2024/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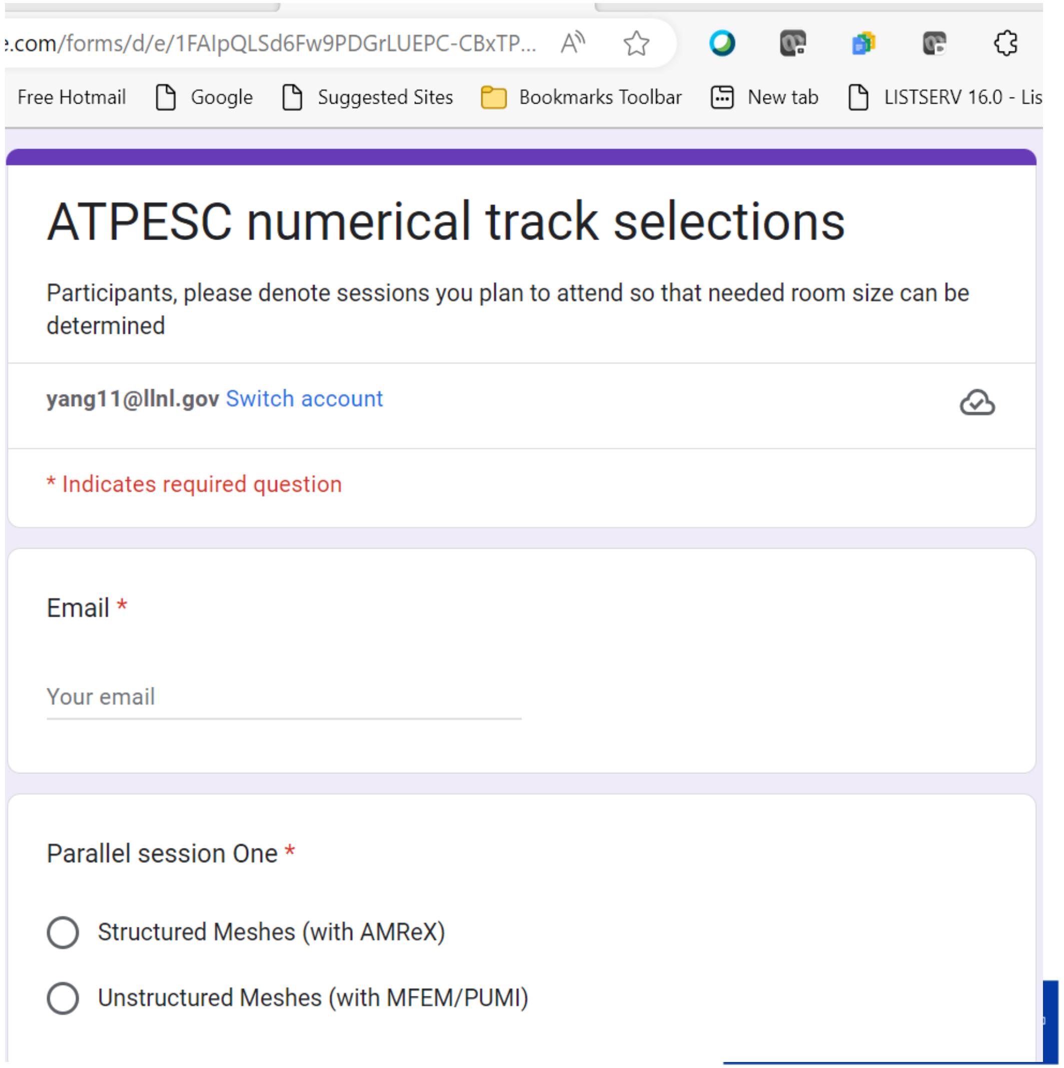

ATPESC numerical track selections

Participants, please denote sessions you plan to attend so that needed room size can be determined

yang11@llnl.gov Switch account

* Indicates required question

Email *

Your email

Parallel session One *

○ Structured Meshes (with AMReX)

○ Unstructured Meshes (with MFEM/PUMI)

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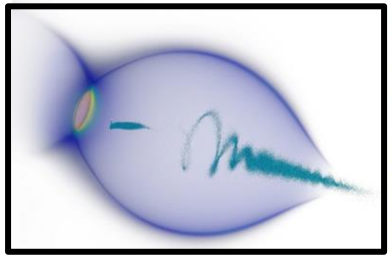
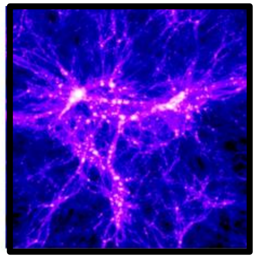
7:30 – 8:30	SME Speed Dating	

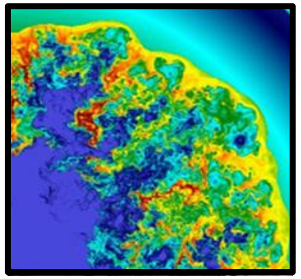
Block-structured adaptive mesh refinement framework. Scalable support for hierarchical mesh and particle data, with embedded boundaries.

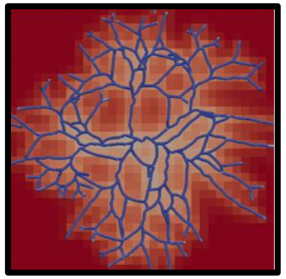
- **Capabilities**
  - Support for PDEs on a hierarchical adaptive mesh with particles and embedded boundary representations of complex geometry
  - Support for multiple modes of time integration
  - Support for explicit and implicit single-level and multilevel mesh operations, multilevel synchronization, particle, particle-mesh and particle-particle operations
  - Hierarchical parallelism –
    - hybrid MPI + OpenMP with logical tiling on multicore architectures
    - hybrid MPI + GPU support for hybrid CPU/GPU systems (NVIDIA CUDA, AMD HIP, Intel SYCL)
  - Native multilevel geometric multigrid solvers for cell-centered and nodal data
  - Highly efficient parallel I/O for checkpoint/restart and for visualization – native format supported by Visit, Paraview, yt
- **Open source software**
  - Used for diverse apps, including accelerator modeling, astrophysics, combustion, cosmology, multiphase flow, phase field modeling, atmospheric modeling and more
  - Source code and development hosted on github with rigorous testing framework
  - Extensive documentation, examples and tutorials

Examples of AMReX applications









https://www.github.com/AMReX-Codes/amrex

MFEM

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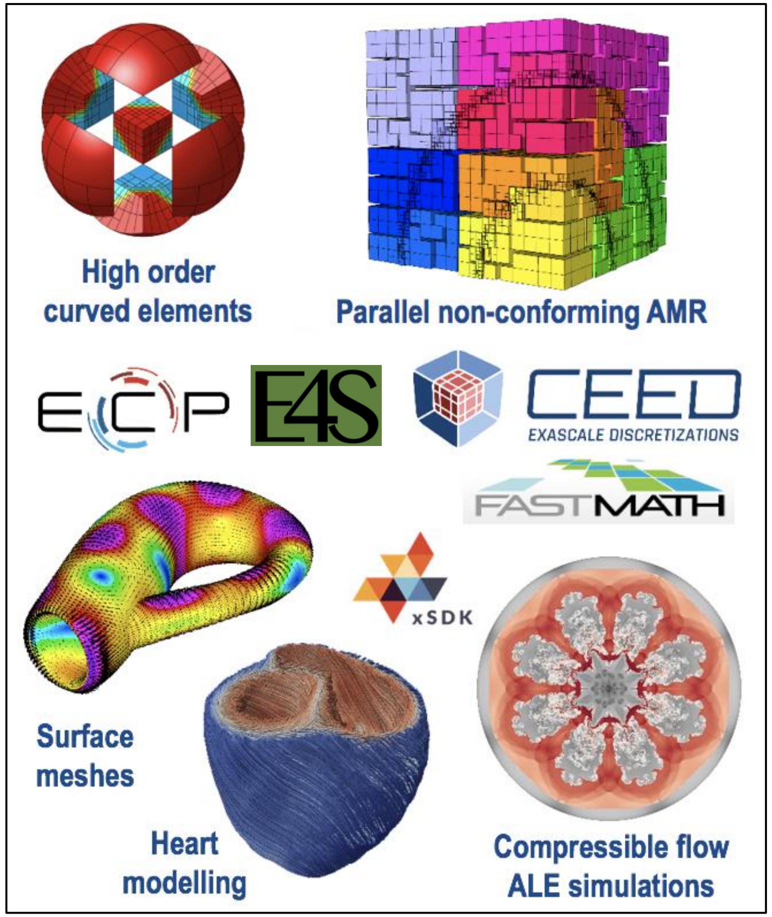
Free, lightweight, scalable C++ library for finite element methods. Supports arbitrary high order discretizations and meshes for wide variety of applications.

- **Flexible discretizations on unstructured grids**
  - Triangular, quadrilateral, tetrahedral and hexahedral meshes.
  - Local conforming and non-conforming refinement.
  - Bilinear/linear forms for variety of methods: Galerkin, DG, DPG, …
- **High-order and scalable**
  - Arbitrary-order H1, H(curl), H(div)- and L2 elements. Arbitrary order curvilinear meshes.
  - MPI scalable to millions of cores and includes initial GPU implementation. Enables application development on wide variety of platforms: from laptops to exascale machines.
- **Built-in solvers and visualization**
  - Integrated with: HYPRE, SUNDIALS, PETSc, SUPERLU, …
  - Accurate and flexible visualization with VisIt and GLVis
- **Open source software**
  - BSD with thousands of downloads/year worldwide.
  - Available on GitHub, also via OpenHPC, Spack. Part of ECP's CEED co-design center.


High order curved elements
Parallel non-conforming AMR
ECP
E4S
CEED
EXASCALE DISCRETIZATIONS
FASTMATH
xSDK
Surface meshes
Heart modelling
Compressible flow ALE simulations

https://mfem.org

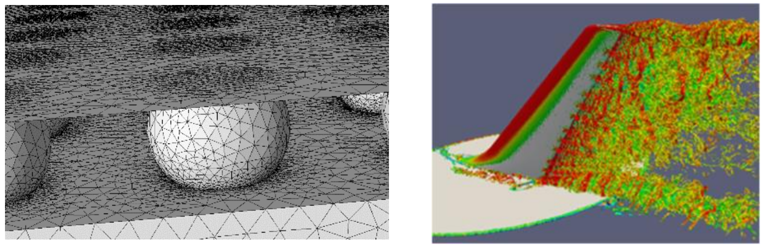
Parallel Unstructured Mesh Infrastructure

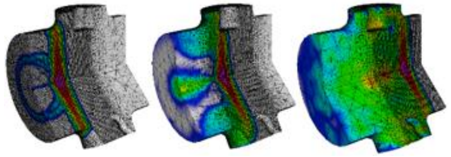
Parallel management and adaptation of unstructured meshes.
Interoperable components to support the development of unstructured mesh simulation workflows

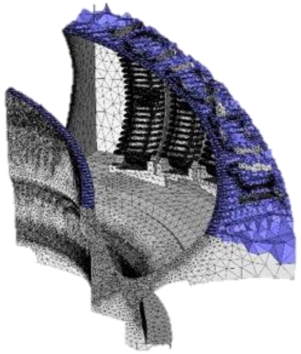
- **Core functionality**
  - Distributed, conformant mesh with entity migration, remote read only copies, fields and their operations
  - Link to the geometry and attributes
  - Mesh adaptation (straight and curved), mesh motion
  - Multi-criteria partition improvement
  - Distributed mesh support for Particle In Cell methods
- **Designed for integration into existing codes**
  - xSDK package; installs with Slack
  - Permissive license enables integration with open and closed-source codes
- **In-memory integrations developed**
  - MFEM: High order FE framework
  - PetraM: Adaptive RF fusion
  - PHASTA: FE for turbulent flows
  - FUN3D: FV CFD
  - Proteus: Multiphase FE
  - ACE3P: High order FE for EM
  - M3D-C1: FE based MHD
  - Nektar++: High order FE for flow
  - Albany/Trilinos: Multi-physics FE

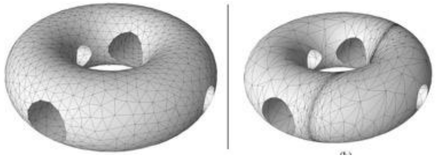
PUMi

SCOREC Rensselaer


Applications with billions of elements: flip-chip (L), flow control (R)


Mesh adaptation for evolving features


RF antenna and plasma surface in vessel.


Anisotropic adaptation for curved meshes

Source Code: github.com/SCOREC/core
User Guide: scorec.rpi.edu/pumi/PUMI.pdf
Paper: scorec.rpi.edu/REPORTS/2014-9.pdf

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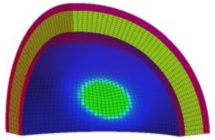
hypre

Lawrence Livermore National Laboratory

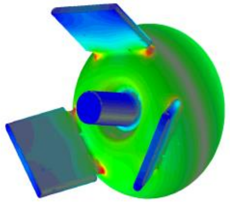
Highly scalable multilevel solvers and preconditioners. Unique user-friendly interfaces. Flexible software design. Used in a variety of applications. Freely available.

- **Conceptual interfaces**
  - Structured, semi-structured, finite elements, linear algebraic interfaces
  - Provide natural “views” of the linear system
  - Provide for efficient (scalable) linear solvers through effective data storage schemes
- **Scalable preconditioners and solvers**
  - Structured and unstructured algebraic multigrid solvers
  - Maxwell solvers, H-div solvers
  - Multigrid solvers for nonsymmetric systems: pAIR
  - Multigrid reduction (MGR) for systems of PDEs
  - Matrix-free Krylov solvers
  - ILU and FSAI preconditioners
- **Exascale early systems GPU-readiness**
  - Nvidia GPU (CUDA), AMD GPU (HIP), Intel GPU (SYCL)
- **Open-source software**
  - Used worldwide in a vast range of applications
  - Can be used through PETSc and Trilinos
  - Available on github: https://www.github.com/hypre-space/hypre

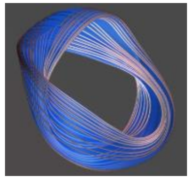
hypre high performance preconditioners



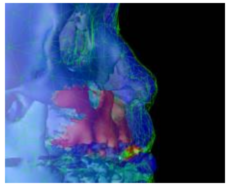
Elasticity / Plasticity



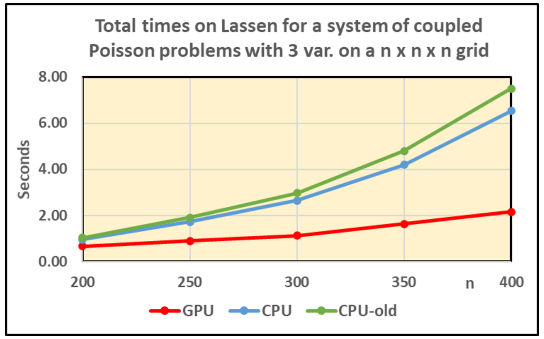
Electro-magnetics



Magneto-hydrodynamics



Facial surgery



Total times on Lassen for a system of coupled Poisson problems with 3 var. on a n x n x n grid

xSDK

E4S

R&D 100

FASTMATH

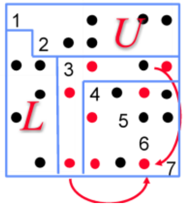
ECP

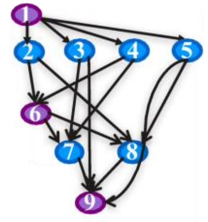
http://www.llnl.gov/CASC/hypre

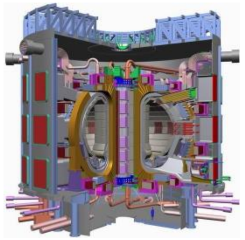
SuperLU

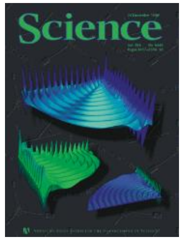
Supernodal Sparse LU Direct Solver. Flexible, user-friendly interfaces. Examples show various use scenarios. Testing code for unit-test. BSD license.

- **Capabilities**
  - Serial (thread-safe), shared-memory (SuperLU_MT, OpenMP or Pthreads), distributed-memory (SuperLU_DIST, hybrid MPI+ OpenM + CUDA/HIP).
    - Written in C, with Fortran interface
  - Sparse LU decomposition (can be nonsymmetric sparsity pattern), triangular solution with multiple right-hand sides
  - Incomplete LU (ILUTP) preconditioner in serial SuperLU
  - Sparsity-preserving ordering: minimum degree or graph partitioning applied to A^TA or A^T+A
  - User-controllable pivoting: partial pivoting, threshold pivoting, static pivoting
  - Condition number estimation, iterative refinement, componentwise error bounds
- **Exascale early systems GPU-readiness**
  - Available: Nvidia GPU (CUDA), AMD GPU (HIP)
  - In progress: Intel GPU (SYCL)
- **Parallel Scalability**
  - Factorization strong scales to 32,000 cores (IPDPS'18, JPDC'19)
  - Triangular solve strong scales to 4000 cores (SIAM CSC'18, SIAM PP'20, SC'23)
- **Open-source software**
  - Used in a vast range of applications, can be used through PETSc and Trilinos, …
  - available on github









ITER tokamak quantum mechanics

Widely used in commercial software, including AMD (circuit simulation), Boeing (aircraft design), Chevron, ExxonMobile (geology), Cray's LibSci, FEMLAB, HP's MathLib, IMSL, NAG, SciPy, OptimaNumerics, Walt Disney Animation.

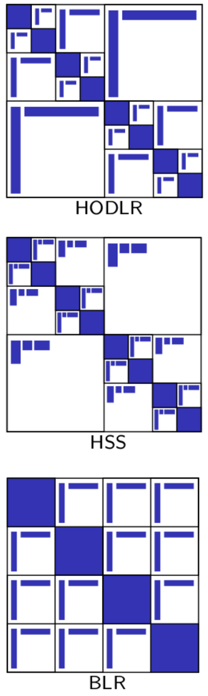
https://portal.nersc.gov/project/sparse/superlu/

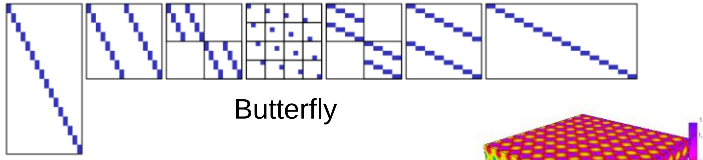
STRUMPACK

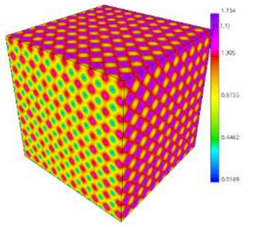
Structured Matrix Package

Hierarchical solvers for dense rank-structured matrices and fast algebraic sparse solver and robust and scalable preconditioners.

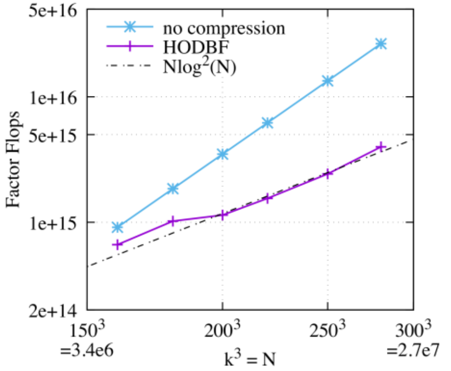
- **Dense Matrix Solvers using Hierarchical Approximations**
  - Hierarchical partitioning, low-rank approximations
  - Hierarchically Semi-Separable (HSS), Hierarchically Off-Diagonal Low-Rank (HODLR), Hierarchically Off-Diagonal Butterfly (HODBF), Block Low-Rank (BLR), Butterfly
  - C++ Interface to ButterflyPACK (Fortran)
  - Applications: BEM, Cauchy, Toeplitz, kernel & covariance matrices, ...
  - Asymptotic complexity much lower than LAPACK/ScaLAPACK routines
- **Sparse Direct Solver**
  - Algebraic sparse direct solver
  - GPU: CUDA, HIP/ROCm, DPC++ (in progress)
  - Orderings: (Par)METIS, (PT)Scotch, RCM
- **Preconditioners**
  - Approximate sparse factorization, using hierarchical matrix approximations
  - Scalable and robust, aimed at PDE discretizations, indefinite systems, …
  - Iterative solvers: GMRES, BiCGStab, iterative refinement
- **Software**
  - BSD license
  - Interfaces from PETSc, MFEM, Trilinos, available in Spack

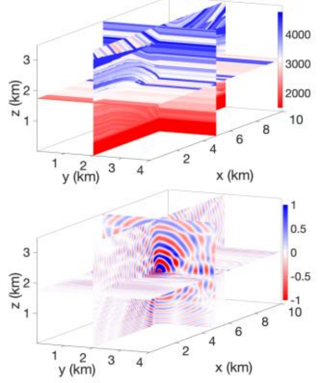






Near linear scaling for high-frequency wave equations





github.com/pghysels/STRUMPACK

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SUNDIALS

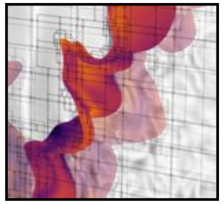
Suite of Nonlinear and Differential /Algebraic Equation Solvers

Adaptive time integrators for ODEs and DAEs and efficient nonlinear solvers

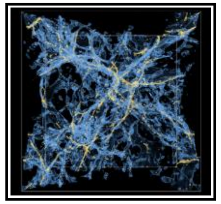
Used in a variety of applications. Freely available. Encapsulated solvers & parallelism.

- **ODE and DAE time integrators:**
  - — *CVODE:* adaptive order and step BDF (stiff) & Adams (non-stiff) methods for ODEs
  - — *ARKODE:* adaptive step implicit, explicit, IMEX, and multirate Runge-Kutta methods for ODEs
  - — *IDA*: adaptive order and step BDF methods for DAEs
  - — *CVODES* and *IDAS:* provide forward and adjoint sensitivity analysis capabilities
- **Nonlinear Solvers:** *KINSOL* – Newton-Krylov; accelerated Picard and fixed point
- **Modular Design:** Easily incorporated into existing codes; Users can supply their own data structures and solvers or use SUNDIALS provided modules
- **Support on NVIDIA, AMD, and Intel GPUs:**
  - — Vectors: CUDA, HIP, OpenMP Offload, RAJA, SYCL (DPC++)
  - — Linear solvers: cuSOLVER, MAGMA, matrix-free Krylov methods
- **Open Source:** BSD License; Download from LLNL site, GitHub, or Spack
  - — Supported by extensive documentation; user email list with an active community
  - — Available through MFEM, AMReX, deal.II, and PETSc

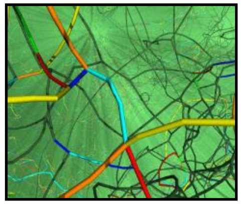
SUNDIALS is used worldwide in applications throughout research and industry



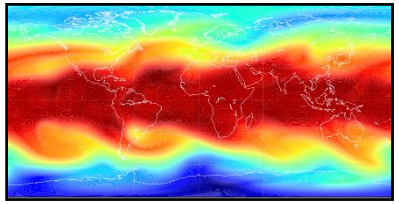
Combustion (Pele)



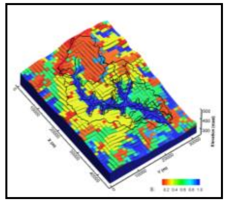
Cosmology (Nyx)



Dislocation dynamics (ParaDiS)



Atmospheric Dynamics (Tempest)



Subsurface flow (ParFlow)

Lawrence Livermore National Laboratory

ECP

FASTMATH

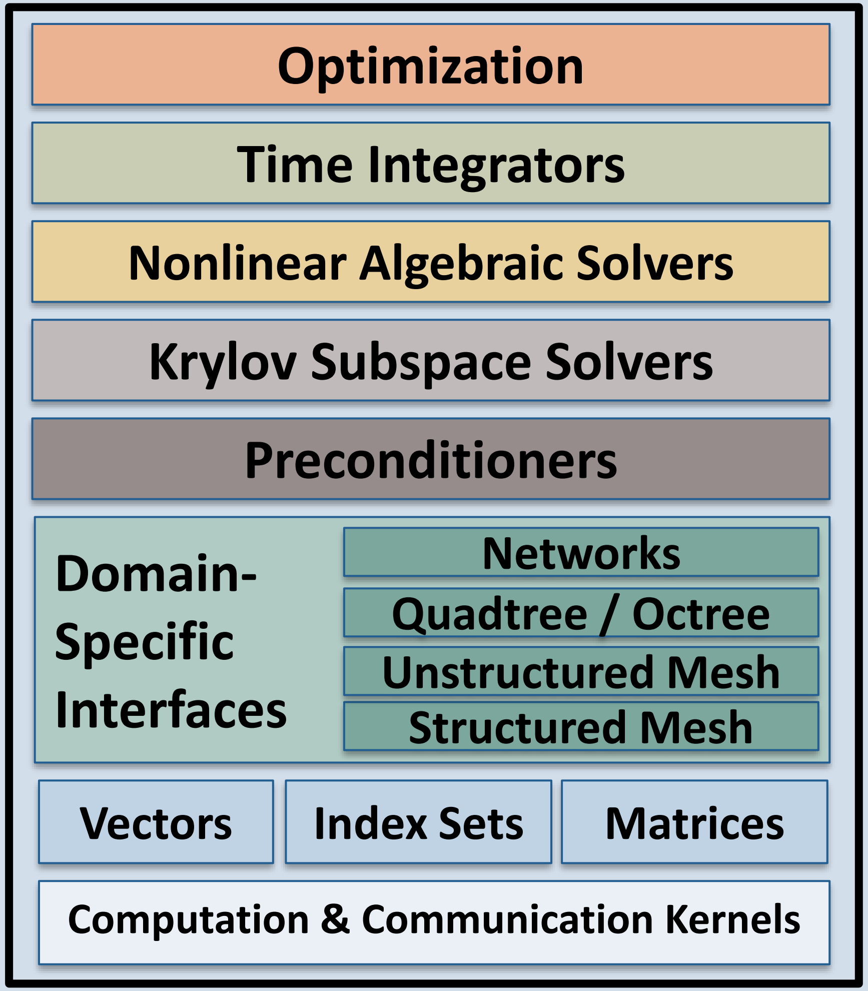
xSDK

http://www.llnl.gov/casc/sundials

PETSc TAO

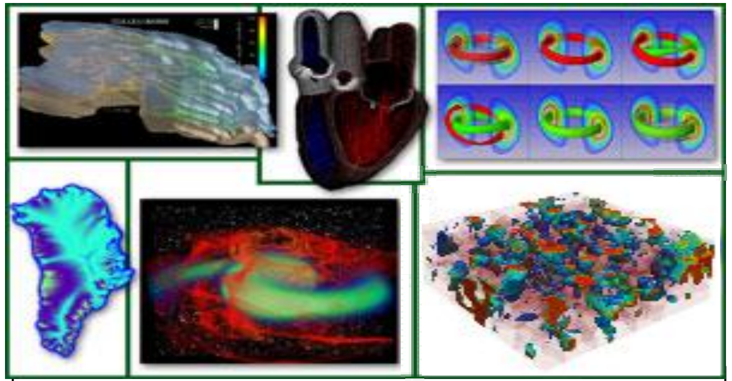
Portable, Extensible Toolkit for Scientific Computation / Toolkit for Advanced

Scalable algebraic solvers for PDEs. Encapsulate parallelism in high-level objects. Active & supported user community. Full API from Fortran, C/C++, Python.



- **Easy customization and composability of solvers <u>at runtime</u>**
  - Enables optimality via flexible combinations of physics, algorithmics, architectures
  - Try new algorithms by composing new/existing algorithms (multilevel, domain decomposition, splitting, etc.)
- **Portability & performance**
  - Largest DOE machines, also clusters, laptops; NVIDIA, AMD, and Intel GPUs
  - Thousands of users worldwide

Argonne NATIONAL LABORATORY



PETSc provides the backbone of diverse scientific applications. clockwise from upper left: hydrology, cardiology, fusion, multiphase steel, relativistic matter, ice sheet modeling

ECP xSDK FASTMATH R&D 100

https://www.mcs.anl.gov/petsc

Agenda

https://extremecomputingtraining.anl.gov/agenda-2024/#Track-5

Time	Room?	Room?
8:30 – 9:30	Introduction to Numerical Software – Ulrike Yang	
9:30 – 10:45	Structured Discretization (AMReX) – Andrew Myers, Weiqun Zhang	Unstructured Discretization (MFEM/PUMI) – Mark Shephard, Cameron Smith, Vladimir Tomov
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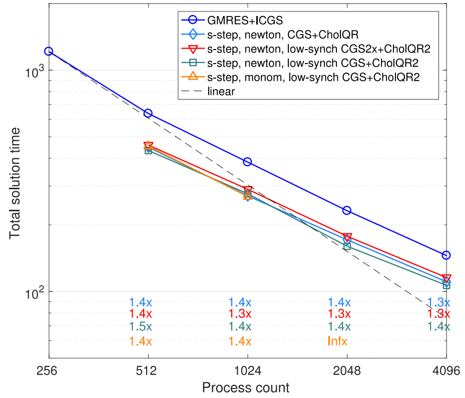
11:15 – 12:30	Iterative Solvers & Algebraic Multigrid (hypre) – Daniel Osei-Kuffuor, Ulrike Yang	Direct Solvers (SuperLU, STRUMPACK) – Sherry Li, Pieter Ghysels
12:30 – 1:30	Lunch	
1:30 – 2:45	Nonlinear Solvers (PETSc) – Toby Isaac	Time Integration (SUNDIALS) – David Gardner
2:45 – 3:15	Break	
3:15 – 4:30	**Optimization (TAO) – Todd Munson**	**Iterative Solvers & Algebraic Multigrid (Trilinos/ Belos/MueLU) – Christian Glusa, Graham Harper**
4:30 – 5:30	Wrap-up (Ann Almgren) / Panel: Extreme-Scale Numerical Algorithms and Software	
6:30 – 7:30	Dinner	
7:30 – 8:30	SME Speed Dating	

Trilinos/Belos

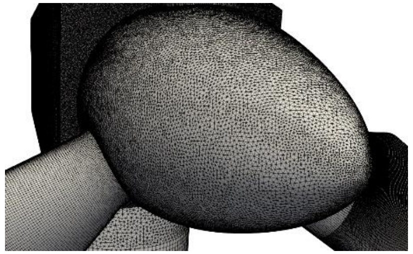
Iterative Krylov-based solvers. Templated C++ allows for generic scalar, ordinal, and compute node types.

- **Ability to solve single or sequence of linear systems**
  - Simultaneously solved systems w/ multiple-RHS: $AX = B$
  - Sequentially solved systems w/ multiple-RHS: $AX_i = B_i,\ i=1,\ldots,t$
  - Sequences of multiple-RHS systems: $A_iX_i = B_i,\ i=1,\ldots,t$
- **Standard methods**
  - Conjugate Gradients (CG), GMRES
  - TFQMR, BiCGStab, MINRES, fixed-point
- **Advanced methods**
  - Block GMRES, block CG/BICG
  - Hybrid GMRES, CGRODR (block recycling GMRES)
  - TSQR (tall skinny QR), LSQR
  - Pipelined and s-step methods
  - Stable polynomial preconditioning
- **Performance portability via Kokkos (CPUs, NVIDIA/Intel/AMD GPUs, Phi)**
- **Ongoing research**
  - Communication avoiding methods

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.



Speed-ups of various s-step Krylov methods within low Mach CFD wind-energy code Nalu-Wind.



Thomas et al., "High-fidelity simulation of wind- turbine incompressible flows", SISC, 2019.

https://trilinos.github.io/belos.html

Trilinos/MueLu

Structured and unstructured aggregation-based algebraic multigrid (AMG) preconditioners

- **Robust, scalable, portable AMG preconditioning critical for many large-scale simulations**
  — Multifluid plasma simulations
  — Shock physics
  — Magneto-hydrodynamics (MHD)
  — Low Mach computational fluid dynamics (CFD)

- **Capabilities**
  — Aggregation-based coarsening
  — Smoothers: Jacobi, GS, *l*1 GS, polynomial, ILU, sparse direct
  — Load-balancing for good parallel performance
  — Structured coarsening, geometric multigrid
  — Setup and solve phases can run on GPUs.
  — Performance portability via Kokkos (CPUs, NVIDIA/Intel/AMD GPUs, Xeon Phi)

- **Research Areas**
  — AMG for multiphysics
  — Multigrid for coupled structured/unstructured meshes
  — Algorithm selection via machine learning

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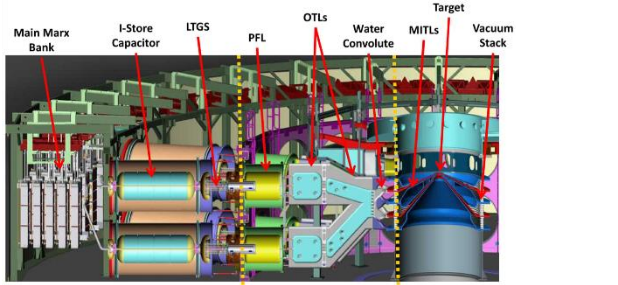
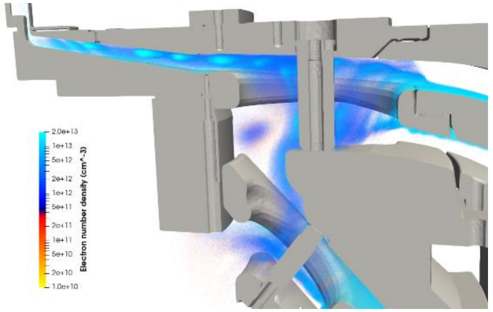


Z machine diagram, from "Redesign of a High Voltage Test Bed for Marxes on Z", W.M. White et al., 2018.

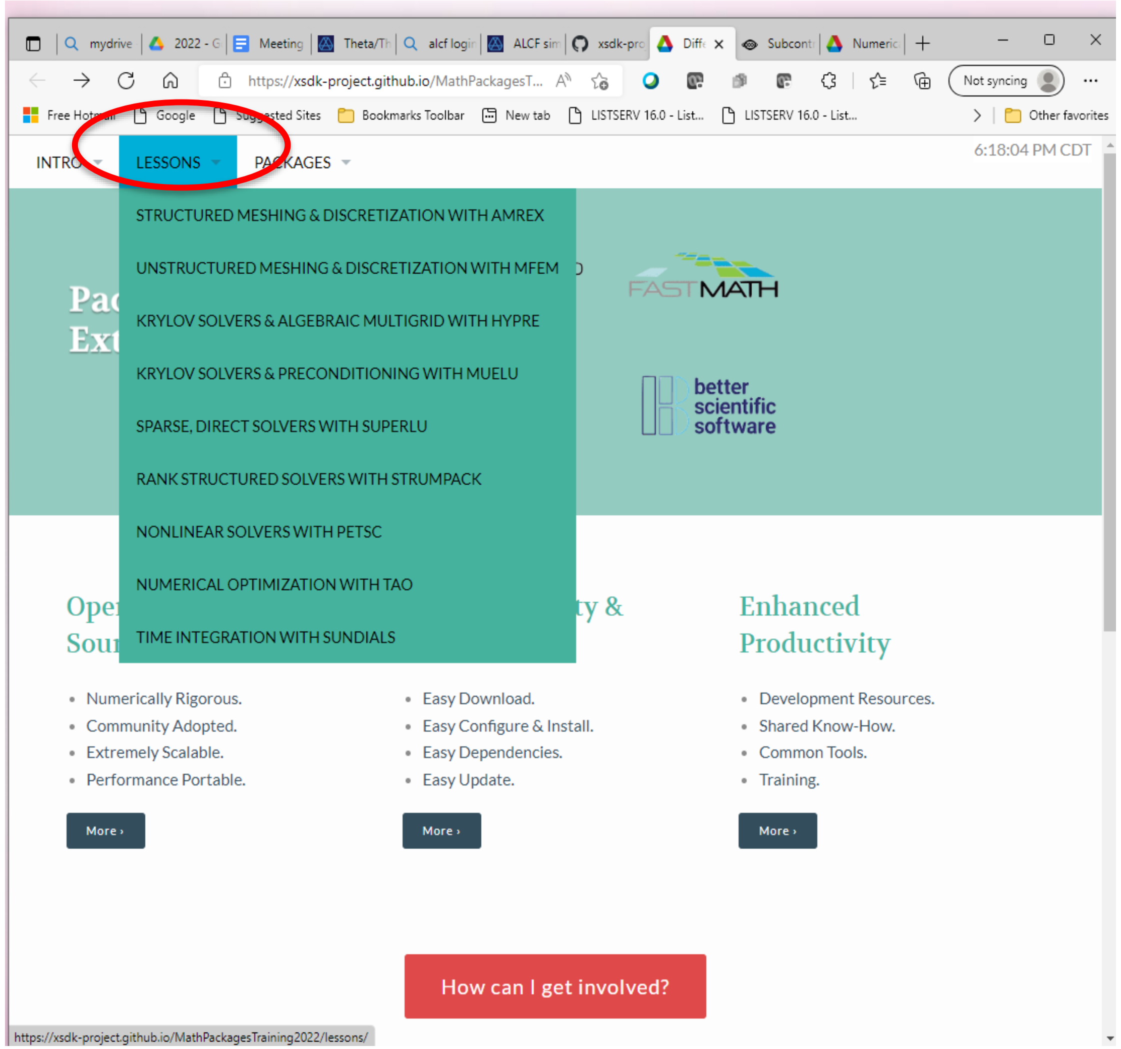
AMG preconditioning for H(curl) systems is key enabling technology in Z machine simulations for determining power from Marx banks to Target.



Plasma density in Z machine Target simulation, courtesy of D. Sirajuddin (SNL).

https://trilinos.github.io/muelu.html

https://xsdk-project.github.io/MathPackagesTraining2024/



- STRUCTURED MESHING & DISCRETIZATION WITH AMREX
- UNSTRUCTURED MESHING & DISCRETIZATION WITH MFEM
- KRYLOV SOLVERS & ALGEBRAIC MULTIGRID WITH HYPRE
- KRYLOV SOLVERS & PRECONDITIONING WITH MUELU
- SPARSE, DIRECT SOLVERS WITH SUPERLU
- RANK STRUCTURED SOLVERS WITH STRUMPACK
- NONLINEAR SOLVERS WITH PETSC
- NUMERICAL OPTIMIZATION WITH TAO
- TIME INTEGRATION WITH SUNDIALS

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- Numerically Rigorous.
- Community Adopted.
- Extremely Scalable.
- Performance Portable.

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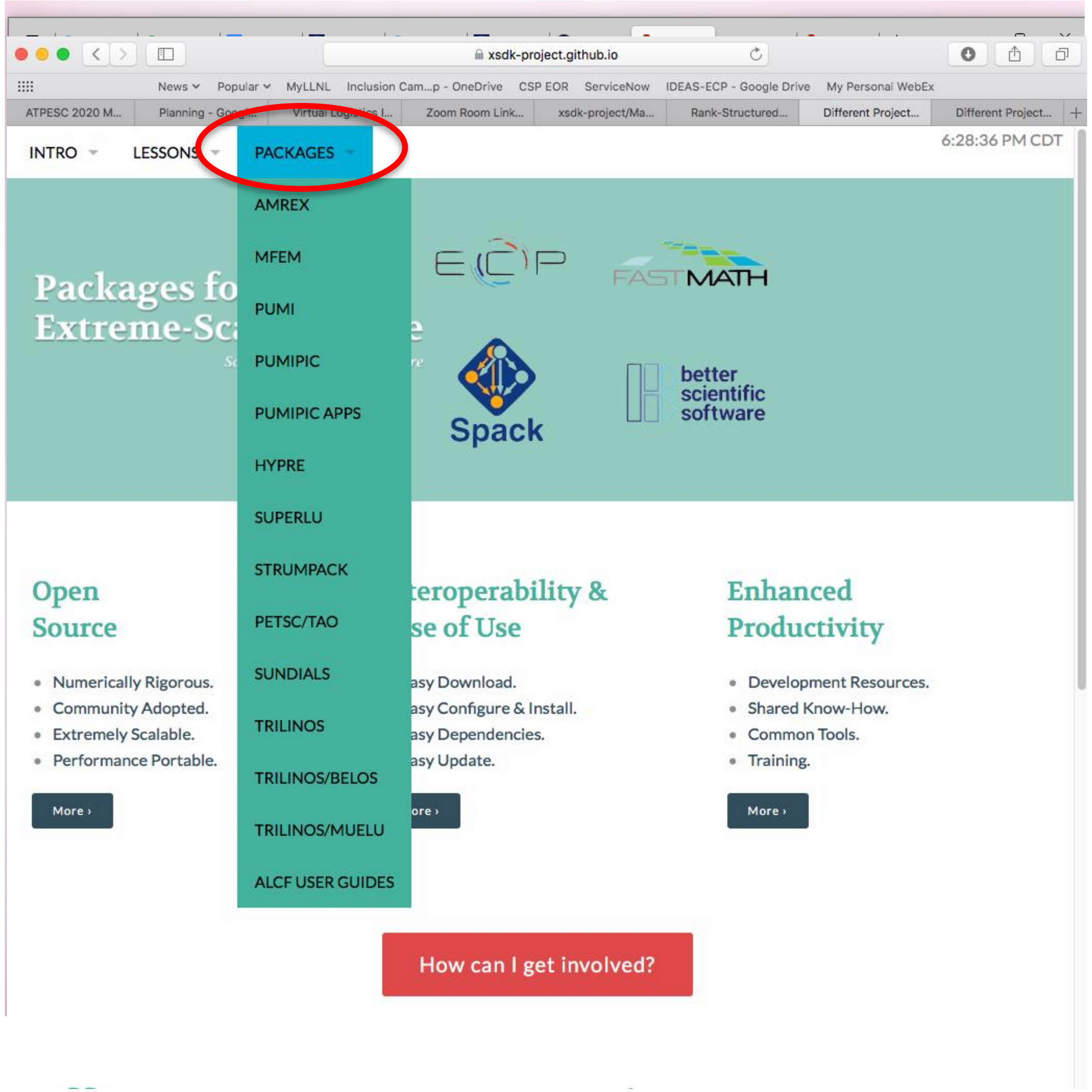
- Easy Download.
- Easy Configure & Install.
- Easy Dependencies.
- Easy Update.

Enhanced Productivity

- Development Resources.
- Shared Know-How.
- Common Tools.
- Training.

- Hands-on Lessons

https://xsdk-project.github.io/MathPackagesTraining2024/



Packages fo
Extreme-Sc

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- Packages

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https://extremecomputingtraining.anl.gov/agenda-2024/#Track-5

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2:45 – 3:15	Break, SME Selections, **Panel Questions Due**	
3:15 – 4:30	Optimization (TAO) – Todd Munson	Iterative Solvers & Algebraic Multigrid (Trilinos, Belos & MueLu) – Christian Glusa, Graham Harper
4:30 – 5:30	**Wrap-up (Toby Isaac) / Panel: Extreme-Scale Numerical Algorithms and Software**	
5:30 – 6:30	Unstructured Time: **SME Selections Due**, Informal Discussion, Continue Hands-on	
6:30 – 7:30	Dinner	
7:30 – 9:30	Optional Activity: SME Speed-dating	

Panel: Extreme-Scale Numerical Algorithms and Software

- **Q&A Session:** ATPESC learners ask questions about working with numerical packages and the community of numerical package developers
  - Questions in **#numerical** slack channel and via Google form
- Panelists

Sherry Li, LBL

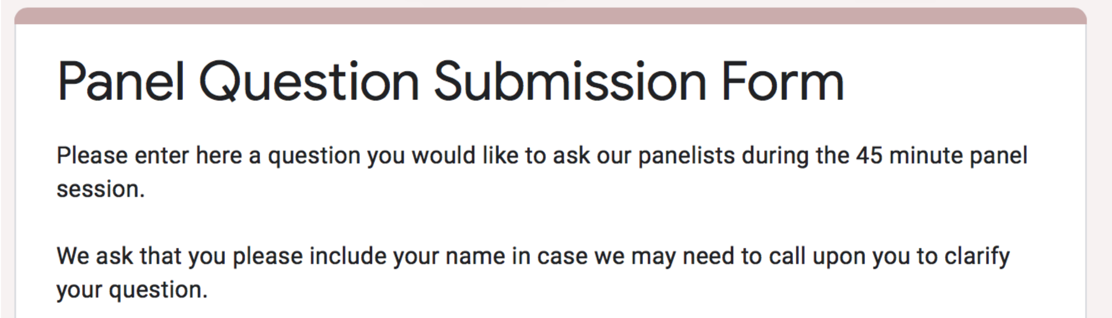
Daniel Osei-Kuffuor, LLNL

Graham Harper, SNL

Vladimir Tomov, LLNL

- Moderator

Todd Munson, ANL


Panel Question Submission Form

Please enter here a question you would like to ask our panelists during the 45 minute panel session.

We ask that you please include your name in case we may need to call upon you to clarify your question.

Next steps: https://xsdk-project.github.io/MathPackagesTraining2024/agenda

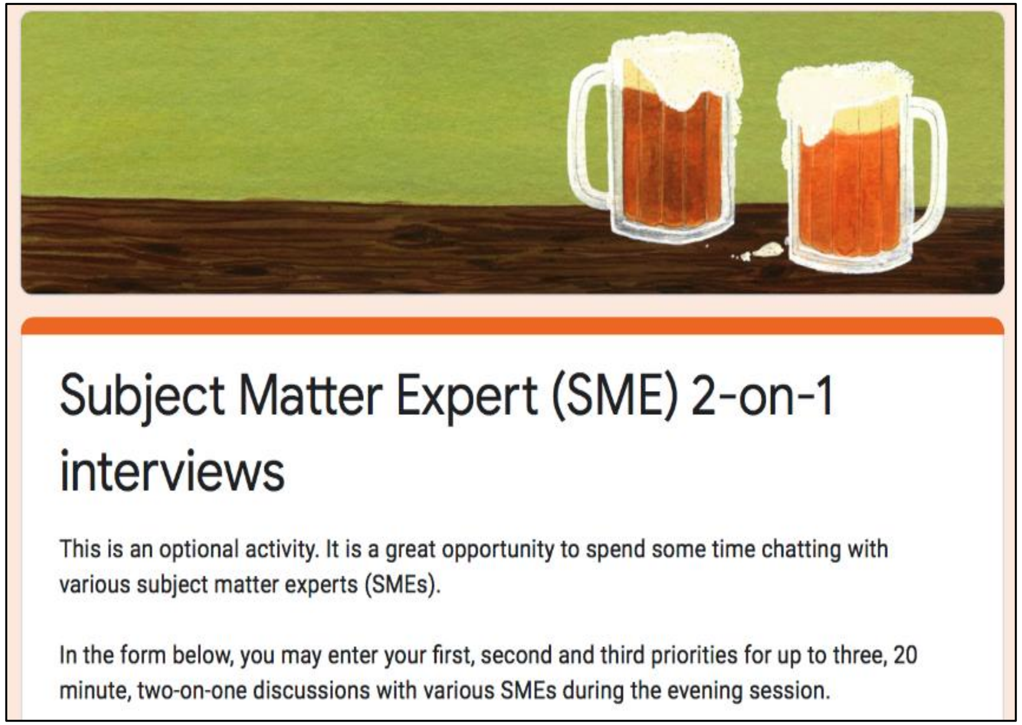
- **WrapUp (Toby Isaac) @ 4:30pm**

  Panel: Main Room @ 4:45 pm

- **SME Speed Dating: @7:30pm**

- **During breaks and lunch**
  - **Provide Panel Questions**
    Due: 3:15 pm
  - **Sign up for discussions with numerical software developers** (optional)
    - Your email address

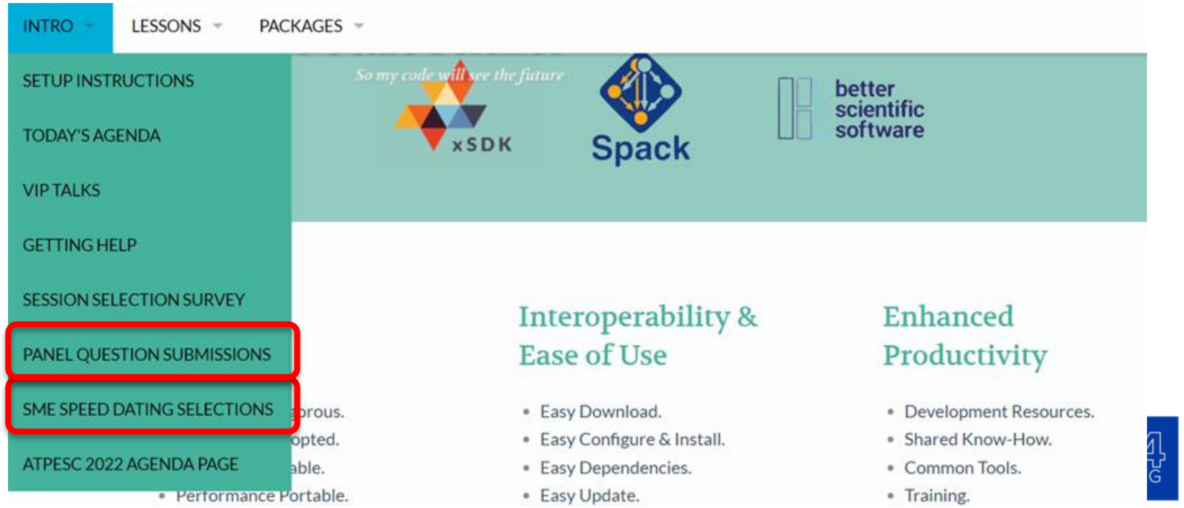
    Due 6:30 pm



Subject Matter Expert (SME) 2-on-1 interviews

This is an optional activity. It is a great opportunity to spend some time chatting with various subject matter experts (SMEs).

In the form below, you may enter your first, second and third priorities for up to three, 20 minute, two-on-one discussions with various SMEs during the evening session.



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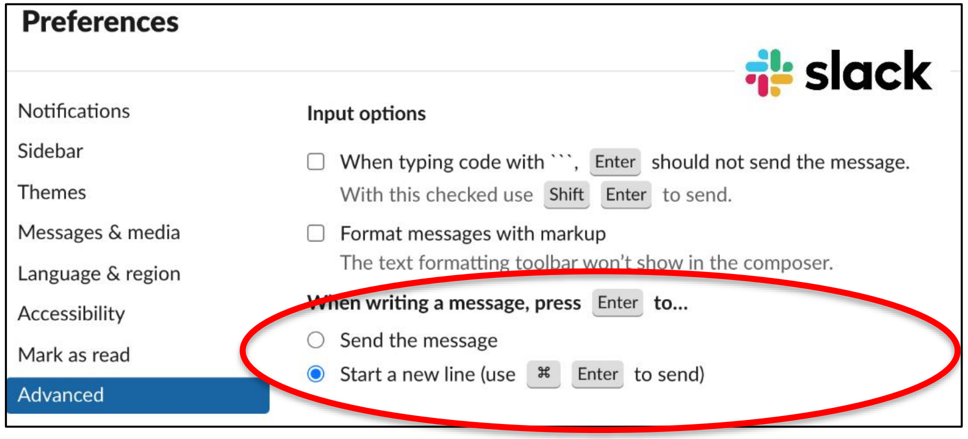
- Development Resources.
- Shared Know-How.
- Common Tools.
- Training.

Using Slack

- Recommend using the desktop app, but browser ok too
- **# atpesc-2024-track-5-numerical** channel
- **# atpesc-2024-helpdesk** channel
  - For all chat during presentations
  - For all chat outside any specific parallel session
  - For general help
  - Recommend using the thread option to help keep track of discussions on subtopics

Tip: Consider setting Preferences to customize when to send



Preferences

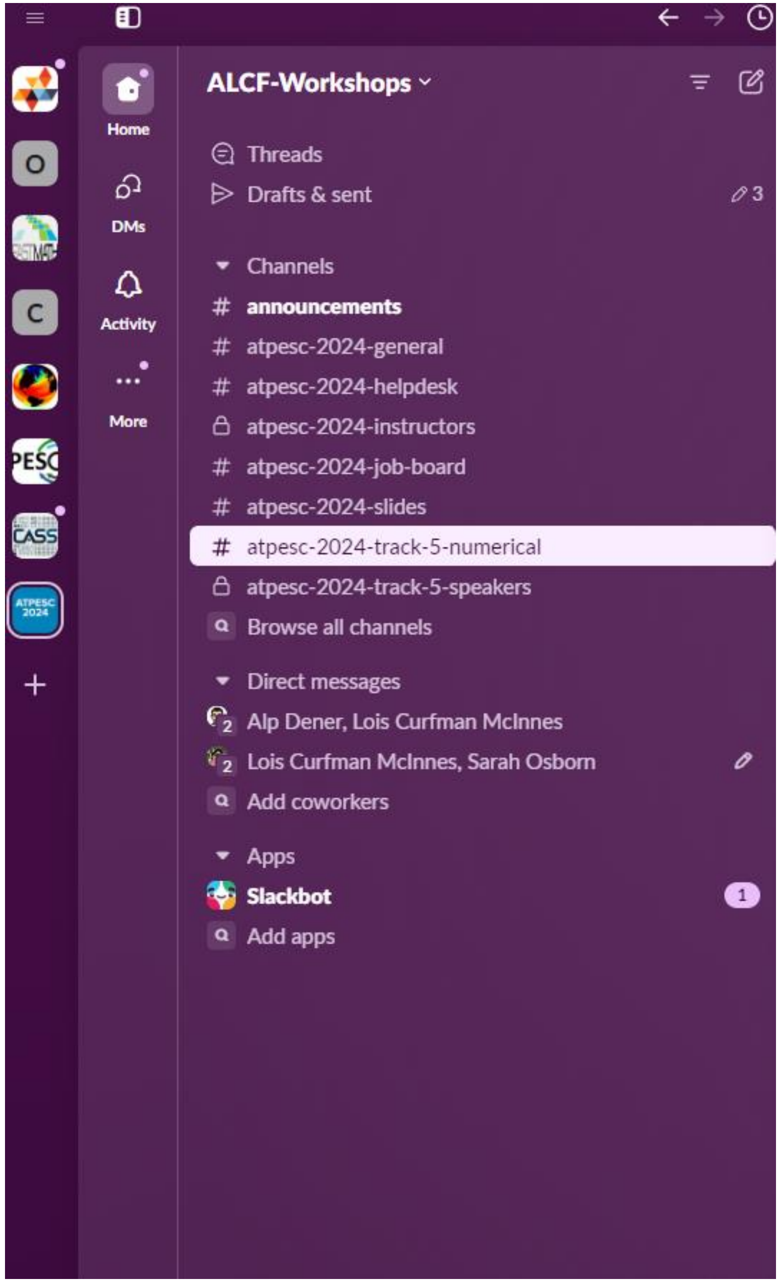
Input options

□ When typing code with ```, Enter should not send the message.
With this checked use Shift Enter to send.

□ Format messages with markup
The text formatting toolbar won't show in the composer.

When writing a message, press Enter to...

○ Send the message
● Start a new line (use ⌘ Enter to send)



VIPs of ATPESC Extreme-Scale Numerical Software Track

- **Jack Dongarra, Univ of Tennessee** [bio]
  - **Growing up at Argonne National Laboratory**
    - ATPESC 2024, Tuesday, July 30, 7:30pm
  - Adaptive Linear Solvers and Eigensolvers, ATPESC 2019 [video]

- **Jim Demmel, UC Berkeley** [bio]
  - **Communication-Avoiding Algorithms for Linear Algebra, Machine Learning and Beyond**
    - ATPESC 2024, Wednesday, August 7, 7:30pm
  - ENLA Seminar, June 2020 [video]

- **David Keyes, KAUST** [bio]
  - **Efficient Computation through Tuned Approximation**
    - ATPESC 2024, Thursday, August 8, 7:30pm
  - Adaptive Nonlinear Preconditioning for PDEs with Error Bounds on Output Functionals, University of Manchester, 2021 [video]

The ATPESC Team 2024

Extreme-scale numerical algorithms and software
Integrated lectures and hands-on examples, panel session, individual discussions … and more!

Toby Isaac, ANL

Andrew Myers, LBL

Vladimir Tomov, LLNL

Mark Shephard, RPI

Cameron Smith, RPI

Ulrike Yang, LLNL

Christian Glusa, SNL

Graham Harper, SNL

Sherry Li, LBL

Pieter Ghysels, LBL

Satish Balay, ANL

Daniel Osei-Kuffuor, LLNL

Todd Munson, ANL

David Gardner, LLNL

Weiqun Zhang, LBL

Track 5: Numerical Algorithms and Software: Tutorial Goals

1. Provide a basic understanding of a variety of applied mathematics algorithms for scalable linear, nonlinear, and ODE solvers, as well as discretization technologies (e.g., adaptive mesh refinement for structured and unstructured grids) and numerical optimization

2. Provide an overview of software tools available to perform these tasks on HPC architectures … including where to go for more info

3. Practice using one or more of these software tools on basic demonstration problems

This presentation provides a high-level introduction to HPC numerical software

- How HPC numerical software addresses challenges in computational science and engineering (CSE)
- Toward extreme-scale scientific software ecosystems
- Using and contributing: Where to go for more info

Why is this important for you?

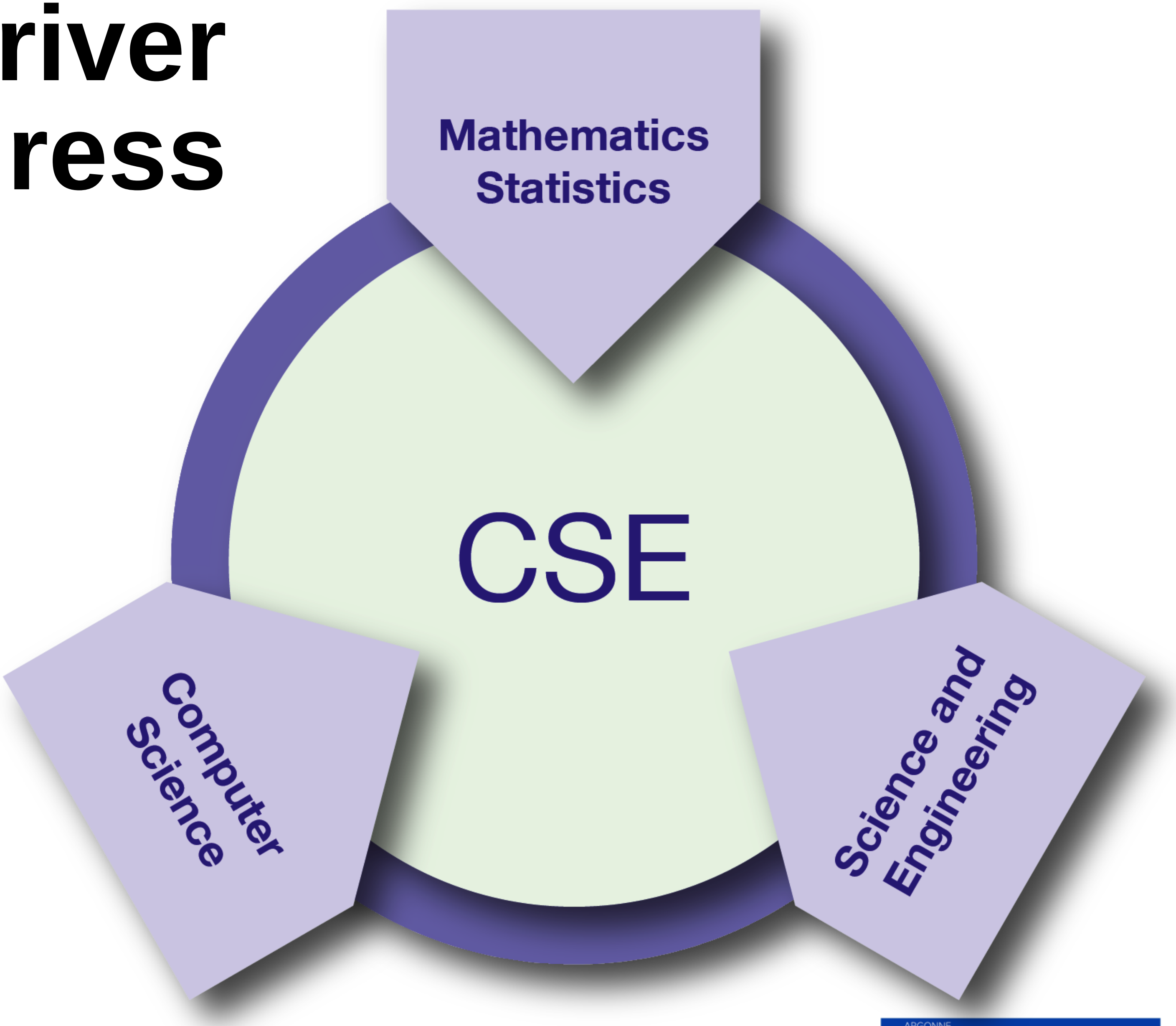
- Libraries enable users to focus on their primary interests
  - Reuse algorithms and data structures developed by experts
  - Customize and extend to exploit application-specific knowledge
  - Cope with complexity and changes over time
- More efficient, robust, reliable, scalable, sustainable scientific software
- Better science, broader impact of your work

CSE: Essential driver of scientific progress

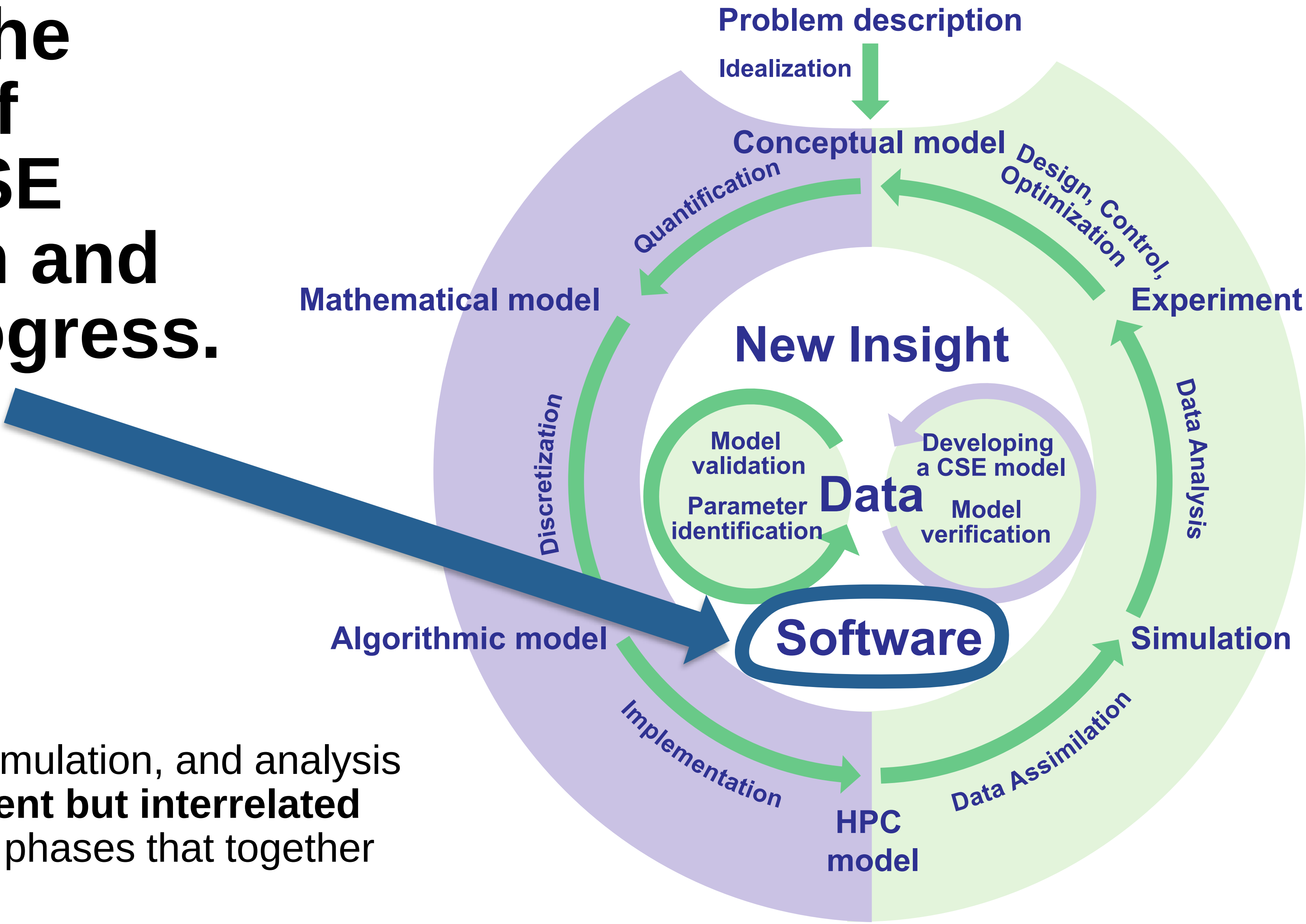
CSE = Computational Science & Engineering

Development and use of computational methods for scientific discovery

- all branches of the sciences
- engineering and technology
- support of decision-making across a spectrum of societally important applications



Software is the foundation of sustained CSE collaboration and scientific progress.

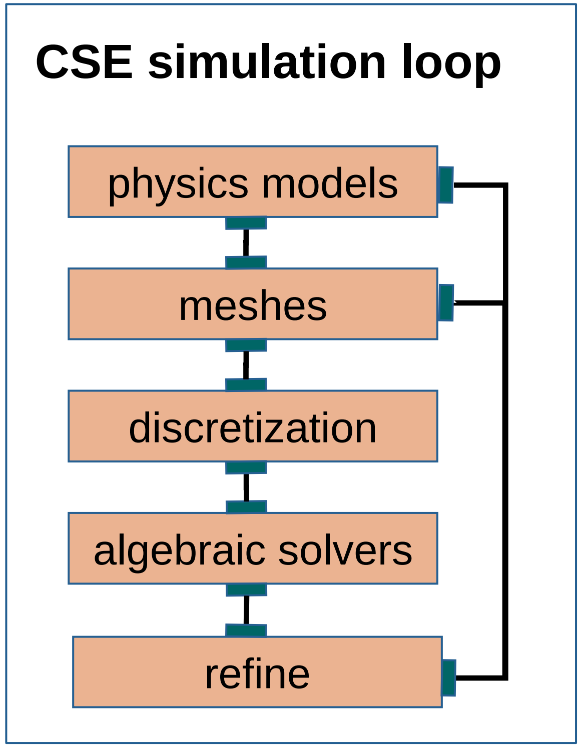


CSE cycle: Modeling, simulation, and analysis

- **Software: independent but interrelated elements** for various phases that together enable CSE

CSE simulation starts with a forward simulation that captures the physical phenomenon of interest

- Develop a mathematical model of the phenomenon of interest
- Approximate the model using a discrete representation
- Solve the discrete representation
- Adapt and refine the mesh or model
- Incorporate different physics, scales


CSE simulation loop

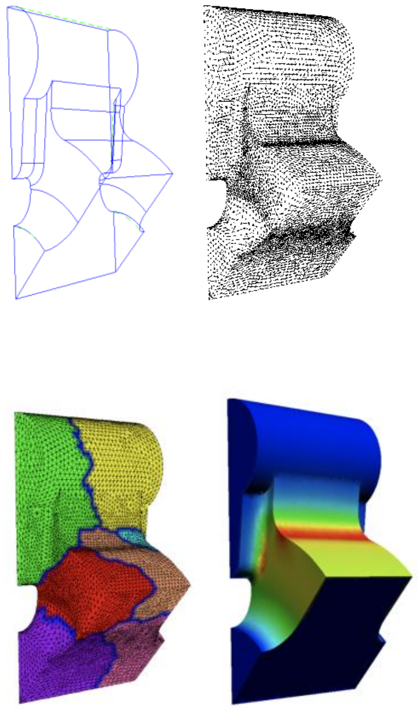
physics models

meshes

discretization

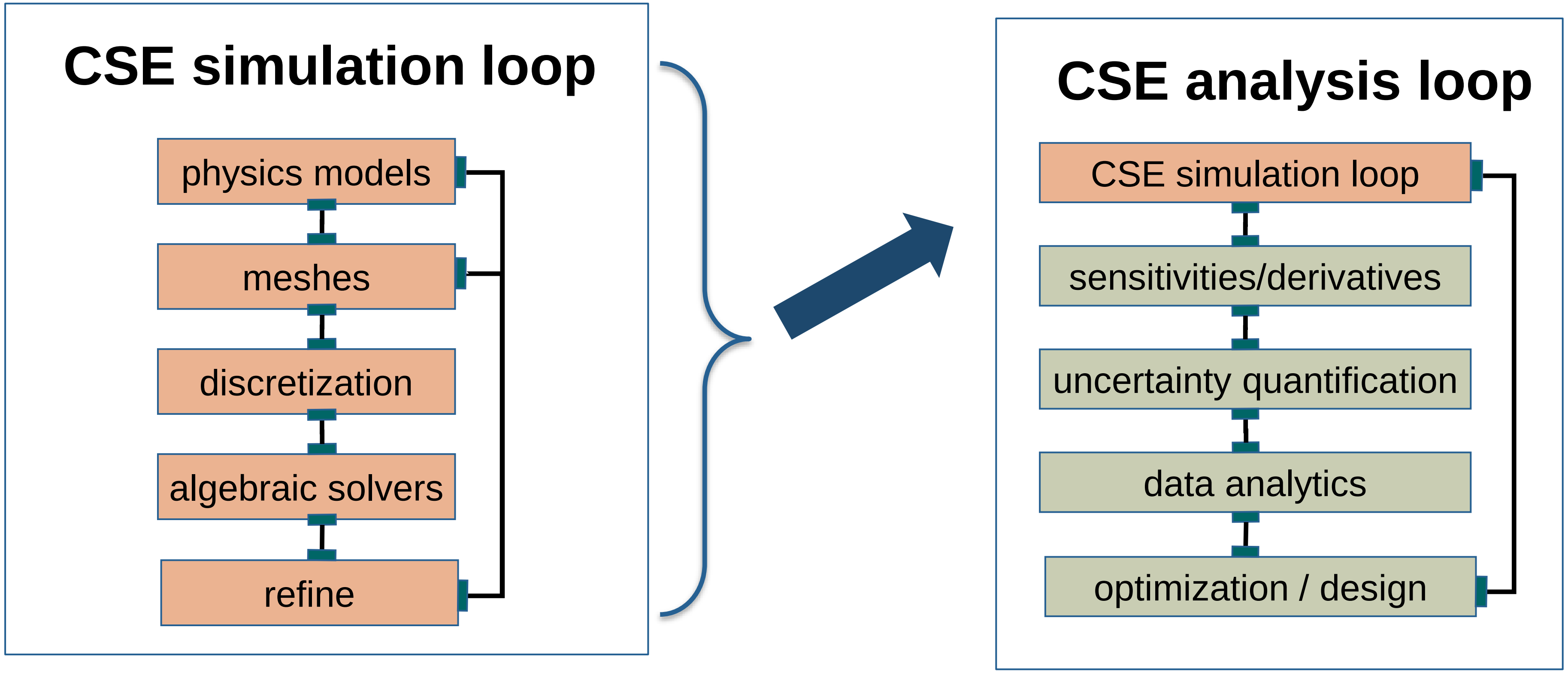
algebraic solvers

refine



Requires: mesh generation, partitioning, load balancing, high-order discretization, time integration, linear & nonlinear solvers, eigensolvers, mesh refinement, multiscale/multiphysics coupling, etc.

CSE analysis builds on the CSE simulation loop … and relies on even more numerical algorithms and software



CSE simulation loop

physics models

meshes

discretization

algebraic solvers

refine

CSE analysis loop

CSE simulation loop

sensitivities/derivatives

uncertainty quantification

data analytics

optimization / design

Beyond interpretive simulations …

working toward predictive science

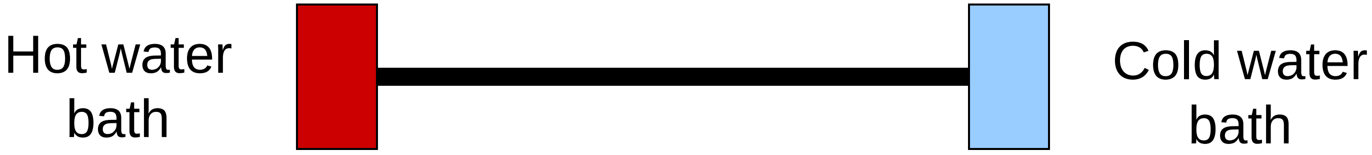
Requires: adjoints, sensitivities, algorithmic differentiation, sampling, ensembles, data analytics, uncertainty quantification, optimization (derivative free & derivative based), inverse problems, etc.

First consider a very simple example

- 1D rod with one end in a hot water bath, the other in a cold water bath
- Mathematical model

$$\nabla^2 T = 0 \in \Omega$$

$$T(0) = 180^o \quad T(1) = 0^o$$

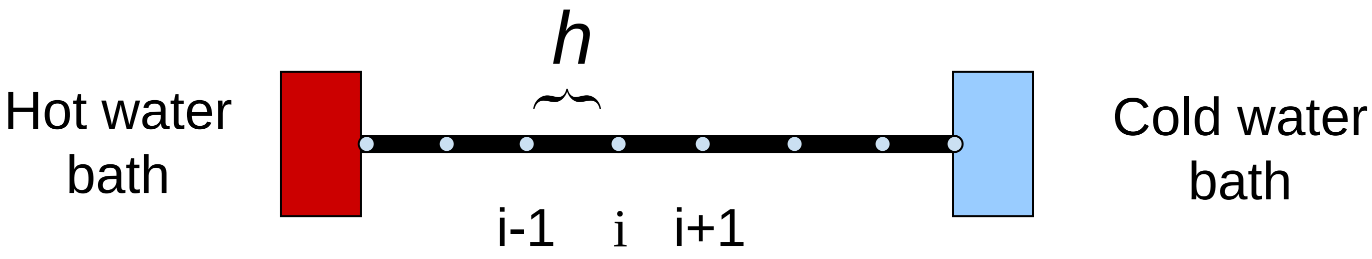


The first step is to discretize the equations

- Approximate the derivatives of the continuous equations with a discrete representation that is easier to solve
- One approach: Finite differences

$$\nabla^2 T \approx (T_{i+1} - 2T_i + T_{i-1})/h^2 = 0$$

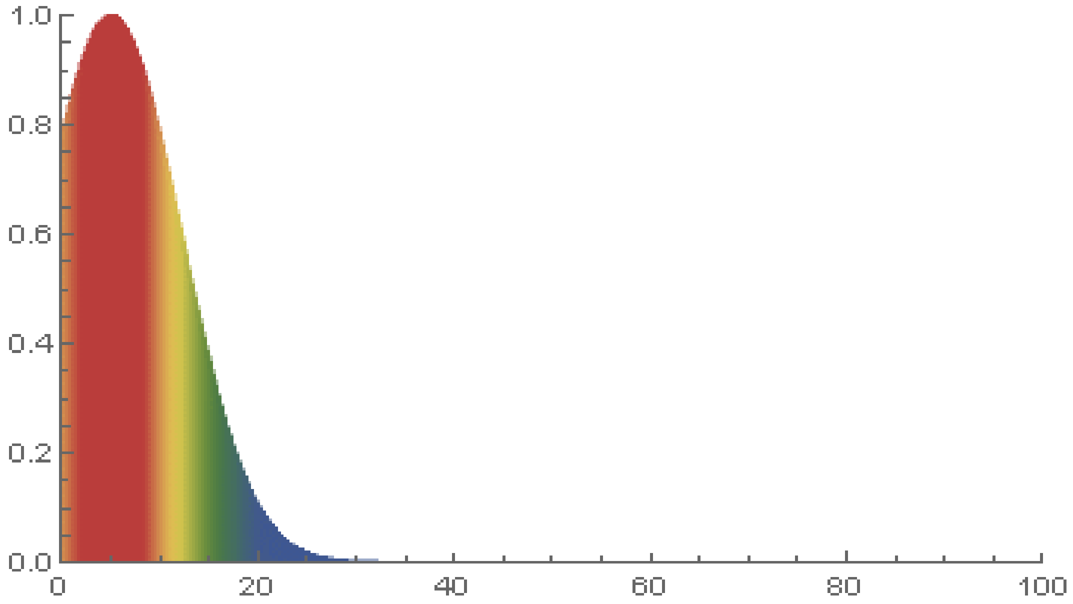
$$T_0 = 180^o \qquad T_n = 0^o$$



Then you can solve for the unknowns T_i

- Set up a matrix of the unknown coefficients
  - include the known boundary conditions
- Solve the linear system for T_i

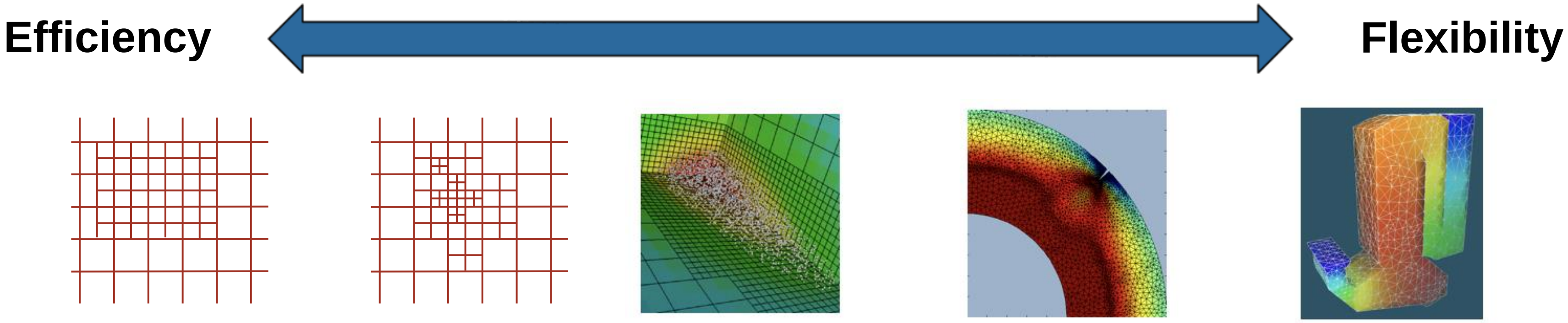
$$\begin{pmatrix} 2 & -1 & 0 & \ldots\ldots\ldots\ldots & 0 \\ -1 & 2 & -1 & 0 \quad \ldots\ldots & 0 \\ 0 & -1 & 2 & -1 \quad 0 \ldots & 0 \\ & & \ldots\ldots\ldots & & \\ 0 & \ldots\ldots\ldots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ . \\ T_{n-1} \end{pmatrix} = \begin{pmatrix} 180\,h^2 \\ 0 \\ 0 \\ . \\ 0 \end{pmatrix}$$



- Visualize and analyze the results

As problems get more complicated, so do the steps in the process

- Different discretization strategies exist for differing needs



Efficiency

Flexibility

- Most problems are time dependent and nonlinear
  - Need higher algorithmic levels than linear solvers
- Increasingly combining multiple physical processes
  - Interactions require careful handling
- Goal-oriented problem solving requires optimization, uncertainty quantification

This work is founded on decades of experience and concerted team efforts to advance numerical software …

https://scidac5-fastmath.lbl.gov

https://exascaleproject.org

- FASTMath SciDAC Institute
- Exascale Computing Project (ECP)
- Developers of xSDK packages

… While improving software productivity & sustainability as key aspects of advancing overall scientific productivity

https://ideas-productivity.org

- IDEAS Software Productivity Project
- Better Scientific Software Community

See also Track 3:
Software Productivity and Sustainability (Aug 2)

Community efforts: Join us!

https://xsdk.info

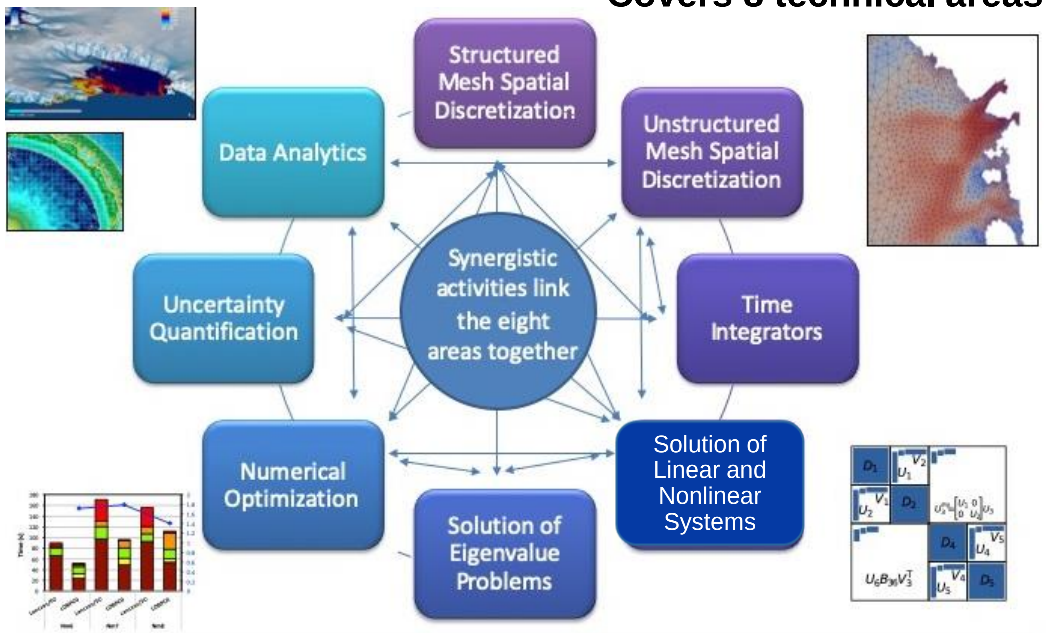
https://bssw.io

https://e4s.io

FASTMath: Frameworks, Algorithms & Scalable Technologies for Mathematics

https://scidac5-fastmath.lbl.gov/

Covers 8 technical areas



Structured Mesh Spatial Discretization

Unstructured Mesh Spatial Discretization

Time Integrators

Solution of Linear and Nonlinear Systems

Solution of Eigenvalue Problems

Numerical Optimization

Uncertainty Quantification

Data Analytics

Synergistic activities link the eight areas together

FASTMath Goals:

- Develop advanced numerical techniques for DOE applications
- Deploy high-performance software on DOE supercomputers
- Demonstrate basic research technologies from applied mathematics
- Engage and support of the computational science community

100’s of person years of experience building math software

SuperLU AMReX sundials ZOLTAN

mfem PETSc hypre

UQTk symPACK

PUMI Trilinos Albany DAKOTA

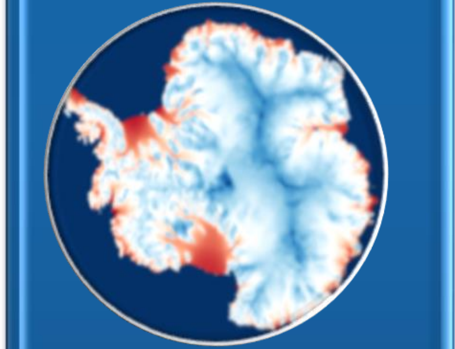
50+ researchers from 6 DOE labs and 6 universities

BERKELEY LAB Argonne NATIONAL LABORATORY OAK RIDGE National Laboratory Sandia National Laboratories NREL

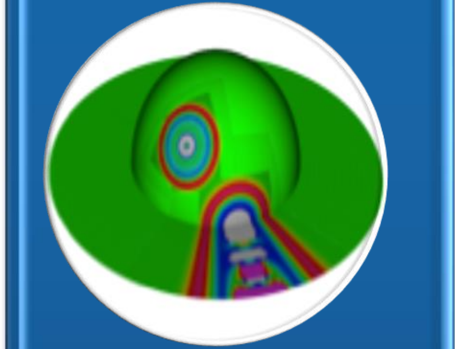
Boulder USC MIT Rensselaer SMU

Esmond G. Ng, FASTMath Institute Director (EGNg@lbl.gov)

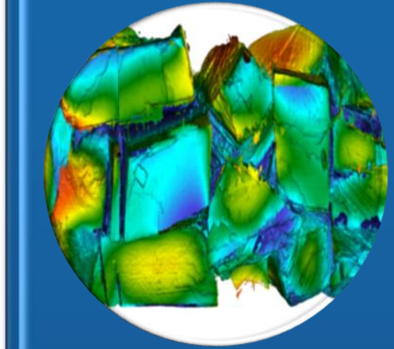
Structured grid efforts focus on high-order, mapped grids, embedded boundaries, AMR, and particles



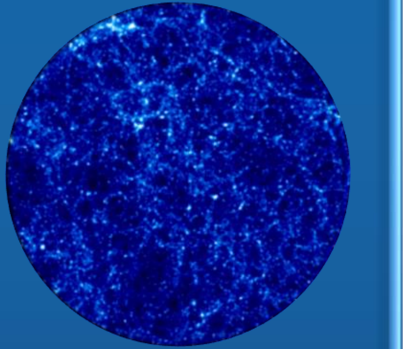
Structured AMR



Mapped-multiblock grids



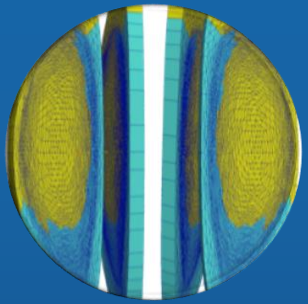
Embedded boundary methods



Particle-based methods

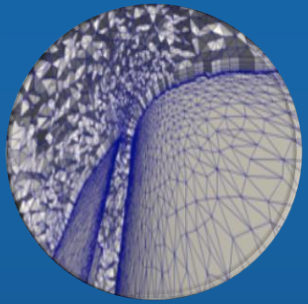
Application to cosmology, astrophysics, accelerator modeling, fusion, climate, subsurface reacting flows, low mach number combustion, etc.

Unstructured grid capabilities focus on adaptivity, high-order, and the tools needed for extreme scaling

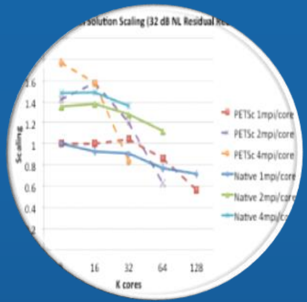


Parallel mesh infrastructures

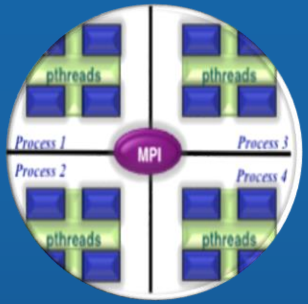
Dynamic load balancing



Mesh adaptation and quality control



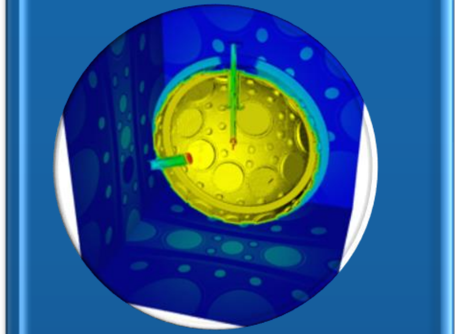
Parallel performance on unstructured meshes



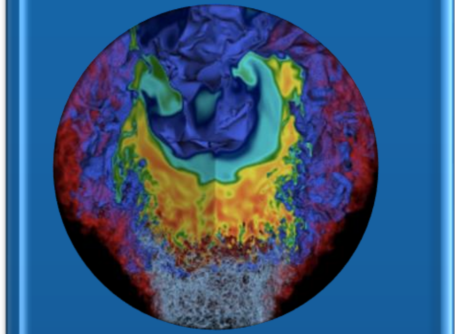
Architecture aware implementations

Application to fusion, climate, accelerator modeling, NNSA applications, nuclear energy, manufacturing processes, etc.

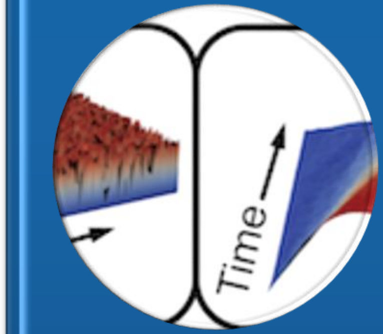
Time discretization methods provide efficient and robust techniques for stiff implicit, explicit and multi-rate systems



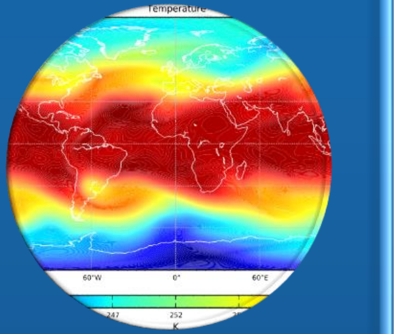
IMEX, multi-rate methods



Spectral deferred correction techniques



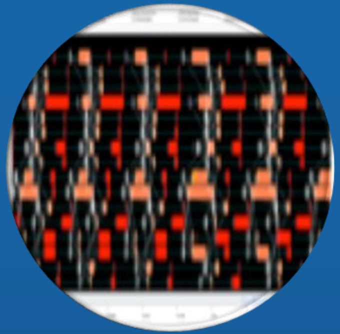
Parallel in time



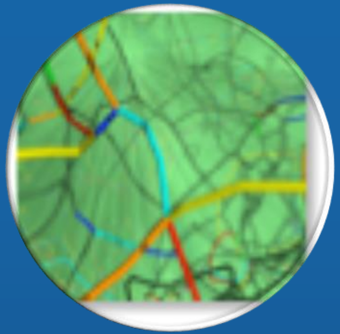
Constrained problems

Application to atmospheric dynamics, ice sheets, combustion, power grid, cosmology, subsurface, etc.

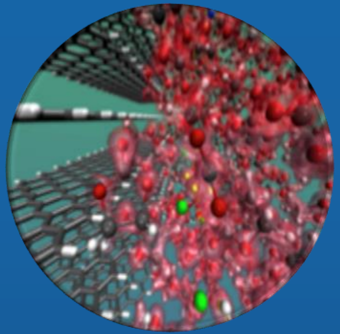
Research on algebraic systems provides key solution technologies to applications



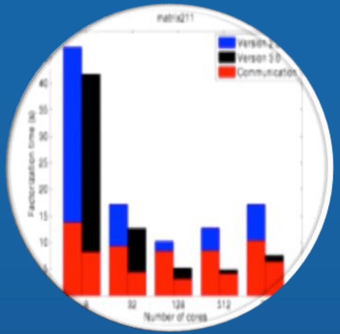
Linear system solution using direct and iterative solvers



Nonlinear system solution using acceleration techniques and globalized Newton methods



Eigensolvers using iterative techniques and optimization



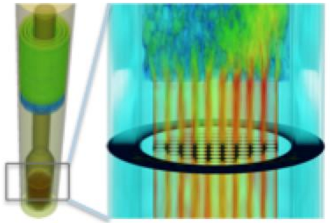
Architecture aware implementations

Application to fusion, nuclear structure calculation, quantum chemistry, accelerator modeling, climate, dislocation dynamics etc,

Multiphysics: A primary motivator for exascale

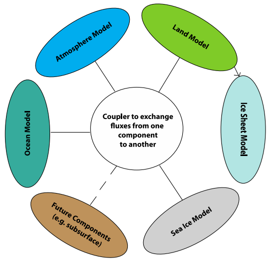
Multiphysics: greater than 1 component governed by its own principle(s) for evolution or equilibrium

- Also: broad class of coarsely partitioned problems possess similarities

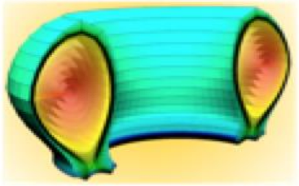


nuclear reactors
A. Siegel, ANL

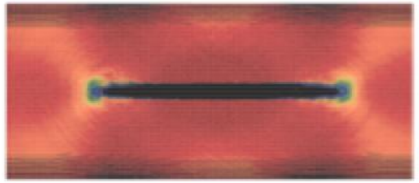
particle accelerators
K. Lee, SLAC


Atmosphere Model
Land Model
Ice Sheet Model
Sea Ice Model
Future Components (e.g. subsurface)
Ocean Model
Coupler to exchange fluxes from one component to another

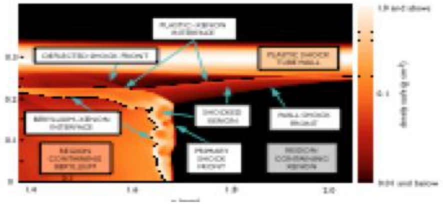
climate
K. Evans, ORNL



fusion
A. Hakim, PPPL

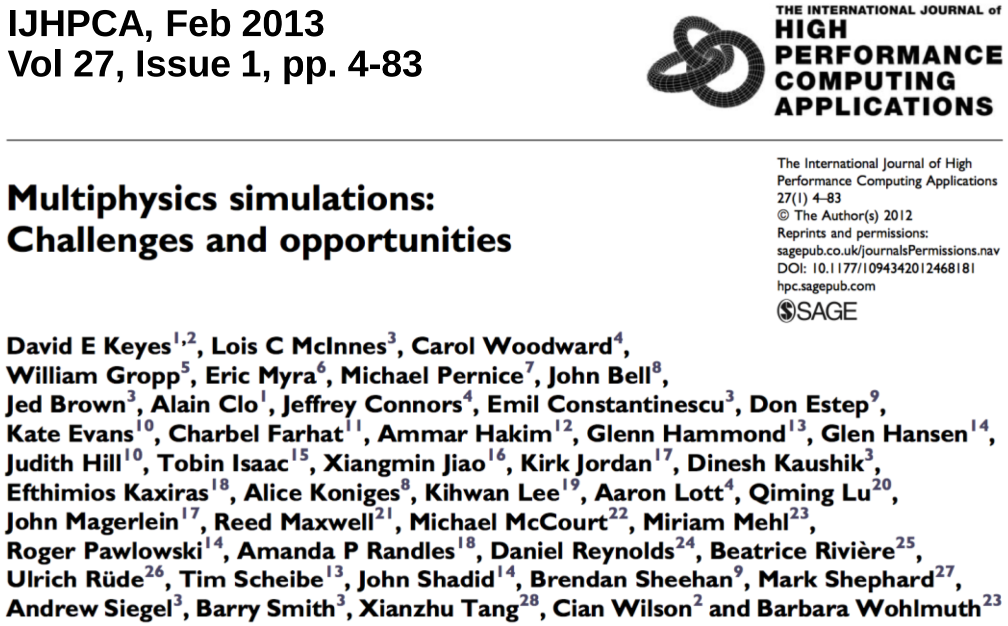


crack propagation
E. Kaxiras, Harvard



radiation hydrodynamics
E. Myra, Univ. of Michigan

IJHPCA, Feb 2013
Vol 27, Issue 1, pp. 4-83



THE INTERNATIONAL JOURNAL of HIGH PERFORMANCE COMPUTING APPLICATIONS

Multiphysics simulations: Challenges and opportunities

The International Journal of High Performance Computing Applications
27(1) 4–83
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DOI: 10.1177/1094342012468181
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David E Keyes[1,2], Lois C McInnes[3], Carol Woodward[4], William Gropp[5], Eric Myra[6], Michael Pernice[7], John Bell[8], Jed Brown[3], Alain Clo[1], Jeffrey Connors[4], Emil Constantinescu[3], Don Estep[9], Kate Evans[10], Charbel Farhat[11], Ammar Hakim[12], Glenn Hammond[13], Glen Hansen[14], Judith Hill[10], Tobin Isaac[15], Xiangmin Jiao[16], Kirk Jordan[17], Dinesh Kaushik[3], Efthimios Kaxiras[18], Alice Koniges[8], Kihwan Lee[19], Aaron Lott[4], Qiming Lu[20], John Magerlein[17], Reed Maxwell[21], Michael McCourt[22], Miriam Mehl[23], Roger Pawlowski[14], Amanda P Randles[18], Daniel Reynolds[24], Beatrice Rivière[25], Ulrich Rüde[26], Tim Scheibe[13], John Shadid[14], Brendan Sheehan[9], Mark Shephard[27], Andrew Siegel[3], Barry Smith[3], Xianzhu Tang[28], Cian Wilson[2] and Barbara Wohlmuth[23]

doi:10.1177/1094342012468181

The Exascale Computing Project was designed to help launch the exascale era

ECP funded teams spanned national labs, universities, and industry

$1.8B over 7 years in a formal Department of Energy 413.3B project

Funded by DOE’s Office of Science and NNSA programs

81 **Total research, development, and deployment projects**

6	Co-Design Centers
25	Application Development
35	Software Technology
17	Hardware and Integration

15
US DOE Labs, 6 of which are Core Partners

57
University Partners

36
Industry Organizations

- A **unique collaboration** brought together some of the brightest application, software, and computational experts from coast to coast
- **Best practices and lessons learned** for how to program GPUs – moving the nation forward
- **1000+ researchers** trained and ready for accelerator-based computing
- **1000+ students** introduced to HPC and Exascale computing through ECP’s outreach, training, and workforce development initiatives

Technical work was largely complete as of Dec 31, 2023

Project leadership team is now working to close out the formal DOE 413.3B project

Next 18 slides courtesy of Lori Diachin

The Exascale Computing Project was started in 2016 and tasked to meet four DOE mission needs in high performance computing

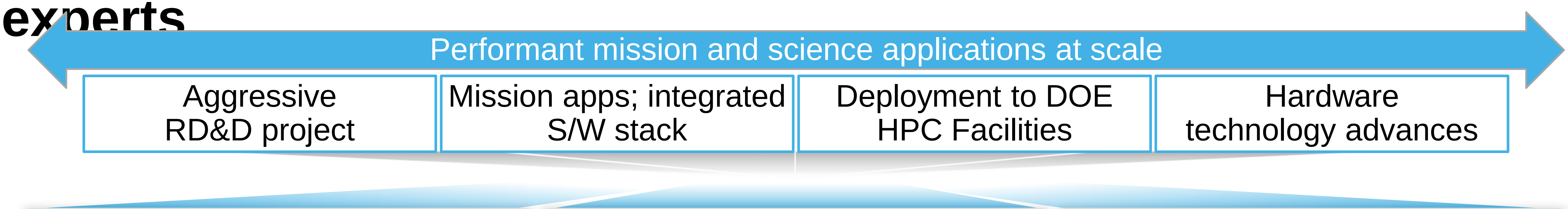
Deliver a long-term, **sustainable software ecosystem** that can be used and maintained for years to come

Promote the **health of the US HPC industry**

Ensure that exascale systems can be used to deliver **mission-critical applications**

Maintain **international leadership in HPC**

To meet mission needs, the ECP was organized into three technical focus areas partnered with formal project management experts



Performant mission and science applications at scale

Aggressive RD&D project

Mission apps; integrated S/W stack

Deployment to DOE HPC Facilities

Hardware technology advances

Application Development (AD)

Develop and enhance the predictive capability of applications critical to DOE

24 applications
National security, energy, Earth systems, economic security, materials, data

6 co-design centers
ML, graph analytics, mesh refinement, PDE discretization, particles, online data analytics

Andrew Siegel, AD Director
Erik Draeger, AD Deputy Director

Software Technology (ST)

Deliver expanded and vertically integrated software stack to achieve full potential of exascale computing

70 unique software products spanning programming models and runtimes, math libraries, data and visualization, development tools

Mike Heroux, ST Director
Lois Curfman McInnes, ST Deputy Director

Hardware and Integration (HI)

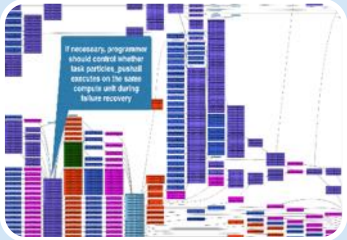
Integrated delivery of ECP products on targeted systems at leading DOE HPC facilities

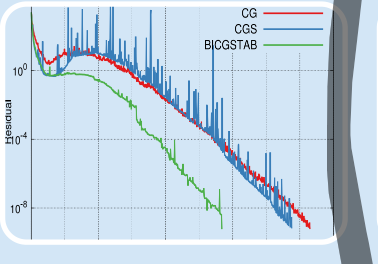
6 US HPC vendors
focused on exascale node and system design; application integration and software deployment to Facilities

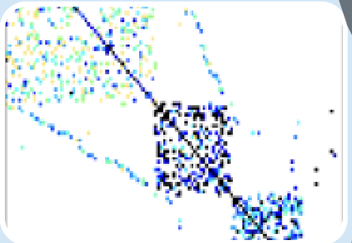
Richard Gerber, HI Director
Susan Coghlan, HI Deputy Director

ECP invested in six software technology areas

Emphasis for this presentation







Programming Models & Runtimes

- Enhance and get ready for exascale the MPI and OpenMP programming models (hybrid programming models, deep memory copies)
- Develop performance portability tools (e.g., Kokkos and Raja)
- Support alternate models for potential benefits and risk mitigation: PGAS (UPC++/GASNet), task-based models (Legion, PaRSEC)
- Libraries for deep memory hierarchy and power management

Development Tools

- Continued, multifaceted capabilities in portable, open-source LLVM compiler ecosystem to support expected ECP architectures, including support for F18
- Performance analysis tools that accommodate new architectures, programming models, e.g., PAPI, Tau

Math Libraries

- Linear algebra, iterative linear solvers, direct linear solvers, integrators and nonlinear solvers, optimization, FFTs, etc
- Performance on new node architectures; extreme strong scalability
- Advanced algorithms for multi-physics, multiscale simulation and outer-loop analysis
- Increasing quality, interoperability, complementarity of math libraries

Data and Visualization

- I/O via the HDF5 API
- Insightful, memory-efficient in-situ visualization and analysis
- Data reduction via scientific data compression
- Checkpoint restart

Software Ecosystem

- Develop features in Spack necessary to support ST products in E4S, and the AD projects that adopt it
- Develop Spack stacks for reproducible turnkey software deployment
- Optimization and interoperability of containers for HPC
- Regular E4S releases of the ST software stack and SDKs with regular integration of new ST products

NNSA ST

- Open source NNSA Software projects
- Projects that have both mission role and open science role
- Major technical areas: New programming abstractions, math libraries, data and viz libraries
- Cover most ST technology areas
- Subject to the same planning, reporting and review processes

Area Leads:

Rajeev Thakur

Jeff Vetter

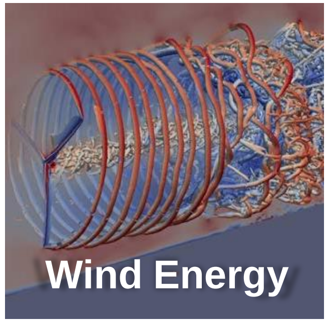
Sherry Li

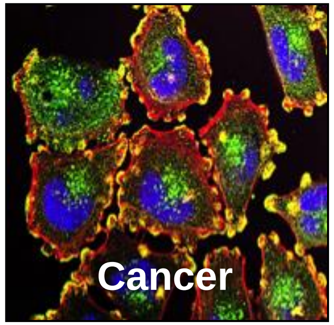
Jim Ahrens

Todd Munson

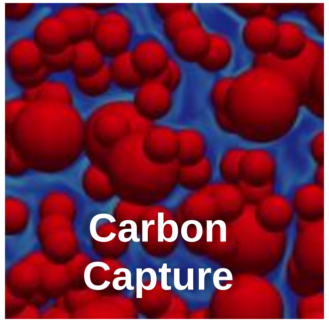
Kathryn Mohror

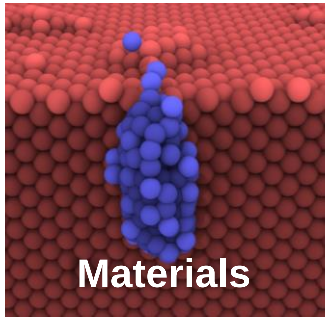
ECP invested in a broad range of critical application areas; some with limited HPC experience at project inception

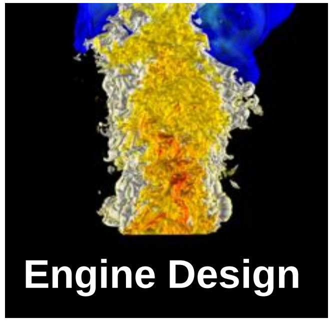

Wind Energy


Cancer

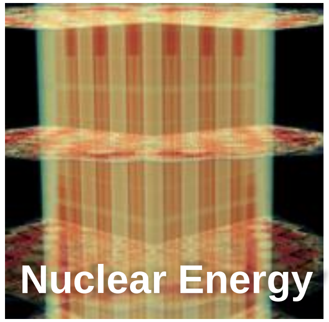
Climate

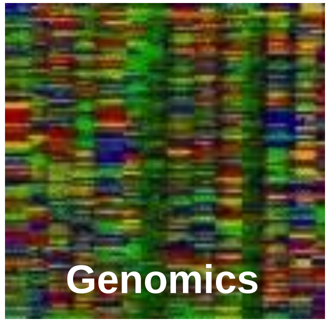

Carbon Capture

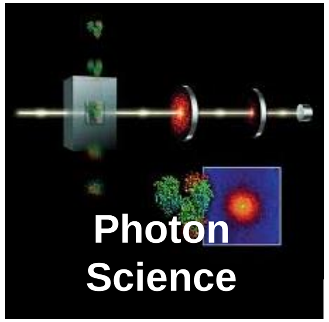

Materials

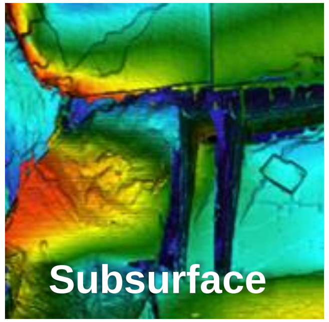

Engine Design

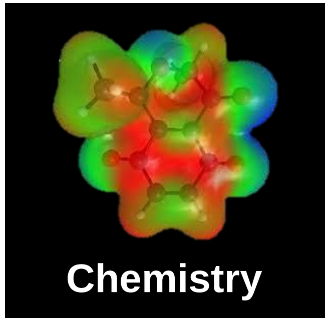
National Security

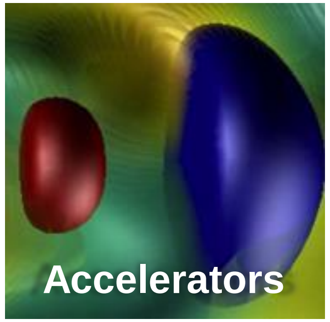

Nuclear Energy

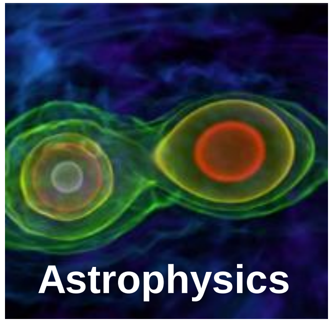

Genomics


Photon Science


Subsurface


Chemistry

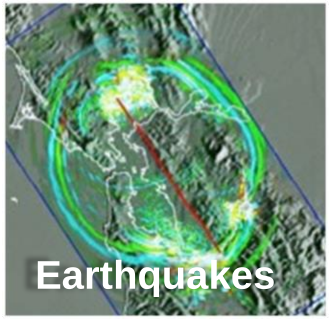

Accelerators

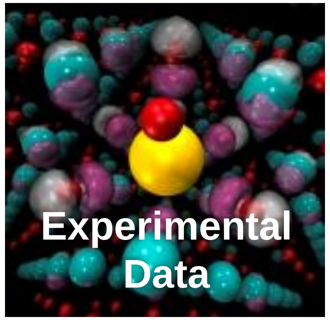

Astrophysics

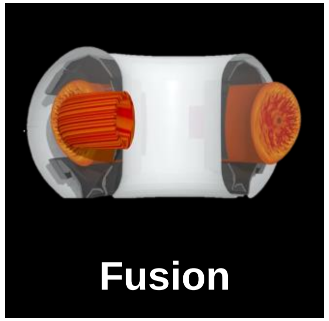
Power Grid

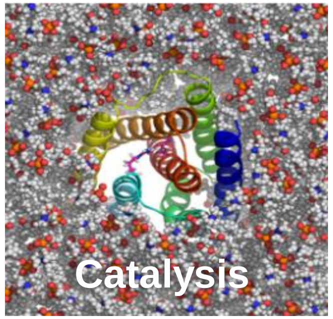
Additive Manufacturing

Quantum Theory


Earthquakes

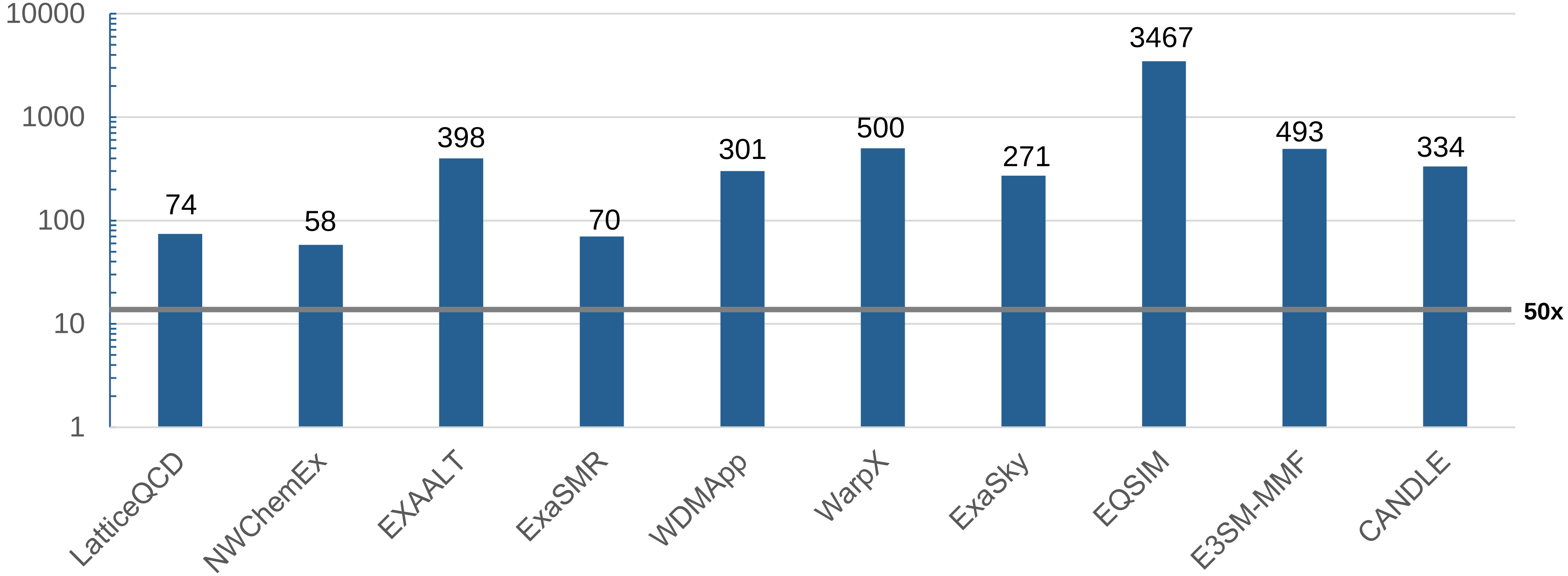

Experimental Data


Fusion

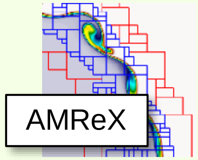

Catalysis

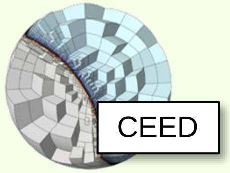
ECP application results exceeded expectations

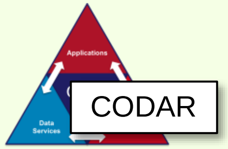
10 out of 11 projects surpassed an ambitious 50x performance target

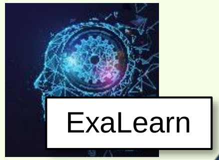


Co-design played a critical role



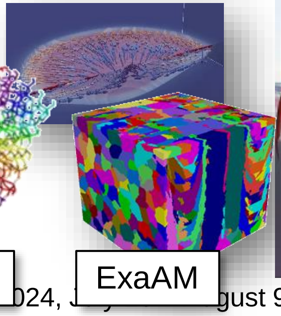


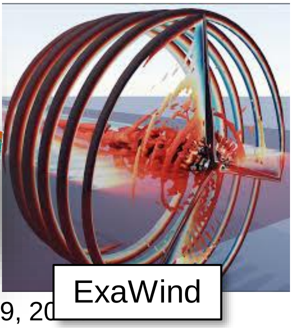


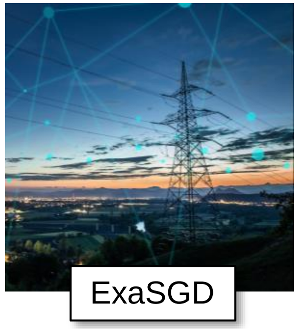


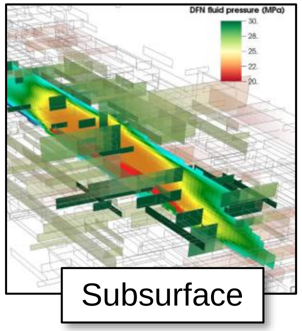
9 out of 10 new HPC science projects completed exascale capability demonstrations

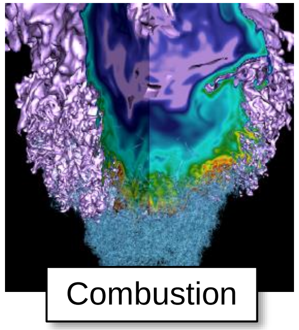
3 out of 4 NNSA applications demonstrated exascale readiness

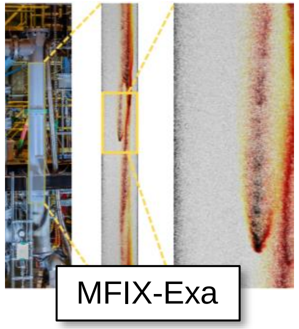


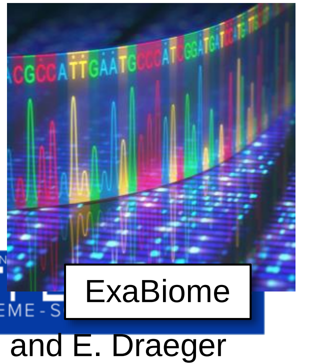












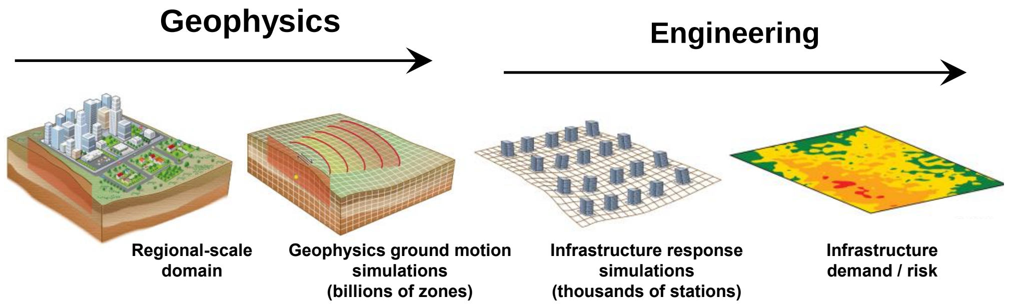
slide credit: A. Siegel and E. Draeger

One example EQSIM: exascale-capable code redesign had massive impact

EQSIM PI: Dave McCallen, LBNL

- **Starting point**: CPU-only code written in C by physicists. Code had complex nested loops (fourth-order finite difference stencil) that the compiler struggled to optimize, find SIMD.

- **ECP accomplishments**
  - Algorithmic improvements using curvilinear mesh refinement improved scientific work-rate by a factor of 2.85
  - Rewrote code in C++ with RAJA, with ZFP data compression to save sufficient data to maintain adequate precision in stored data
  - Infrastructure simulations now include strong coupling with OpenSees soil/building modeling and using in soil-structure interaction models; help gain insight into areas of maximum risk.



Geophysics

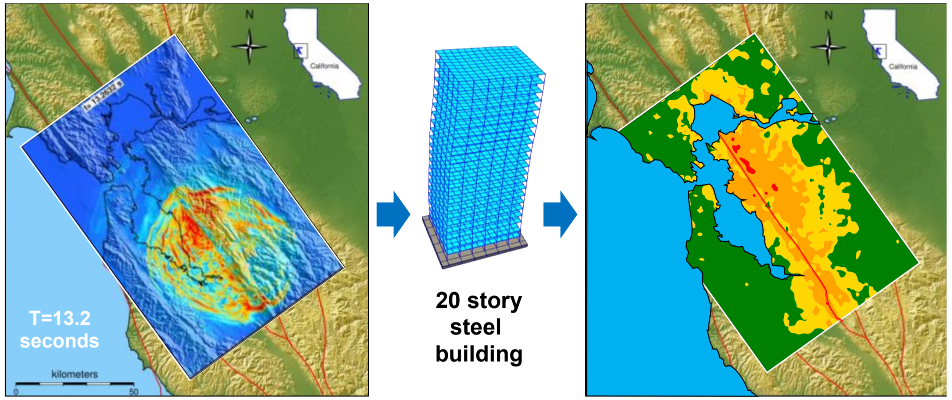
Engineering

Regional-scale domain

Geophysics ground motion simulations (billions of zones)

Infrastructure response simulations (thousands of stations)

Infrastructure demand / risk



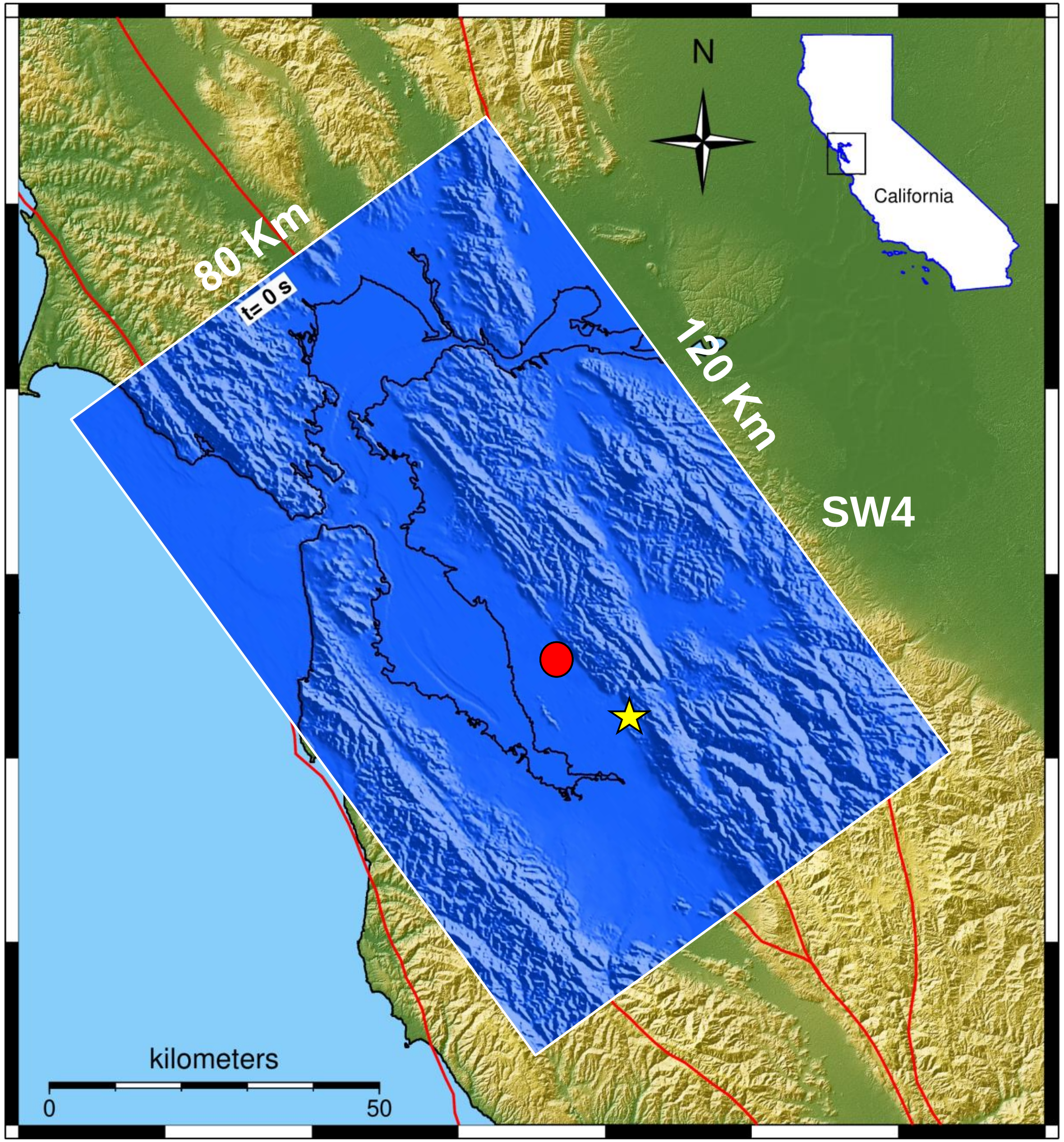
T=13.2 seconds

20 story steel building

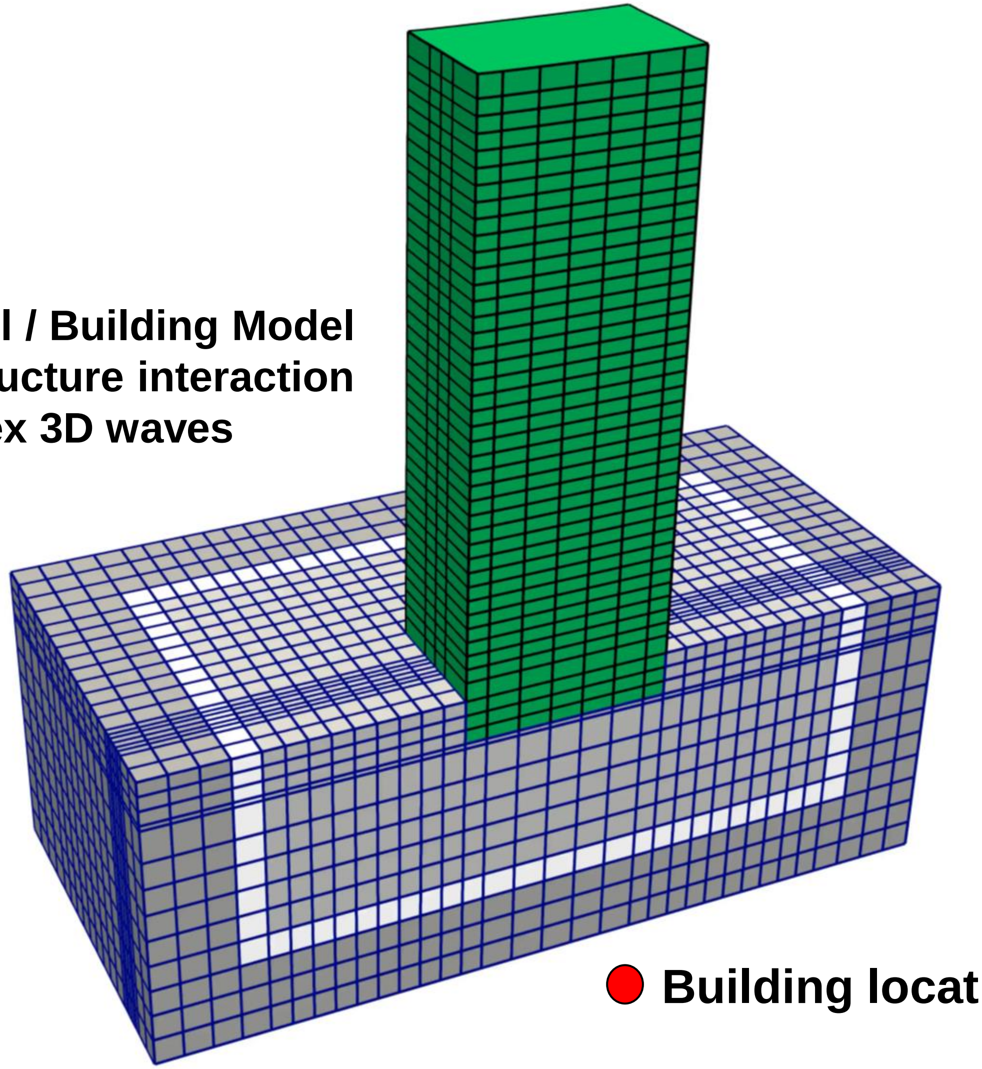
Achieved a **3500X improvement in computational performance** compared to initial baseline on Cori (~30 PF KNL system); Simulation of regional-scale ground motions at frequencies of engineering interest (5-10 Hz) now within reach.

Regional Geophysics Model (M7 Hayward fault earthquake)

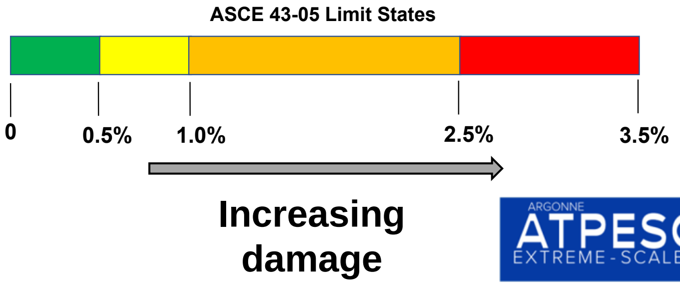
Fmax 10 Hz Vsmin 140 m/s 391 Billion grid points



Local Soil / Building Model
- Soil-structure interaction
- Complex 3D waves



● Building location



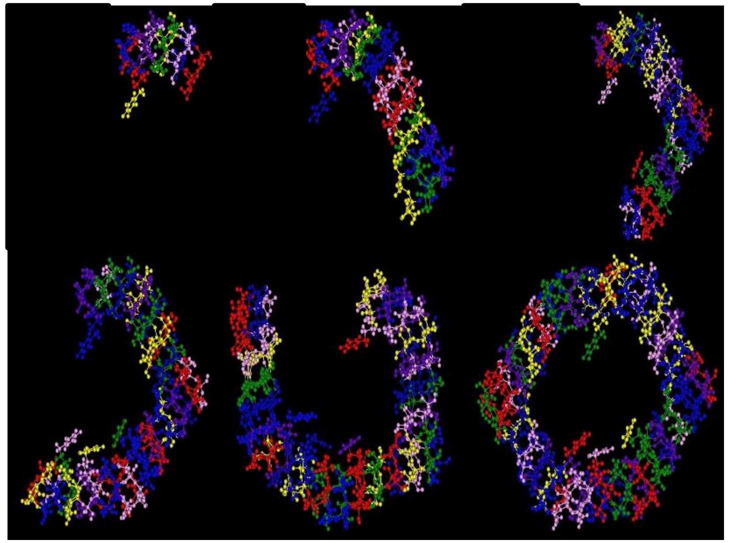
There where several key ingredients required for a successful ECP Application Development Project

Algorithmic innovation

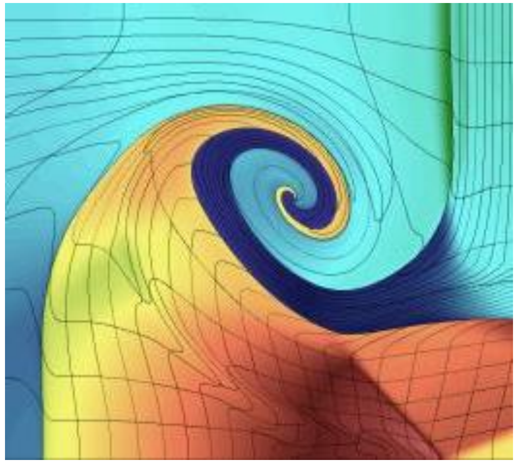
Porting

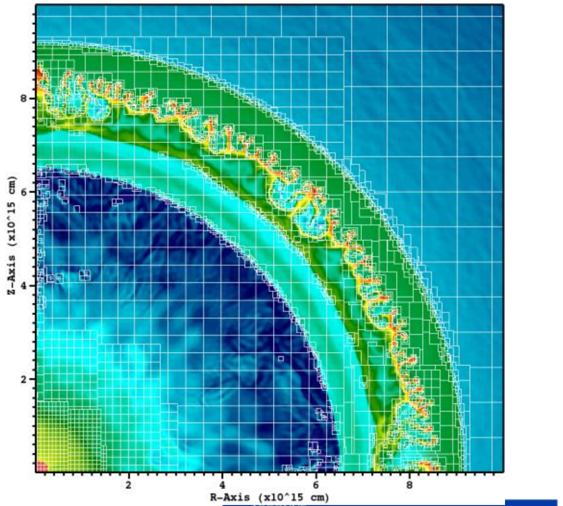
Integration

Algorithmic innovation: domain-driven adaptations critical for making efficient use of exascale systems

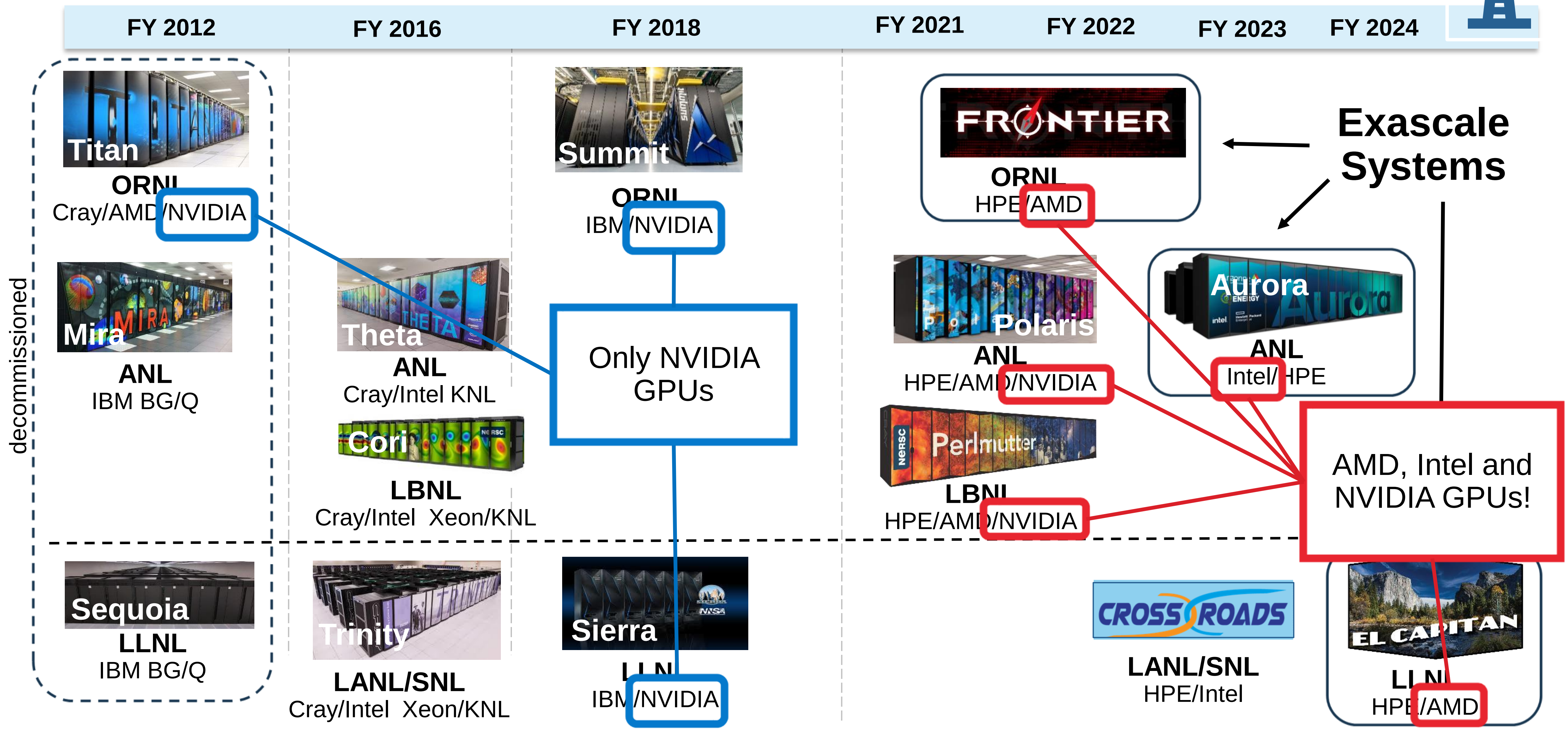


- Inherent strong scaling challenges on GPU-based systems
  - Ensembles vs. time averaging
  - Fluid dynamics, seismology, molecular dynamics, time-stepping
- Increase dimensions of (fine-grained) parallelism to feed GPUs
  - Ray tracing, Markov Chain Monte Carlo, fragmentation methods
- Localized physics models to maximize "free flops”
  - MMF, electron subcycling, enhanced subgrid models, high-order discretizations
- Alternatives to sparse linear systems
  - Higher order methods, Monte Carlo
- Reduced branching
  - Event-based models





HPC systems have come a long way since ECP's inception



FY 2012 | FY 2016 | FY 2018 | FY 2021 | FY 2022 | FY 2023 | FY 2024

decommissioned

Titan
ORNL
Cray/AMD/NVIDIA

Mira
ANL
IBM BG/Q

Sequoia
LLNL
IBM BG/Q

Theta
ANL
Cray/Intel KNL

Cori
LBNL
Cray/Intel Xeon/KNL

Trinity
LANL/SNL
Cray/Intel Xeon/KNL

Summit
ORNL
IBM/NVIDIA

Only NVIDIA GPUs

Sierra
LLNL
IBM/NVIDIA

FRONTIER
ORNL
HPE/AMD

Polaris
ANL
HPE/AMD/NVIDIA

Perlmutter
LBNL
HPE/AMD/NVIDIA

Aurora
ANL
Intel/ HPE

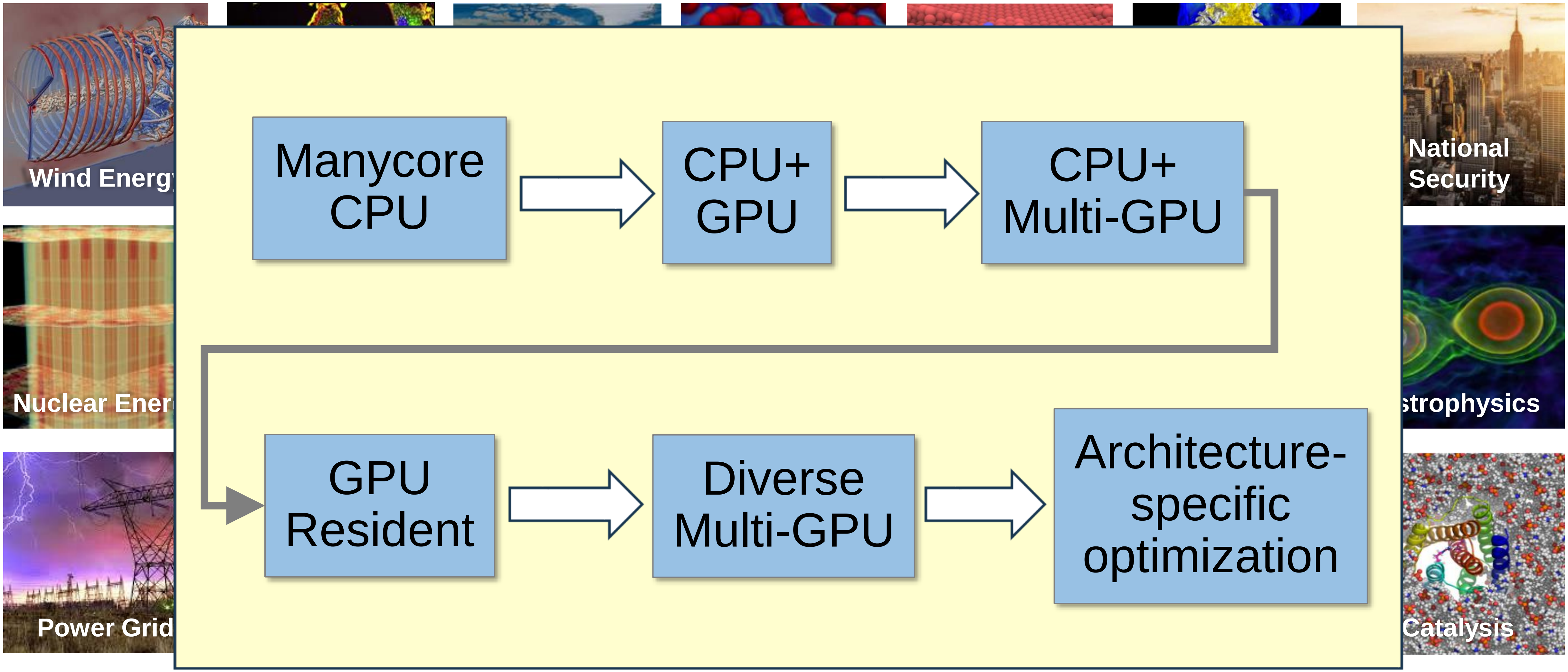
Exascale Systems

AMD, Intel and NVIDIA GPUs!

CROSSROADS
LANL/SNL
HPE/Intel

EL CAPITAN
LLNL
HPE/AMD

Exascale applications were designed to be flexible and adaptive



Manycore CPU → CPU+ GPU → CPU+ Multi-GPU → GPU Resident → Diverse Multi-GPU → Architecture-specific optimization

ECP applications teams used several different programming models to achieve performance portability

GPU-specific kernels

- Isolate the computationally-intensive parts of the code into CUDA/HIP/SYCL kernels.
- Refactoring the code to work well with the GPU is the majority of effort.

Loop pragma models

- Offload loops to GPU with OpenMP or OpenACC.
- Most common portability strategy for Fortran codes.

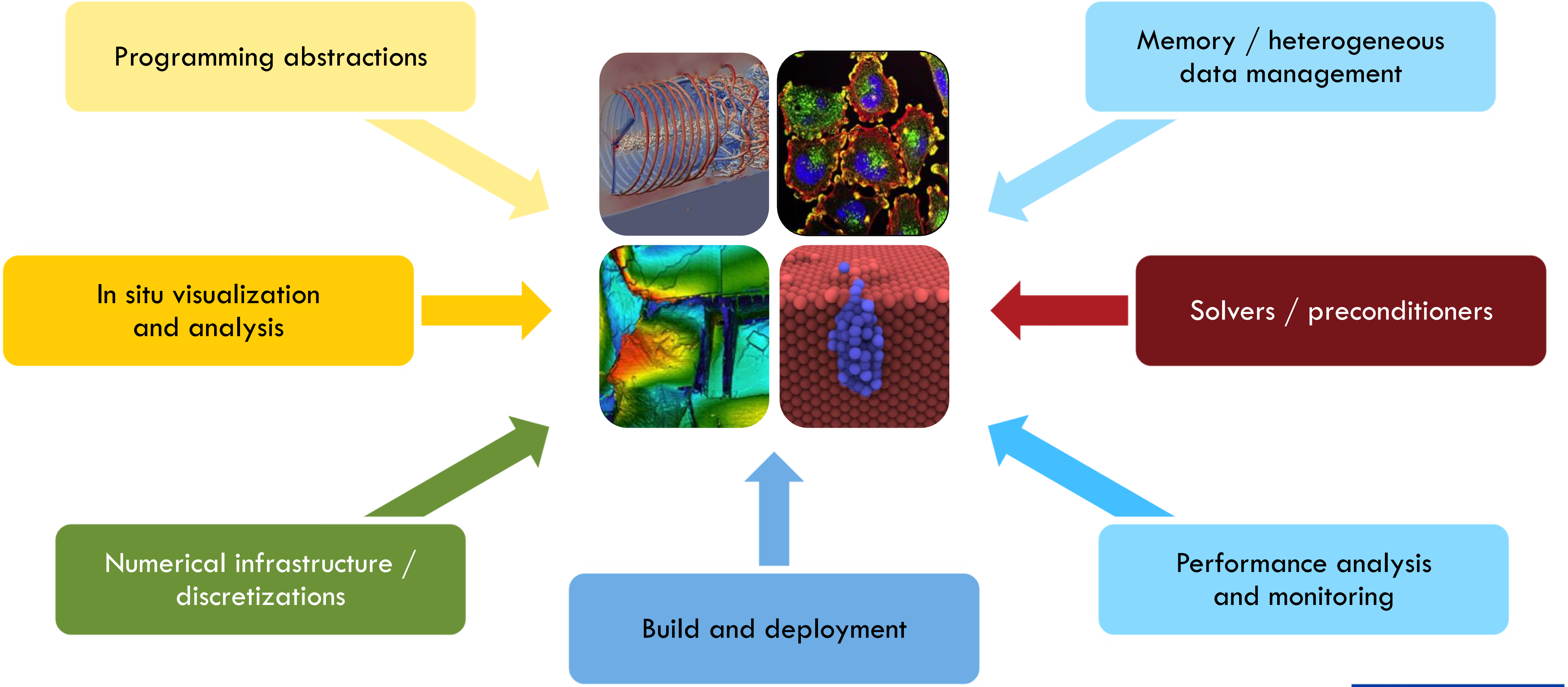
C++ abstractions

- Fully abstract loop execution and data management using advanced C++ features.
- Kokkos and RAJA developed by NNSA in response to increasing hardware diversity.

Co-design frameworks

- Design application with a specific motif to use common software components
- Depend on co-design code (e.g. CEED, AMReX) to implement key functions on GPU.

The success of exascale applications relied on significant software infrastructure



Programming abstractions

Memory / heterogeneous data management

In situ visualization and analysis

Solvers / preconditioners

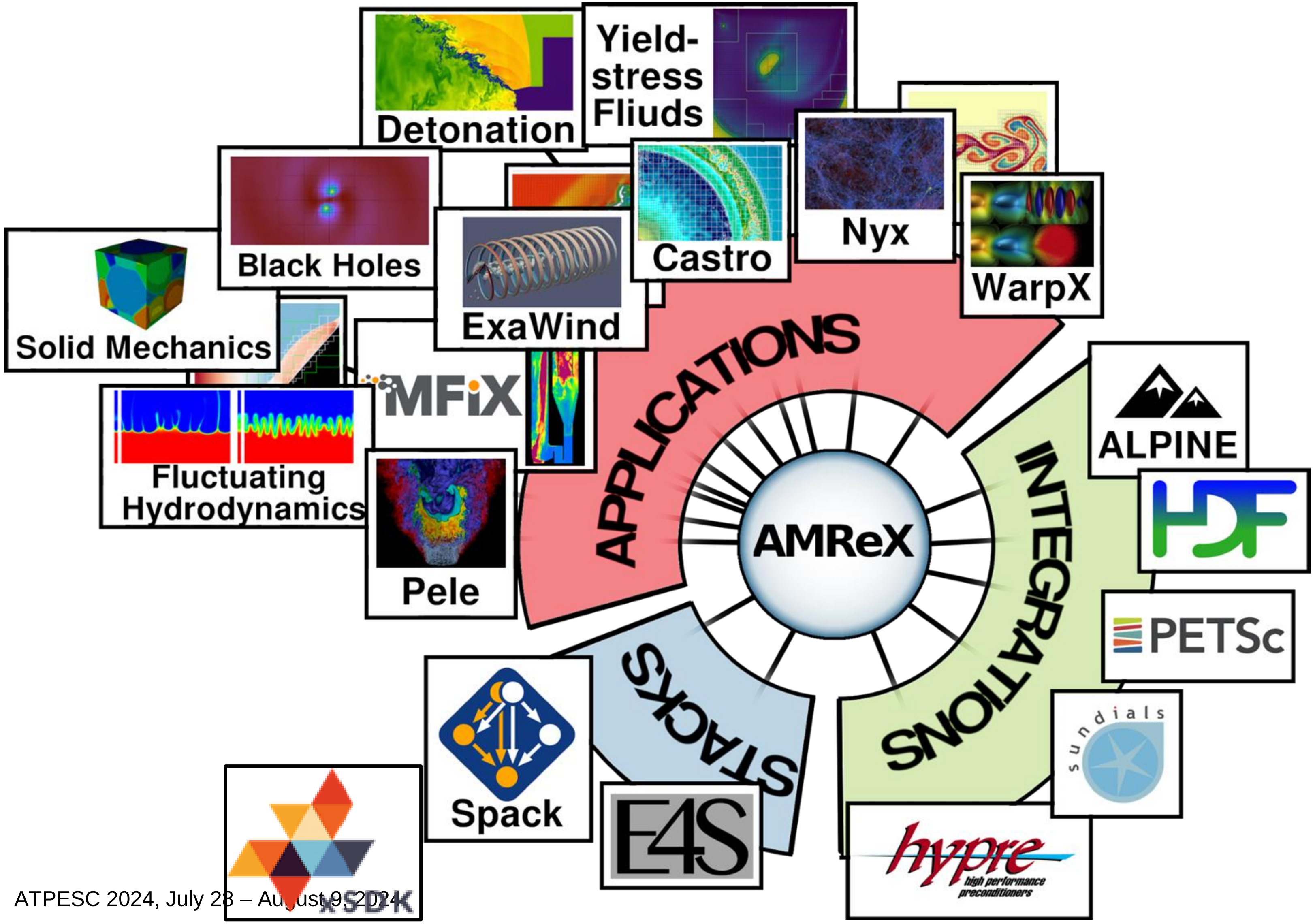
Numerical infrastructure / discretizations

Build and deployment

Performance analysis and monitoring

slide credit: A. Siegel and E. Draeger

Integration of multiple technologies allow users of higher-level frameworks, e.g., AMReX, access many different technologies



Software Integrations:

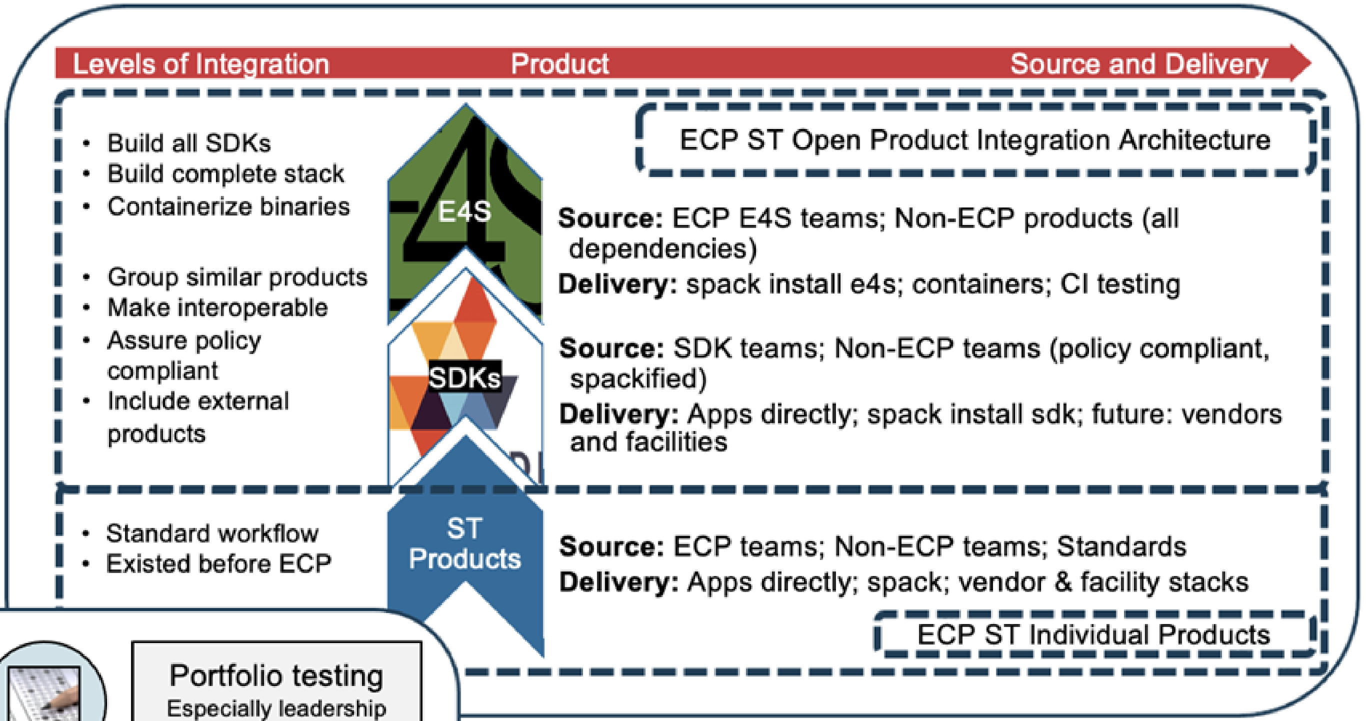
- SUNDIALS – Chemical reactions, time integrators
- *hypre*, PETSc – Linear solvers on mesh data
- In-situ: Ascent, Sensei
- Offline visualization: VisIt, Paraview, yt
- IO: HDF5, ADIOS

Software Stacks:

- Spack
  - Smoke test – CUDA, AMD HIP
- xSDK
- E4S

ECP software technologies were broadly deployed through the Extreme Scale Scientific Software Stack (E4S)

- ECP Software Technology lead: Mike Heroux (SNL)
- E4S: HPC software ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source**, **containers**, **cloud, binary caches**
- Not a commercial product – an open resource for all
- Supported by DOE and commercial entities (Paratools)
- Growing functionality: November 2023: E4S 23.11 – 100+ full release products



Levels of Integration
Product
Source and Delivery
ECP ST Open Product Integration Architecture
E4S
SDKs
ST Products
ECP ST Individual Products

- Build all SDKs
- Build complete stack
- Containerize binaries

Source: ECP E4S teams; Non-ECP products (all dependencies)
Delivery: spack install e4s; containers; CI testing

- Group similar products
- Make interoperable
- Assure policy compliant
- Include external products

Source: SDK teams; Non-ECP teams (policy compliant, spackified)
Delivery: Apps directly; spack install sdk; future: vendors and facilities

- Standard workflow
- Existed before ECP

Source: ECP teams; Non-ECP teams; Standards
Delivery: Apps directly; spack; vendor & facility stacks

Community Policies
Commitment to SW quality

DocPortal
Single portal to all E4S product info

Portfolio testing
Especially leadership platforms

Curated collection
The end of dependency hell

Quarterly releases

Build caches
10X build time improvement

Turnkey stack
A new user experience

https://e4s.io

Post-ECP Strategy
LSSw, ASCR Task Force

https://e4s.io

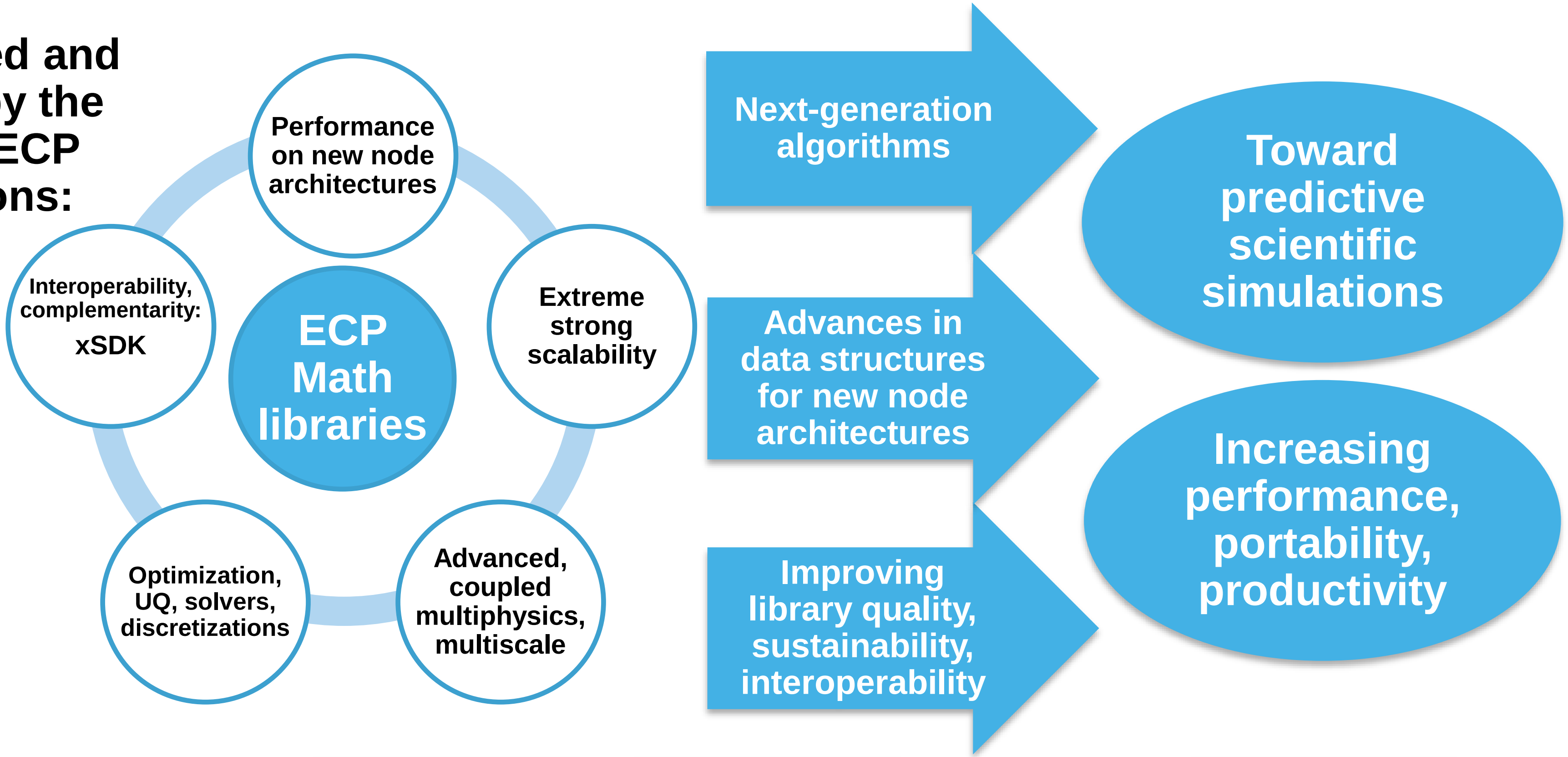
E4S lead: Sameer Shende (U Oregon)

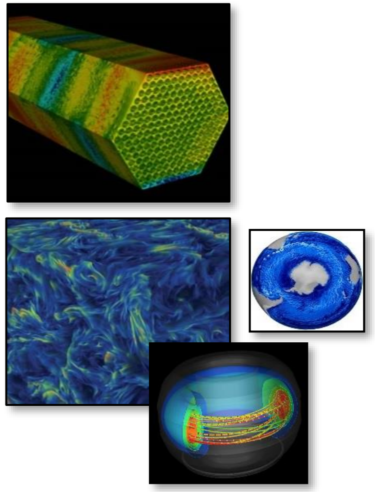
Spack https://spack.io

Spack lead: Todd Gamblin (LLNL)

xSDK: Primary delivery mechanism for ECP math libraries' continual advancements toward predictive science

As motivated and validated by the needs of ECP applications:


ECP Math libraries
Performance on new node architectures
Extreme strong scalability
Advanced, coupled multiphysics, multiscale
Optimization, UQ, solvers, discretizations
Interoperability, complementarity: xSDK
Next-generation algorithms
Advances in data structures for new node architectures
Improving library quality, sustainability, interoperability
Toward predictive scientific simulations
Increasing performance, portability, productivity



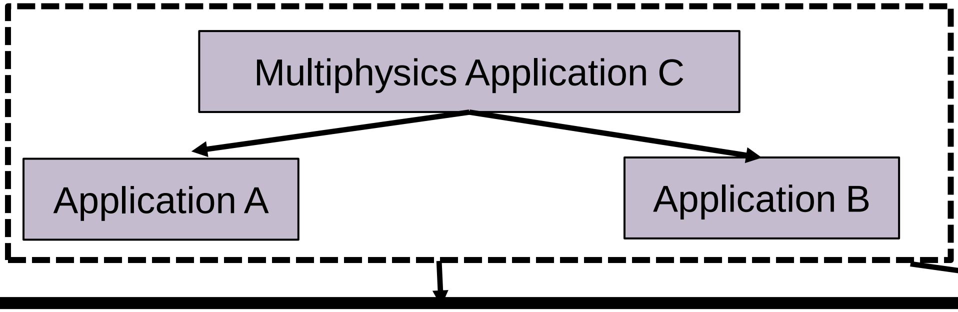
Timeline: xSDK release 1 | xSDK release 2 | . . . . . | xSDK release n

xSDK Version 1.0.0: November 2023

https://xsdk.info

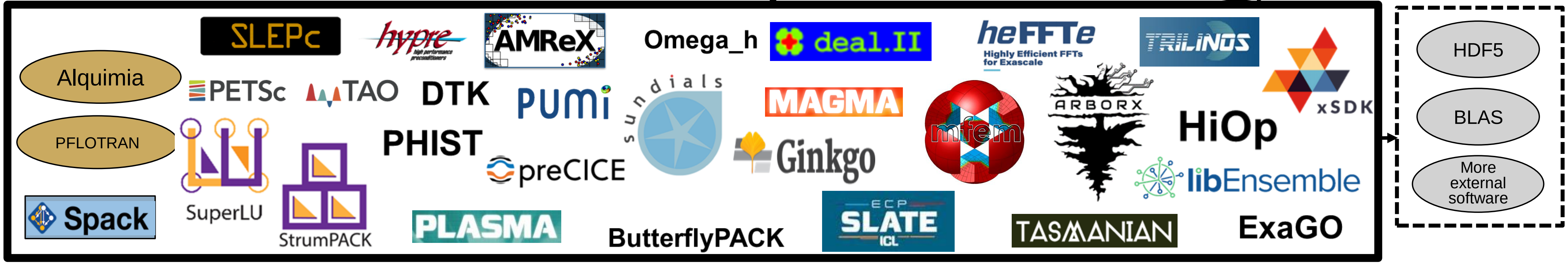
https://xsdk.info

Each xSDK member package uses or can be used with one or more xSDK packages, and the connecting interface is regularly tested for regressions.



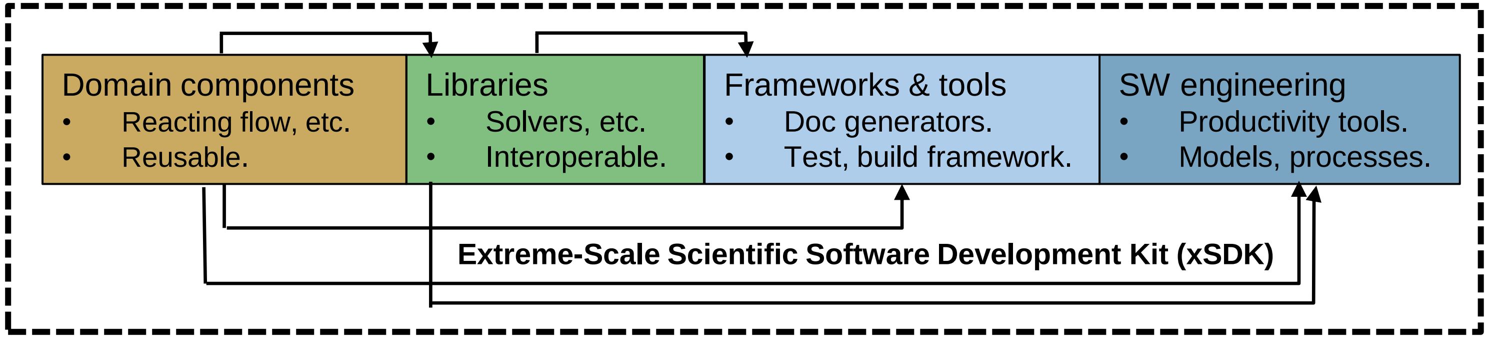
xSDK functionality, Nov 2023

Tested on key machines at ALCF, NERSC, OLCF, also Linux



November 2023

- 26 math libraries
- 2 domain components
- 17 mandatory xSDK community policies
- Spack xSDK installer



Domain components
- Reacting flow, etc.
- Reusable.

Libraries
- Solvers, etc.
- Interoperable.

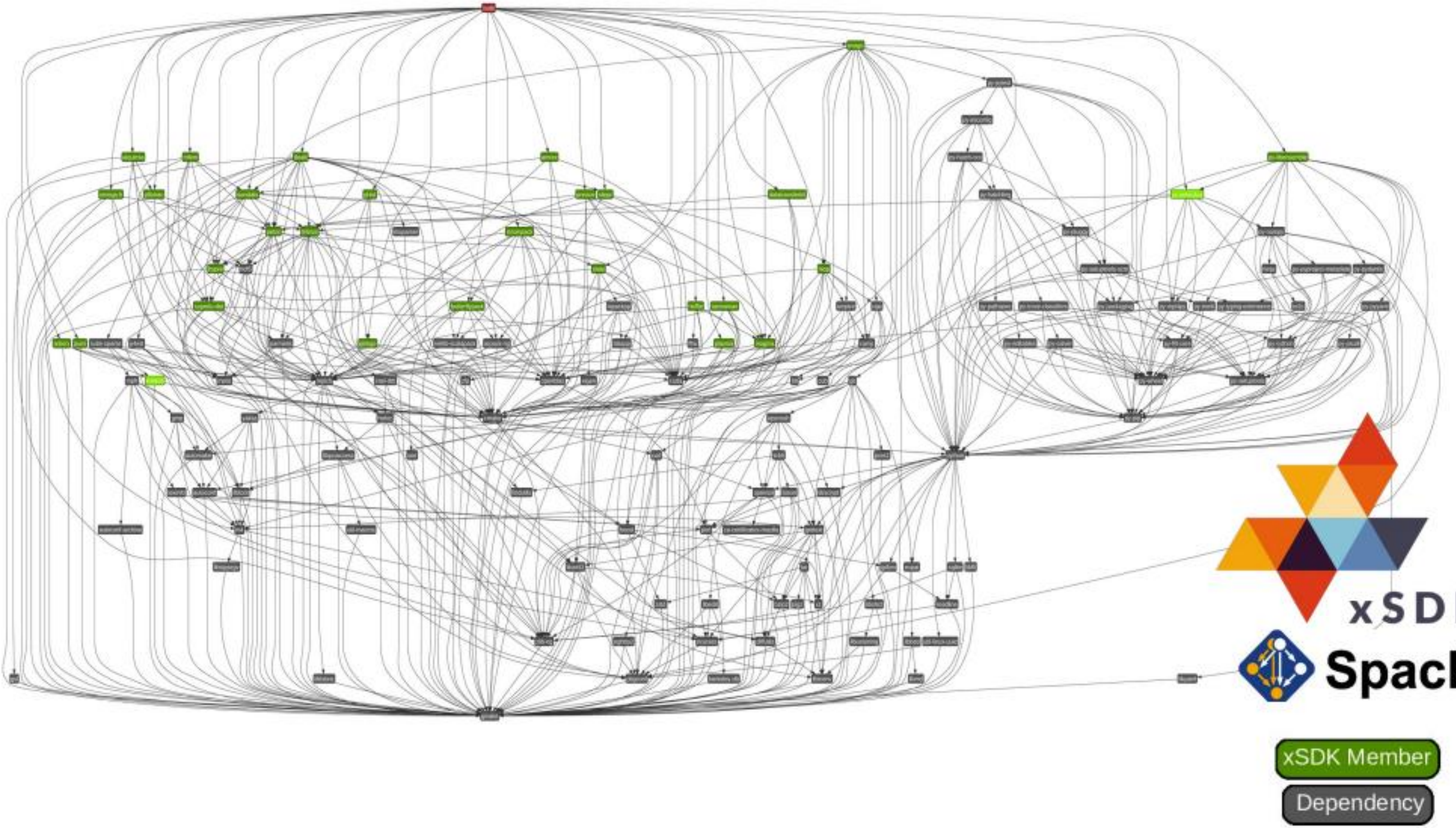
Frameworks & tools
- Doc generators.
- Test, build framework.

SW engineering
- Productivity tools.
- Models, processes.

Extreme-Scale Scientific Software Development Kit (xSDK)

Impact: Improved code quality, usability, access, sustainability

Foundation for work on performance portability, deeper levels of package interoperability


xSDK
Spack
xSDK Member
Dependency

xSDK: https://xsdk.info

Building the foundation of an extreme-scale scientific software ecosystem

xSDK community policies: Help address challenges in interoperability and sustainability of software developed by diverse groups at different institutions

https://github.com/xsdk-project/xsdk-community-policies

xSDK compatible package: must satisfy the mandatory xSDK policies (M1, ..., M17)

Topics include configuring, installing, testing, MPI usage, portability, contact and version information, open-source licensing, namespacing, and repository access

Also specify **recommended policies**, which currently are encouraged but not required (R1, ..., R8)

Topics include public repository access, error handling, freeing system resources, and library dependencies, documentation quality

xSDK member package:

(1) Must be an xSDK-compatible package, *and*

(2) it uses or can be used by another package in the xSDK, and the connecting interface is regularly tested for regressions.

xSDK policies 1.0.0: Feb 2023

- Facilitate combined use of independently developed packages

Impact:

- Improved code quality, usability, access, sustainability
- Foundation for work on deeper levels of interoperability and performance portability

We encourage feedback and contributions!

The Exascale Computing Project has delivered on its mission needs

Deliver a long-term, **sustainable software ecosystem** that can be used and maintained for years to come

- ❖ E4S deployed at HPC facilities around the US and the world
- ❖ 76 HPC products available for computing at all scales
- ❖ Performance portability tools developed and widely used

Ensure that exascale systems can be used to deliver **mission-critical applications**

- ❖ ECP applications demonstrate outstanding performance and capabilities at exascale
- ❖ Previously unattainable results in real-world challenge problems
- ❖ ECP lessons learned pave the way for many additional applications to leverage accelerator-based computing

Promote the **health of the US HPC industry**

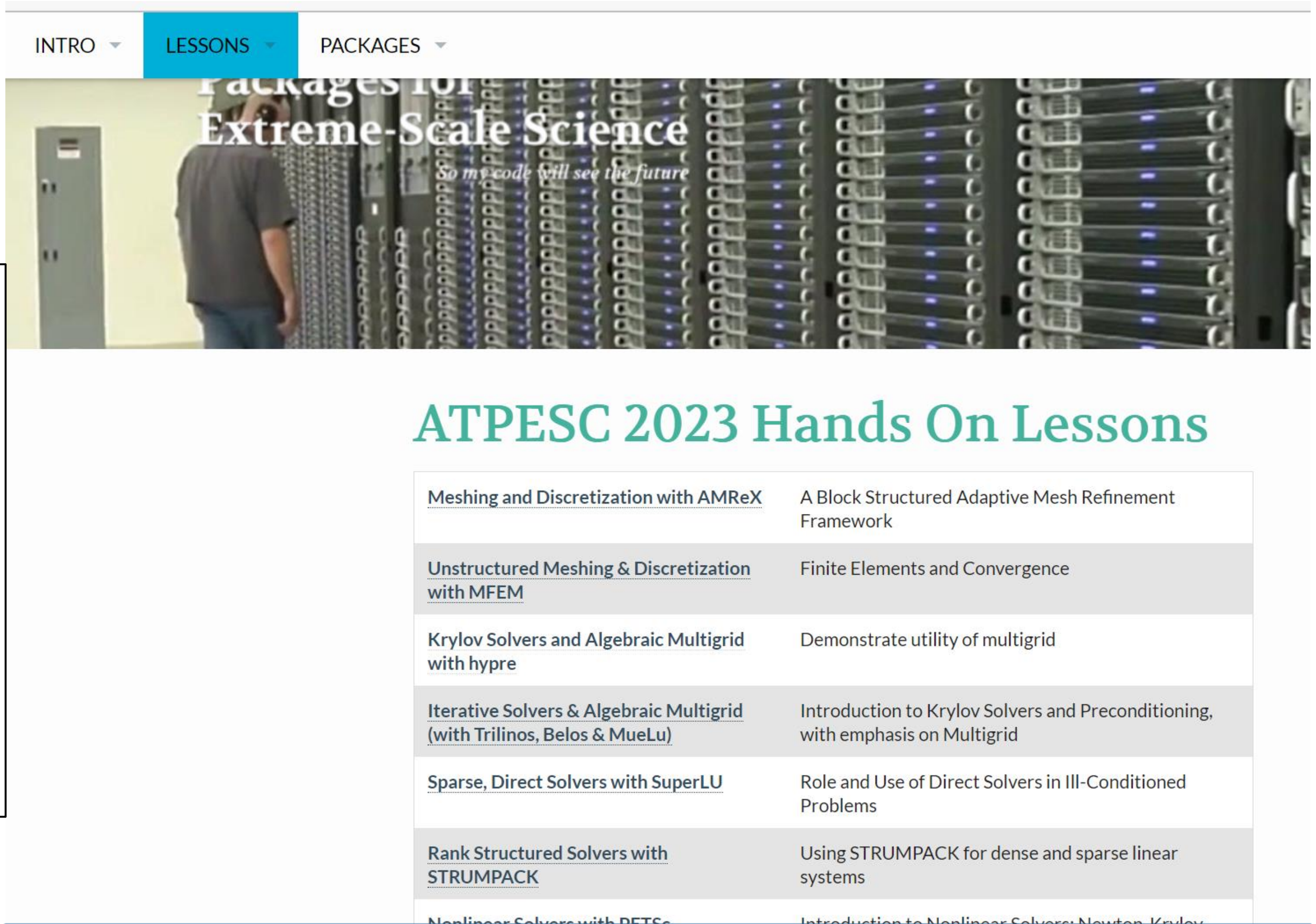
- ❖ Six vendors funded under PathForward; outcomes realized in exascale systems
- ❖ Accelerator-based computing lowers cost of energy across the board
- ❖ The ECP Industry and Agency Council stimulates consumption of HPC resources

Maintain **international leadership in HPC**

- ❖ Frontier is the world’s first exascale machine – in part due to ECP/ECI investments
- ❖ Aurora is the world’s second exascale system
- ❖ 1000+ researchers trained in GPU computing

HandsOn Lessons

- Structured meshing & discretization
- Unstructured meshing & discretization
- Krylov solvers & preconditioners
- Sparse direct solvers
- Nonlinear solvers
- Time integration
- Numerical optimization



ATPESC 2023 Hands On Lessons

Meshing and Discretization with AMReX	A Block Structured Adaptive Mesh Refinement Framework
Unstructured Meshing & Discretization with MFEM	Finite Elements and Convergence
Krylov Solvers and Algebraic Multigrid with hypre	Demonstrate utility of multigrid
Iterative Solvers & Algebraic Multigrid (with Trilinos, Belos & MueLu)	Introduction to Krylov Solvers and Preconditioning, with emphasis on Multigrid
Sparse, Direct Solvers with SuperLU	Role and Use of Direct Solvers in Ill-Conditioned Problems
Rank Structured Solvers with STRUMPACK	Using STRUMPACK for dense and sparse linear systems
Nonlinear Solvers with PETSc	Introduction to Nonlinear Solvers: Newton-Krylov

And more …

Github pages site:

https://xsdk-project.github.io/MathPackagesTraining2024/lessons/

If you haven’t yet done so, please choose which session you plan to attend!

Time	Room?	Room?
8:30 – 9:30	Introduction to Numerical Software – Ulrike Yang	
9:30 – 10:45	Structured Discretization (AMReX) – Andrew Myers, Weiqun Zhang	Unstructured Discretization (MFEM/PUMI) – Mark Shephard, Cameron Smith, Vladimir Tomov
10:45 – 11:15	Break, Subject Matter Expert (SME) Selections, Panel Questions	
11:15 – 12:30	Iterative Solvers & Algebraic Multigrid (hypre) – Daniel Osei-Kuffuor, Ulrike Yang	Direct Solvers (SuperLU, STRUMPACK) – Sherry Li, Pieter Ghysels
12:30 – 1:30	Lunch, SME Selections, Panel Questions	
1:30 – 2:45	Nonlinear Solvers (PETSc) – Toby Isaac	Time Integration (SUNDIALS) – David Gardner
2:45 – 3:15	Break, SME Selections, **Panel Questions Due**	
3:15 – 4:30	Optimization (TAO) – Todd Munson	Iterative Solvers & Algebraic Multigrid (Trilinos/ Belos/MueLU) – Christian Glusa, Graham Harper
4:30 – 5:30	Wrap-up (Ann Almgren) / Panel: Extreme-Scale Numerical Algorithms and Software	
5:30 – 6:30	Unstructured Time: **SME Selections Due**, Informal Discussion, Continue Hands-on	
6:30 – 7:30	Dinner	
7:30 – 9:30	Optional Activity: SME Speed-dating	

Room Choice

- Please raise your hand if you want to attend
  - Structured meshing

    AMReX

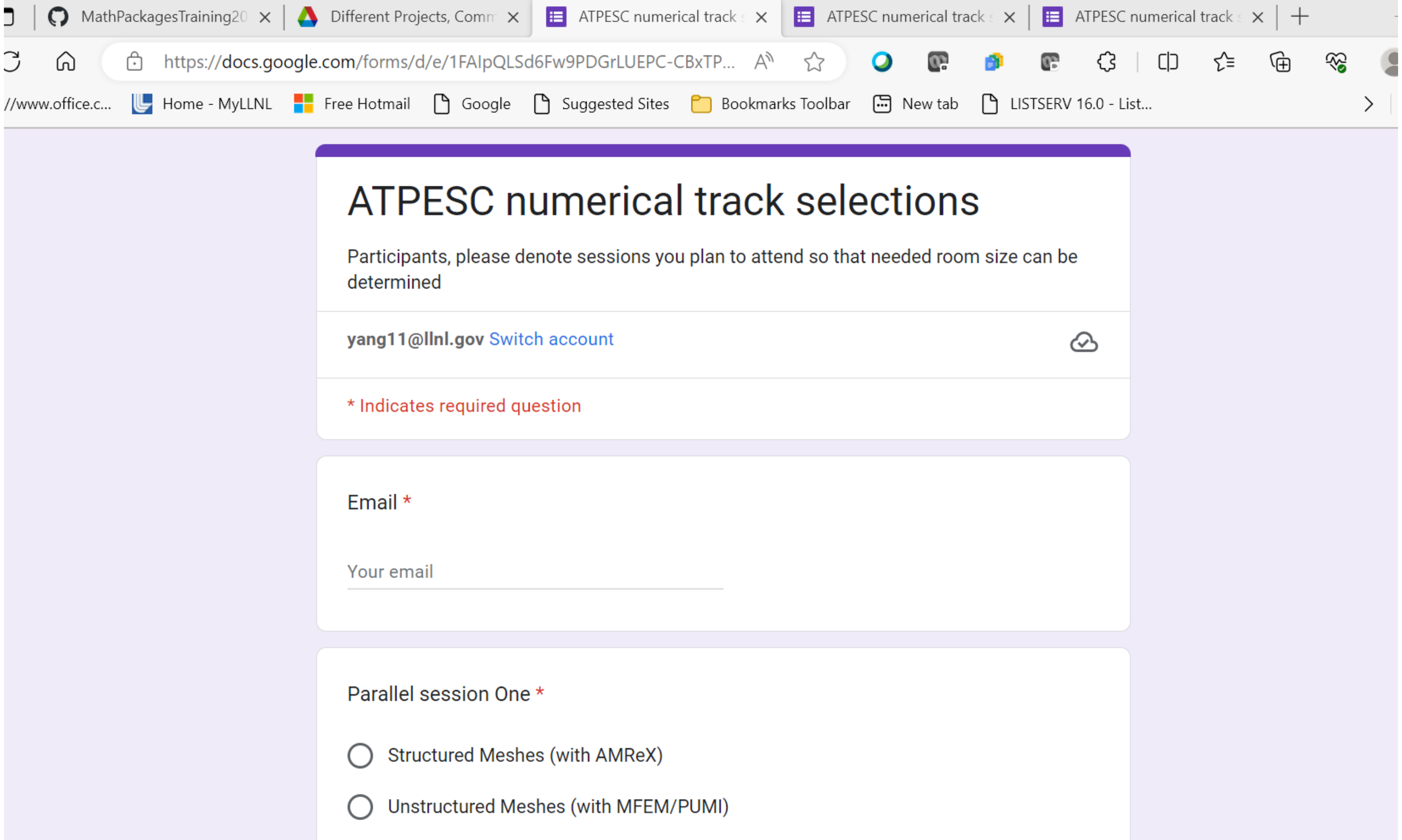
  - Unstructured meshing

    mfem

    PUMi

Choose which lecture you want to attend!

Access form here



ATPESC numerical track selections

Participants, please denote sessions you plan to attend so that needed room size can be determined

yang11@llnl.gov Switch account

* Indicates required question

Email *

Your email

Parallel session One *

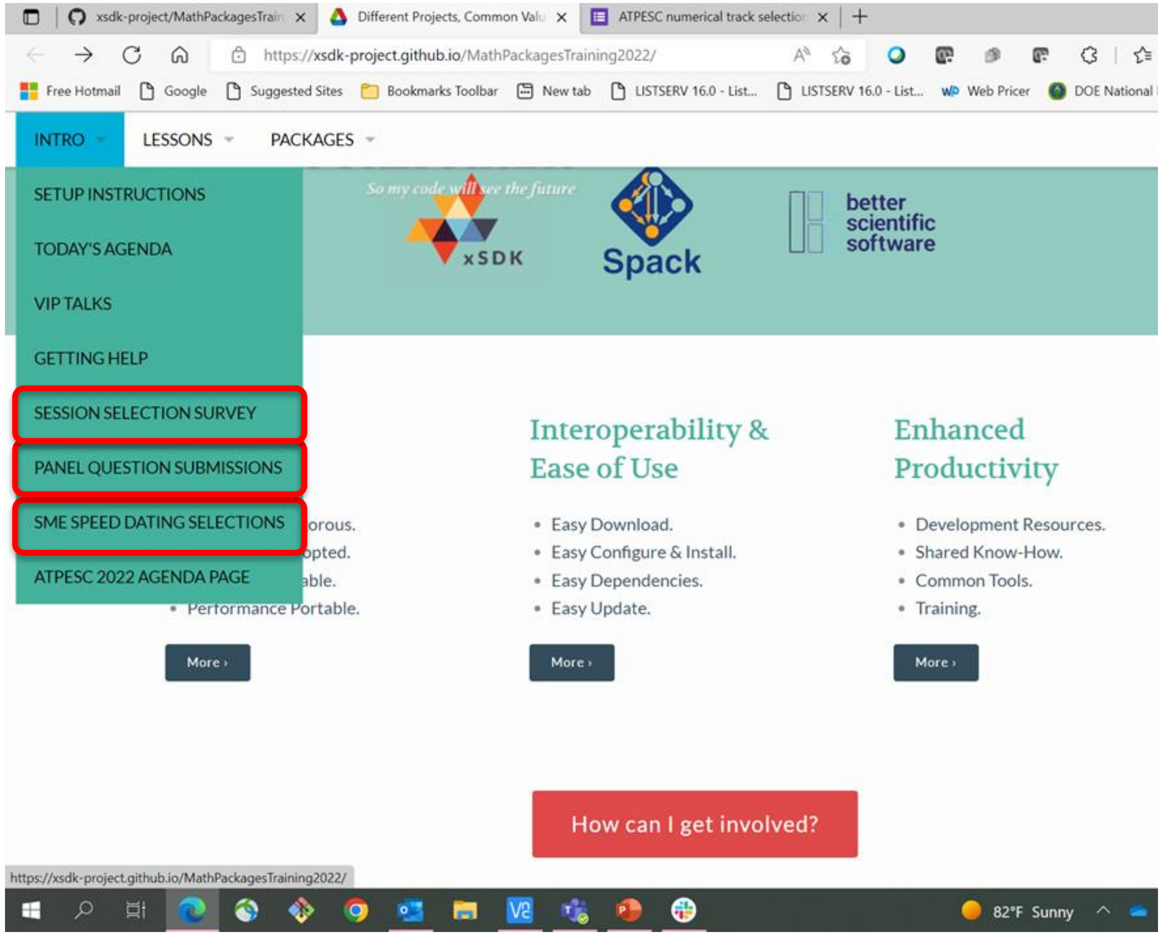
○ Structured Meshes (with AMReX)

○ Unstructured Meshes (with MFEM/PUMI)

Next steps

- **If you haven’t done so**
  – **Choose which session you will attend!**

- **During breaks and lunch**
  – **Submit questions for panelists** (optional)
  – **Sign up for discussions with numerical software developers** (optional)
    - **Your email address**
    - Complete by 3:30 pm CDT


xsdk-project/MathPackagesTrain
Different Projects, Common Valu
ATPESC numerical track selectio
https://xsdk-project.github.io/MathPackagesTraining2022/
Free Hotmail
Google
Suggested Sites
Bookmarks Toolbar
New tab
LISTSERV 16.0 - List...
LISTSERV 16.0 - List...
Web Pricer
DOE National
INTRO
LESSONS
PACKAGES
SETUP INSTRUCTIONS
TODAY'S AGENDA
VIP TALKS
GETTING HELP
SESSION SELECTION SURVEY
PANEL QUESTION SUBMISSIONS
SME SPEED DATING SELECTIONS
ATPESC 2022 AGENDA PAGE
So my code will see the future
xSDK
Spack
better scientific software
More ›
More ›
More ›
How can I get involved?
https://xsdk-project.github.io/MathPackagesTraining2022/
82°F Sunny

orous.
opted.
able.
- Performance Portable.

Interoperability & Ease of Use

- Easy Download.
- Easy Configure & Install.
- Easy Dependencies.
- Easy Update.

Enhanced Productivity

- Development Resources.
- Shared Know-How.
- Common Tools.
- Training.

Thank you to all ATPESC staff

Special thanks to Ray Loy and Yasaman Ghadar

For their outstanding work in running the 2-week ATPESC program

And thank you to all ATPESC attendees for engaging questions and discussions!

CASC

Center for Applied Scientific Computing

Lawrence Livermore National Laboratory

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC. LLNL-PRES-852746

This work was supported by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research (ASCR), Scientific Discovery through Advanced Computing (SciDAC) program, and by the Exascale Computing Project, a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

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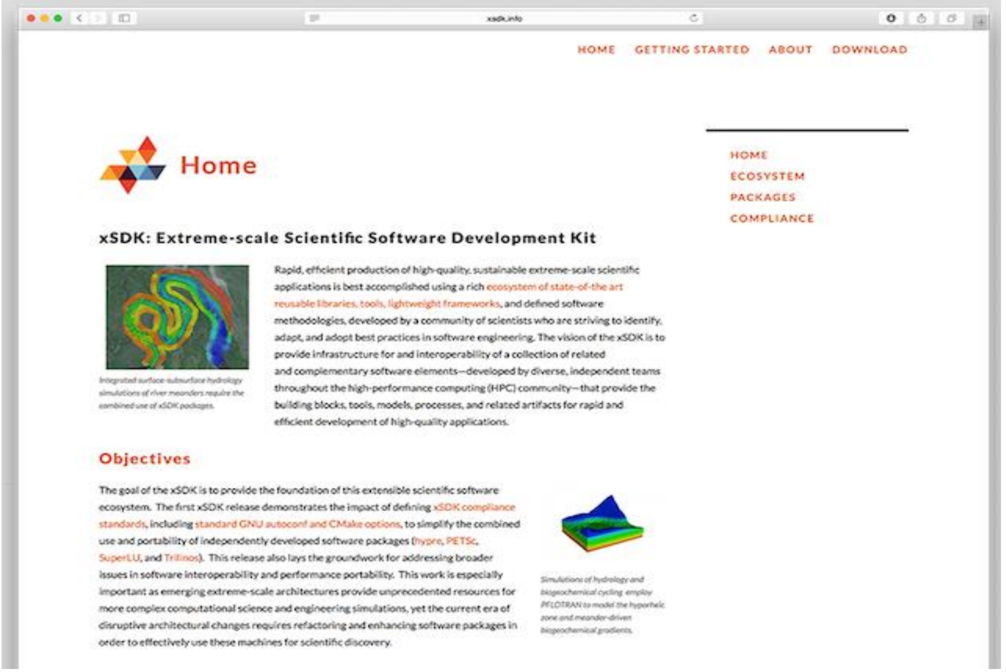
Building the foundation of a highly effective extreme-scale scientific software ecosystem

Focus: Increasing the functionality, quality, and interoperability of important scientific libraries, domain components, and development tools

Impact:

- Improved code quality, usability, access, sustainability
- Inform potential users that an xSDK member package can be easily used with other xSDK packages
- Foundation for work on performance portability, deeper levels of package interoperability



Home

xSDK: Extreme-scale Scientific Software Development Kit

Rapid, efficient production of high-quality, sustainable extreme-scale scientific applications is best accomplished using a rich ecosystem of state-of-the art reusable libraries, tools, lightweight frameworks, and defined software methodologies, developed by a community of scientists who are striving to identify, adapt, and adopt best practices in software engineering. The vision of the xSDK is to provide infrastructure for and interoperability of a collection of related and complementary software elements—developed by diverse, independent teams throughout the high-performance computing (HPC) community—that provide the building blocks, tools, models, processes, and related artifacts for rapid and efficient development of high-quality applications.

Integrated surface-subsurface hydrology simulations of river meanders require the combined use of xSDK packages.

Objectives

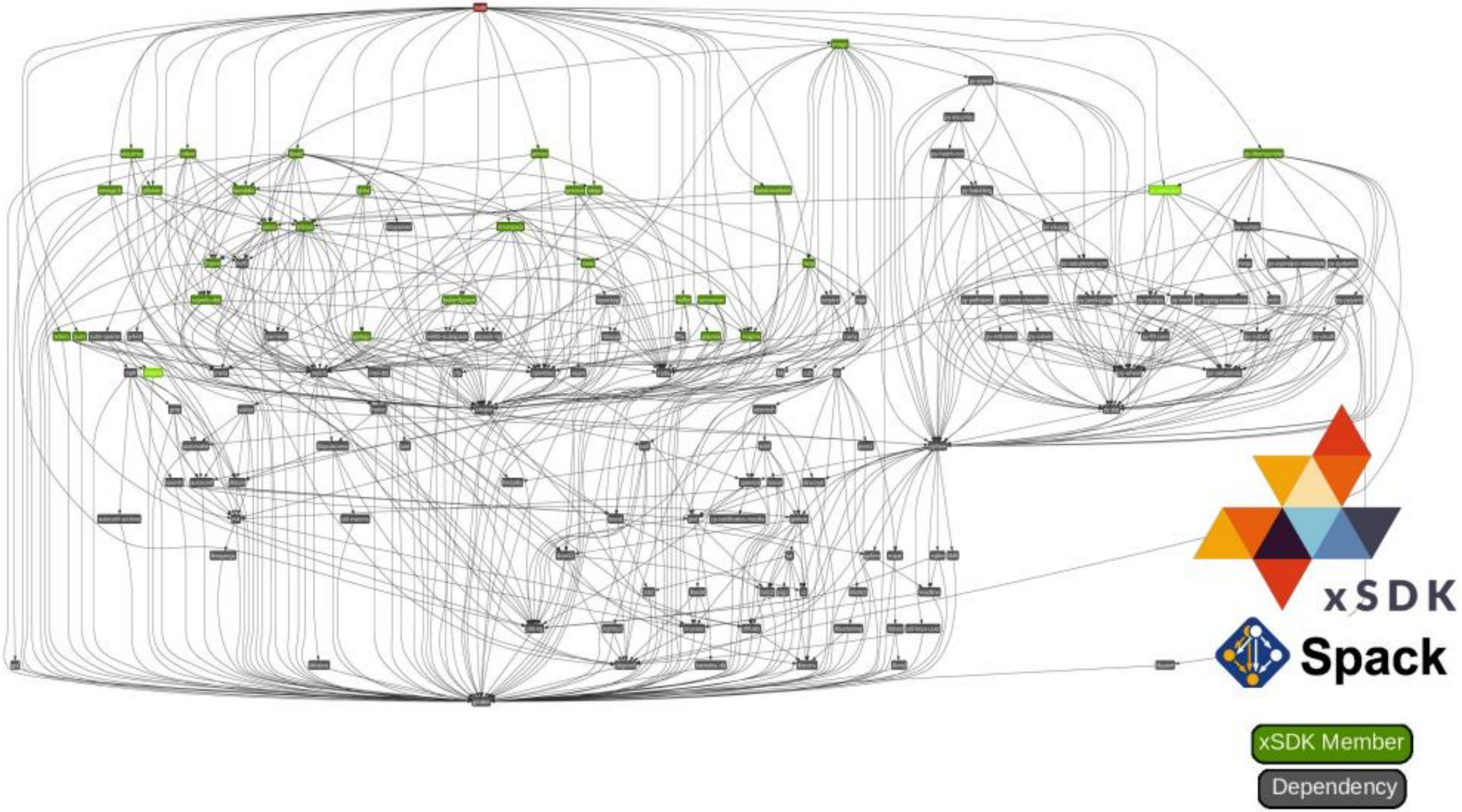
The goal of the xSDK is to provide the foundation of this extensible scientific software ecosystem. The first xSDK release demonstrates the impact of defining xSDK compliance standards, including standard GNU autoconf and CMake options, to simplify the combined use and portability of independently developed software packages (hypre, PETSc, SuperLU, and Trilinos). This release also lays the groundwork for addressing broader issues in software interoperability and performance portability. This work is especially important as emerging extreme-scale architectures provide unprecedented resources for more complex computational science and engineering simulations, yet the current era of disruptive architectural changes requires refactoring and enhancing software packages in order to effectively use these machines for scientific discovery.

Simulations of hydrology and biogeochemical cycling employ PFLOTRAN to model the hyporheic zone and meander-driven biogeochemical gradients.

website: xSDK.info

The xSDK is using Spack to deploy its software

- The xSDK packages depend on a number of open-source libraries
- Spack is a flexible package manager for HPC (see Track 3: Software Productivity and Sustainability)
- Spack allows the xSDK to be deployed with a single command
  - User can optionally choose compilers, build options, etc.



https://spack.io github.com/spack