

Overview of Numerical Algorithms and Software for Extreme-Scale Science

Presented to
ATPESC 2020 Participants

Lois Curfman McInnes
Argonne National Laboratory

Mark C. Miller
Lawrence Livermore National Laboratory

Date 08/04/2020



ATPESC Numerical Software Track

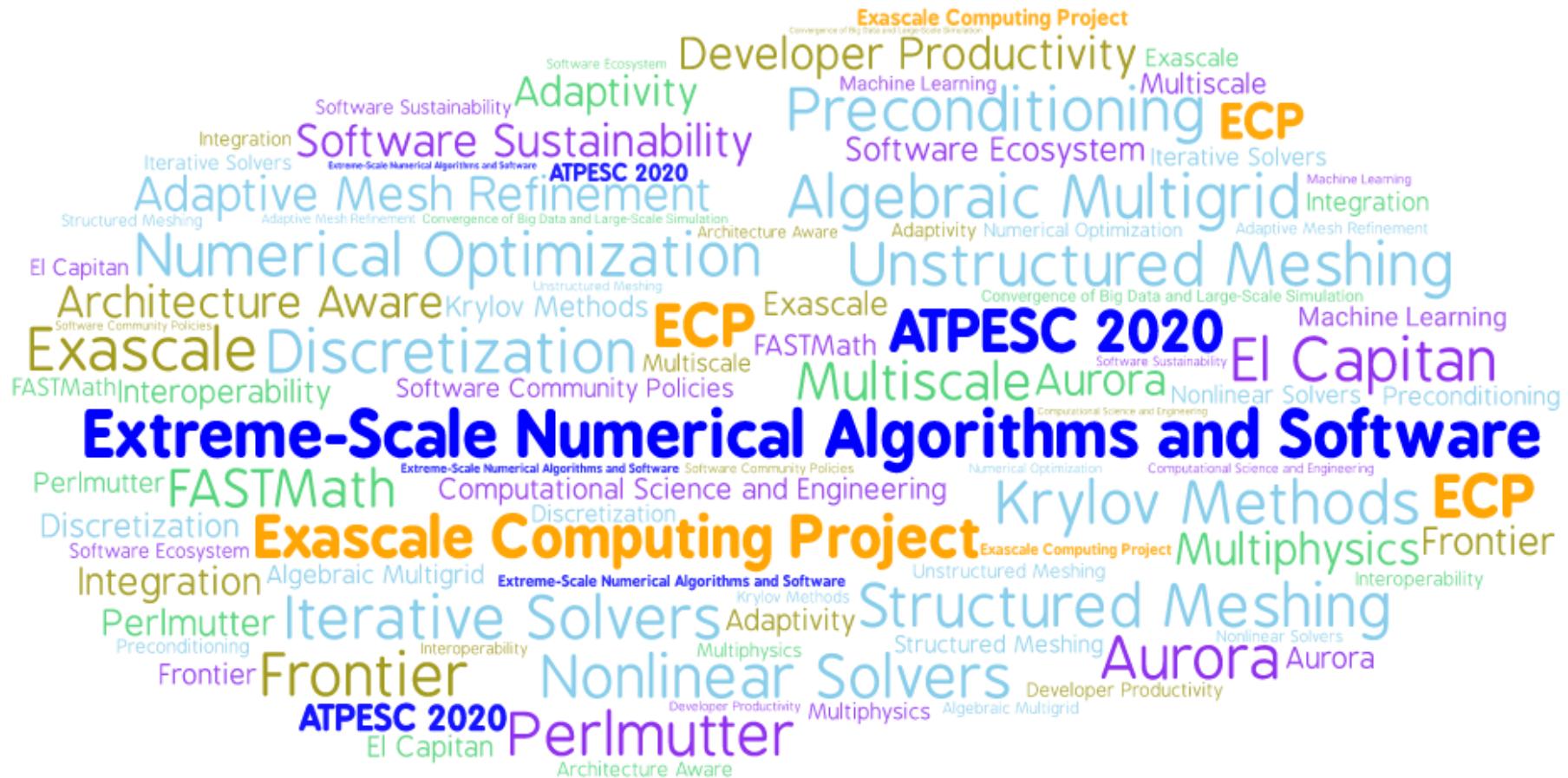


Rensselaer

SMU

Outline

- Logistics for the day
 - Intro to numerical algorithms and software for extreme-scale science
 - Gallery of highlights: HPC numerical software packages
 - Hands-on example: “Hello world” for numerical packages



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-2020/#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/MathPackagesTraining2020/agenda>

Agenda

<https://extremecomputingtraining.anl.gov/agenda-2020/#Track-5>

9:30 Introduction to Numerical Libraries and Virtual Logistics

Lois Curfman McInnes, ANL
and Mark Miller, LLNL

10:30 Session 1

- **ROOM FRONTIER:** Structured Discretization (with AMReX)
- **ROOM AURORA:** Unstructured Discretization (with MFEM/PUMI)
- **ROOM PERLMUTTER:** Iterative Solvers+Preconditioners (with Trilinos/MueLu)
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack)

Ann Almgren, LBL and Don Willcox, LBL

Mark Shephard, RPI
and Aaron Fisher, LLNL

Jonathan Hu, SNL
and Christian Glusa, SNL

Sherry Li, LBL and Pieter Ghysels, LBL

11:30 Break

11:45 Session 2

- **ROOM FRONTIER:** Structured Discretization (with AMReX)
- **ROOM AURORA:** Unstructured Discretization (with MFEM/PUMI)
- **ROOM PERLMUTTER:** Iterative Solvers+Algebraic Multigrid (with HYPRE)
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack)

Ann Almgren, LBL and Don Willcox, LBL

Mark Shephard, RPI
and Aaron Fisher, LLNL

Ulrike Yang, LLNL

Sherry Li, LBL and Pieter Ghysels, LBL

12:45 p.m. Lunch

1:45 Panel Discussion: Contributing to the Numerical Package Community

Panel Moderator: [Mark Miller](#), LLNL

Panelists: [Jonathan Hu](#), SNL; [Richard Mills](#), ANL; [Sherry Li](#), LBL; [Cameron Smith](#), RPI; and [Ulrike Yang](#), LLNL

2:35 Session 3

- **ROOM FRONTIER:** Nonlinear Solvers (with PETSc)
- **ROOM AURORA:** Optimization (with TAO)
- **ROOM PERLMUTTER:** Time Integration (with SUNDIALS)
- **ROOM EL CAPITAN:** Iterative Solvers+Preconditioners (with Trilinos/MueLu)

[Richard Mills](#), ANL

[Alp Dener](#), ANL

[Dan Reynolds](#), SMU

[Jonathan Hu](#), SNL and [Christian Glusa](#), SNL

3:25 Break

3:40 Session 4

- **ROOM FRONTIER:** Nonlinear Solvers (with PETSc)
- **ROOM AURORA:** Optimization (with TAO)
- **ROOM PERLMUTTER:** Time Integration (with SUNDIALS)
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack)

[Richard Mills](#), ANL

[Alp Dener](#), ANL

[Dan Reynolds](#), SMU

[Sherry Li](#), LBL and [Pieter Ghysels](#), LBL

[Ann Almgren](#), LBL

4:30 Working with Numerical Packages in Practice

5:00 Adjourn

5:15 Optional Activity: SME speed-dating in pairs

[Mark Miller](#), LLNL

6:35 Optional Activity Concludes

Agenda Overview

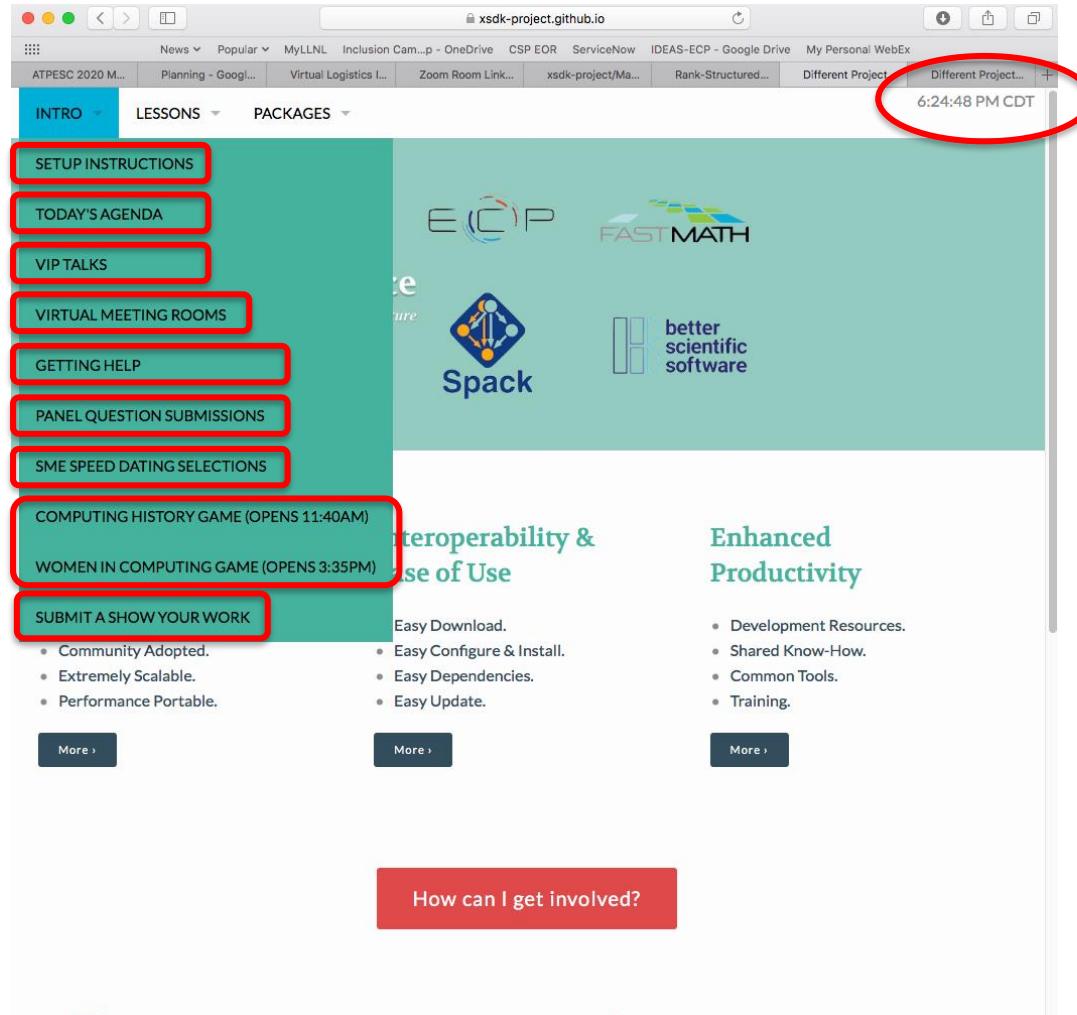
Start CDT	Activity	Virtual Room
9:30	Introduction	Main room
10:30	Parallel Session #1	Four parallel rooms
11:30	Break	
11:45	Parallel Session #2	Four parallel rooms
12:45	Lunch	
1:45	Panel	Main room
2:35	Parallel Session #3	Four parallel rooms
3:25	Break	
3:40	Parallel Session #4	Four parallel rooms
4:30	Wrap-up	Main room
5:00	Break	
5:15	Subject Matter Expert (SME) Speed Dating (optional)	Individual SME rooms

Mix-n-Match topics
to your interests

See Synopses from Agenda

- #1
 - Structured Discretization (AMReX)
 - Unstructured Discretization (MFEM/PUMI)
 - Iterative Solvers & Preconditioners (Trilinos/MueLU)
 - Direct Solvers (SuperLU/Strumpack)
- #2
 - Structured Discretization (AMReX)
 - Unstructured Discretization (MFEM/PUMI)
 - Iterative Solvers & Preconditioners (hypre)
 - Direct Solvers (SuperLU/Strumpack)
- #3
 - Nonlinear Solvers (PETSc)
 - Optimization (TAO)
 - Time Interation (SUNDIALS)
 - Iterative Solvers & Preconditioners (Trilinos/MueLU)
- #4
 - Nonlinear Solvers (PETSc)
 - Optimization (TAO)
 - Time Interation (SUNDIALS)
 - Direct Solvers (SuperLU/Strumpack)

<https://xsdk-project.github.io/MathPackagesTraining2020/>



- Clock
- Setup instructions
- Today's agenda
- VIP talks
- Virtual meeting rooms
- Getting help
- Panel question submission
- SME speed dating selections
- Break games
- Submit a "Show your work"

Today's agenda

<https://xsdk-project.github.io/MathPackagesTraining2020/agenda>

Structured Discretization (with AMReX)

Slides

Block-structured adaptive mesh refinement (AMR) provides a natural framework in which to focus computing power on the most critical parts of the problem in the most computationally efficient way possible. AMReX supports the development of block-structured AMR algorithms for solving systems of partial differential equations (PDE's) and other algorithms that require structured mesh and/or particle discretizations. We will begin with an overview of block-structured AMR, including several different time-stepping strategies, and then discuss the features of AMReX we might want to use to solve a multiphysics problem on machines from laptops to supercomputers. Hands-on exercises will include passive scalar advection with time-dependent adaptivity, the use of native linear solvers to impose incompressibility on a flow around obstacles, and "AMReX-Pachinko", which demonstrates the interaction of particles with objects.

Iterative Solvers & Preconditioners (with MueLu)

Slides

In this session, attendees will learn about linear solvers and preconditioners available in the Trilinos project. We will focus on Krylov solvers such as conjugate gradients (CG) and generalized minimum residual (GMRES); simple preconditioners like Jacobi, Gauss-Seidel, and Chebyshev polynomials; and scalable aggregation-based algebraic multigrid preconditioning. The two hands-on lessons will provide an opportunity to run a variety of stand-alone examples that demonstrate some of the many Trilinos solver capabilities on a model linear problem.

Mix-n-Match topics
to your interests
See Synopses from Agenda

CDT Start	Mins	Topic	Speaker(s)	Virtual Venue
09:30	55	Intro. to Numerical Libraries	Lois Curfman McInnes Mark Miller	Main-Room
10:25	5	Telecon Transition		
10:30	60	Parallel Session One		
		Structured Discretization (with AMReX)	Ann Almgren Don Willcox	Frontier
		Unstructured Discretization (with MFEM/PUMI)	Aaron Fisher Mark Shephard	Aurora
		Iterative Solvers & Preconditioners (with MueLu)	Jonathan Hu Christian Glusa	Perlmutter
		Direct Solvers (with SuperLU/Strumpack)	Sherry Li Pieter Ghysels	El-Capitan

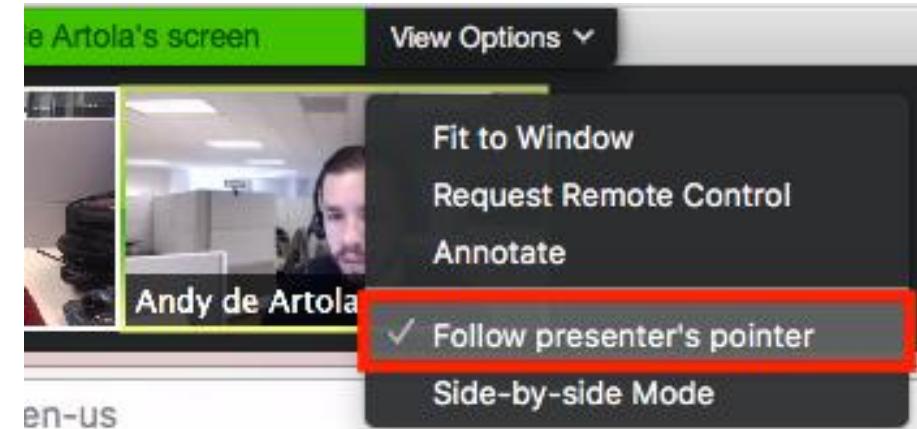
<https://xsdk-project.github.io/MathPackagesTraining2020/>

The screenshot shows a web browser window with the URL <https://xsdk-project.github.io/MathPackagesTraining2020/>. The page is titled "Math Packages Training 2020". The navigation bar includes links for News, Popular, MyLLNL, Inclusion Cam..., OneDrive, CSP EOR, ServiceNow, IDEAS-ECP - Google Drive, and My Personal WebEx. A red circle highlights the "PACKAGES" button in the top navigation menu. The main content area features a sidebar with "Open Source" packages: AMREX, MFEM, PUMI, PUMIPIC, PUMIPIC APPS, HYPRE, SUPERLU, STRUMPACK, PETSC/TAO, SUNDIALS, TRILINOS, TRILINOS/BELOS, TRILINOS/MUELU, and ALCF USER GUIDES. The main content area has two sections: "Interoperability & Ease of Use" and "Enhanced Productivity". The "Interoperability & Ease of Use" section lists: "Numerically Rigorous.", "Community Adopted.", "Extremely Scalable.", and "Performance Portable.". The "Enhanced Productivity" section lists: "Development Resources.", "Shared Know-How.", "Common Tools.", and "Training.". Logos for ECP, FASTMATH, Spack, and better scientific software are visible. A red button at the bottom says "How can I get involved?".

- Hands-on Lessons
- Packages

Using Zoom

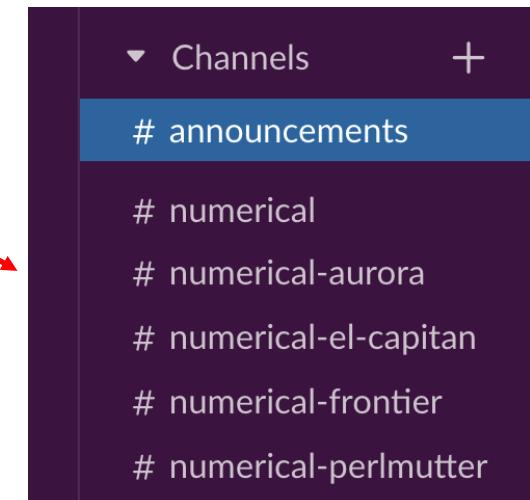
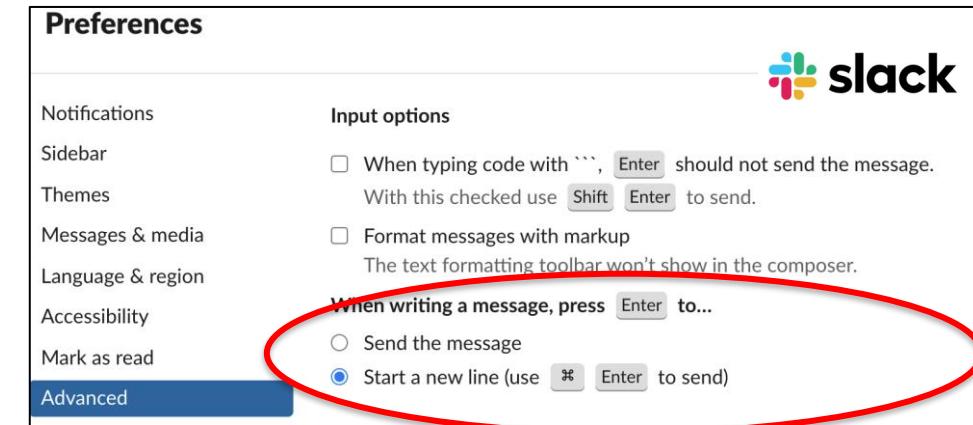
- Please stay muted unless asked to un-mute
- We're using Slack for chat, not Zoom's chat
- "Follow presenter's pointer" might be helpful
 - Available only if NOT in "Fit to Window" mode
- Download slide PDFs from ATPESC web site (agenda page) ahead of presentation as a backup
- Other useful tips
 - Better performance if also disable your video
 - Stop other streaming activity in your home if you can



Using Slack

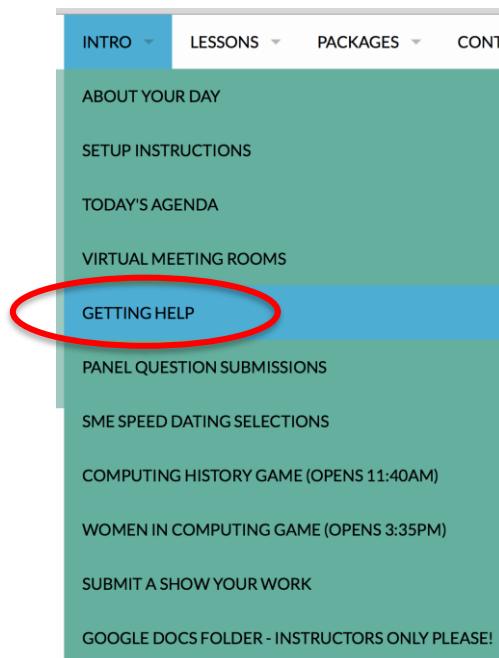
- Recommend using the desktop app, but browser ok too
- **#numerical** channel
 - For all chat during presentations in “Main room”
 - For all chat outside any specific parallel session
 - For general help
 - Recommend using the thread option to help keep track of discussions on subtopics
- **#numerical-<room-name>** (e.g., **#numerical-aurora**)
 - For all chat during presentations in the associated room
 - Room chat restricted to discussion on the current presentation topic only
 - To continue questions/discussion on topics presented earlier in the day, transition to the **#numerical** channel or direct slack messages to individuals in the ATPESC numerical software team

Tip: Consider setting Preferences to customize when to send



Getting help (“Getting help” menu item)

- **#numerical** Slack channel
- IT Support Rooms under the “Getting Help” menu



Getting help

Use the **#numerical** slack channel for general help and it support.

Launch **#numerical** Slack in
[new browser window](#) or [desktop app](#)

IT Support Zoom Rooms

Also individual tech support is available from specialists in these Zoom rooms...

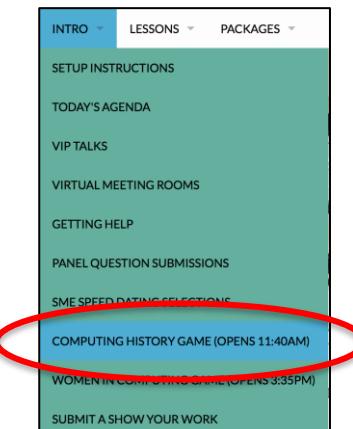
- **Ampere**
- **Volta**
- **Navi** (morning sessions only; viz-tool issues only)
- **Vega** (morning sessions only; viz-tool issues only)

As a last resort, you can try emailing...

- **Satish Balay**,
- **Cameron Smith**
- **Mark Miller**

During breaks and lunch

- During mid-morning and mid-afternoon 15-minute breaks, we will keep Zoom meetings open and allow unmuting for some informal dialog for those interested.
- During lunch will do the same with the “Main Room” – again, for anyone interested.
- Some simple computing history games for those interested
 - Ignore the points, scoring



Row 1:
• Dan Reynolds
• Lois Curfman McInnes
• Don Willcox
• Ann Almgren
• Satish Balay

Row 2:
• Pieter Ghysels
• Christian Glusa
• Mark Miller
• Aaron Fisher
• Sherry Li

Row 3:
• Sara Osborn
• David Gardner
• Mark Shephard
• Ulrike Yang
• Alp Dener

Row 4:
• Richard Mills
• Jonathan Hu

Not shown:
• Cameron Smith
• Carol Woodward

The ATPESC Team 2020 on Zoom



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

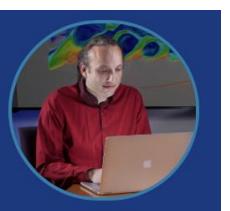
The ATPESC Team 2020

Extreme-scale numerical algorithms and software

Integrated lectures and hands-on examples, panel session, individual discussions ... and more!



Ann Almgren, LBL



Aaron Fisher, LLNL



Jonathan Hu, SNL



Mark Miller, LLNL



Cameron Smith, RPI



Carol Woodward, LLNL



Satish Balay, ANL



Pieter Ghysels, LBL



Sherry Li, LBL



Dan Reynolds, SMU



Richard Mills, ANL



Don Willcox, LBL



Ulrike Yang, LLNL

Thank you to David Gardner and Sara Osborn, LLNL

Additional contributors to gallery of highlights:

Various HPC package developers



Alp Dener, ANL



Christian Glusa, SNL



Lois Curfman McInnes, ANL



Mark Shephard, RPI

VIPs of ATPESC Extreme-Scale Numerical Software Track



- **Jim Demmel, UC Berkeley** [[bio](#)]
 - Communication-Avoiding Algorithms for Linear Algebra, Machine Learning, and Beyond
 - ATPESC 2019 [[slides](#), [video](#)]
 - ENLA Seminar, June 2020 [[video](#)]
- **Jack Dongarra, Univ of Tennessee** [[bio](#)]
 - Adaptive Linear Solvers and Eigensolvers, ATPESC 2019 [[slides](#), [video](#)]
- **David Keyes, KAUST** [[bio](#)]
 - The Convergence of Big Data and Large-scale Simulation: Leveraging the Continuum, ATPESC 2019 [[slides](#), [video](#)]
 - Algorithmic Adaptations to Extreme Scale Computing, ATPESC 2018 [[slides](#), [video](#)]

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



<https://exascaleproject.org>



<https://fastmath-scidac.llnl.gov>

- Exascale Computing Project
- FASTMath SciDAC Institute
- Developers of xSDK packages

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



- IDEAS Software Productivity Project
- Better Scientific Software Community

See also Track 7:
Software Productivity and Sustainability (Aug 6)

Community efforts:
Join us!



<https://xsdk.info>

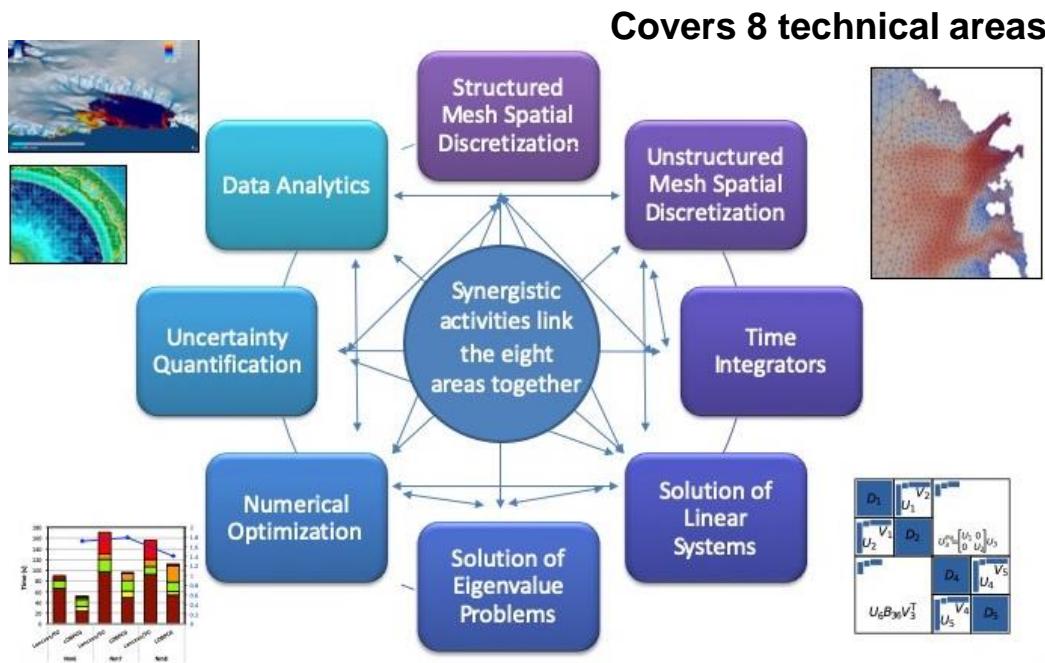


<https://e4s.io>



FASTMath: Frameworks, Algorithms & Scalable Technologies for Mathematics

<https://fastmath-scidac.llnl.gov>



50+ researchers from 5 DOE labs and 5 universities



Argonne
NATIONAL LABORATORY



OAK
RIDGE
National Laboratory

Sandia
National
Laboratories



USC Rensselaer



Rensselaer



SMU



PUMI
Parallel Unstructured Mesh Infrastructure



mfem



AMReX

PETSc

UQTk

Trilinos



symPACK

Albany

ZOLTAN

hypre
high performance preconditioners



FASTMath Goals:

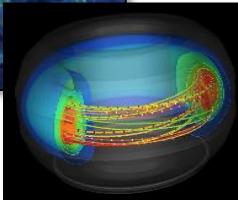
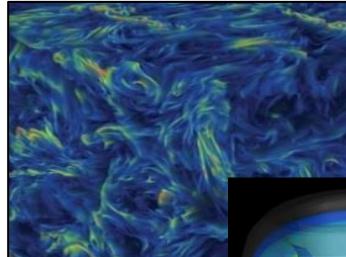
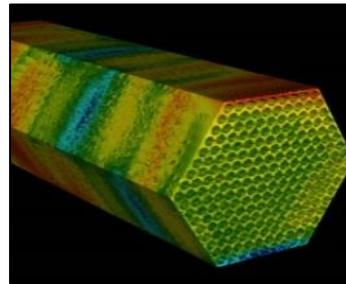
- Develop advanced numerical techniques for DOE applications
- Deploy high-performance software on DOE supercomputers
- Demonstrate basic research technologies from applied mathematics
- Engage and support of the computational science community

100's of person years of experience building math software

ECP's holistic approach uses co-design and integration to achieve exascale computing

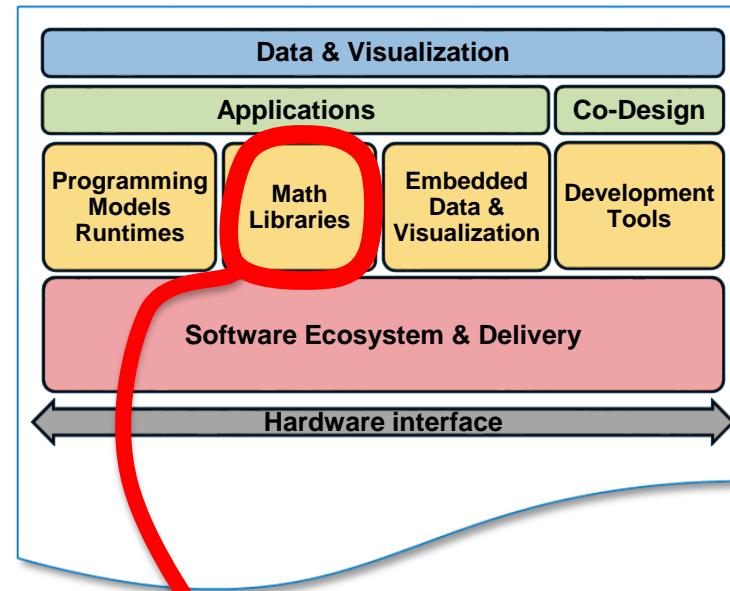
Application Development

Science and mission applications



Software Technology

Scalable software stack



Emphasis for this presentation

Hardware and Integration

Relationships: facilities with AD/ST, with vendors

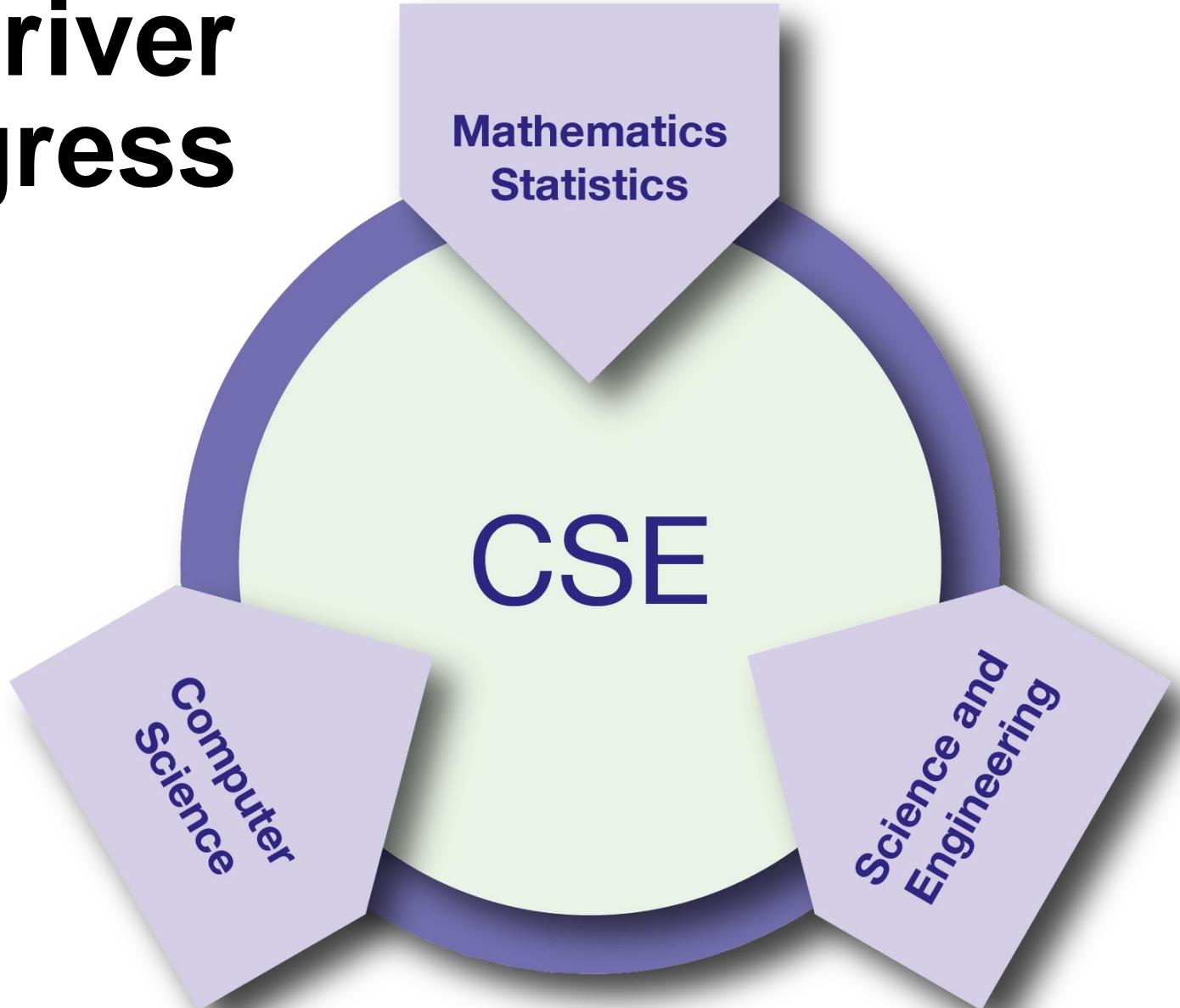


CSE: Essential driver of scientific progress

CSE = Computational Science & Engineering

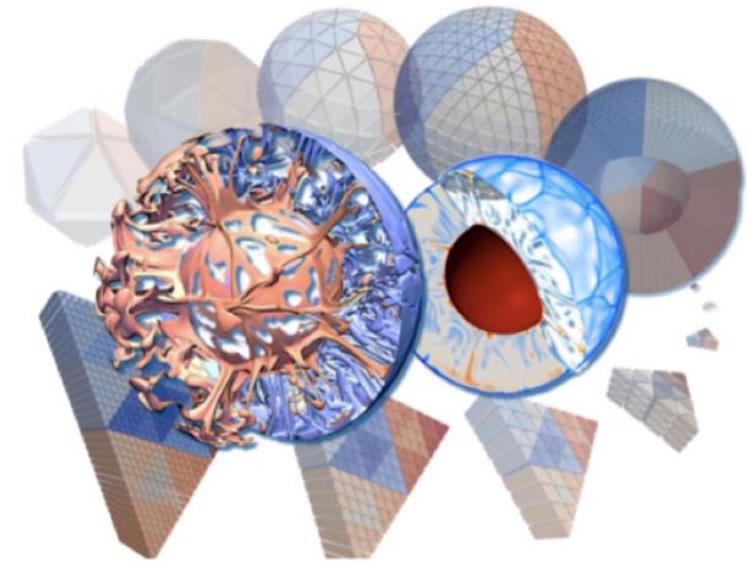
Development and use of computational methods for scientific discovery

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



Rapidly expanding role of CSE: New directions toward predictive science

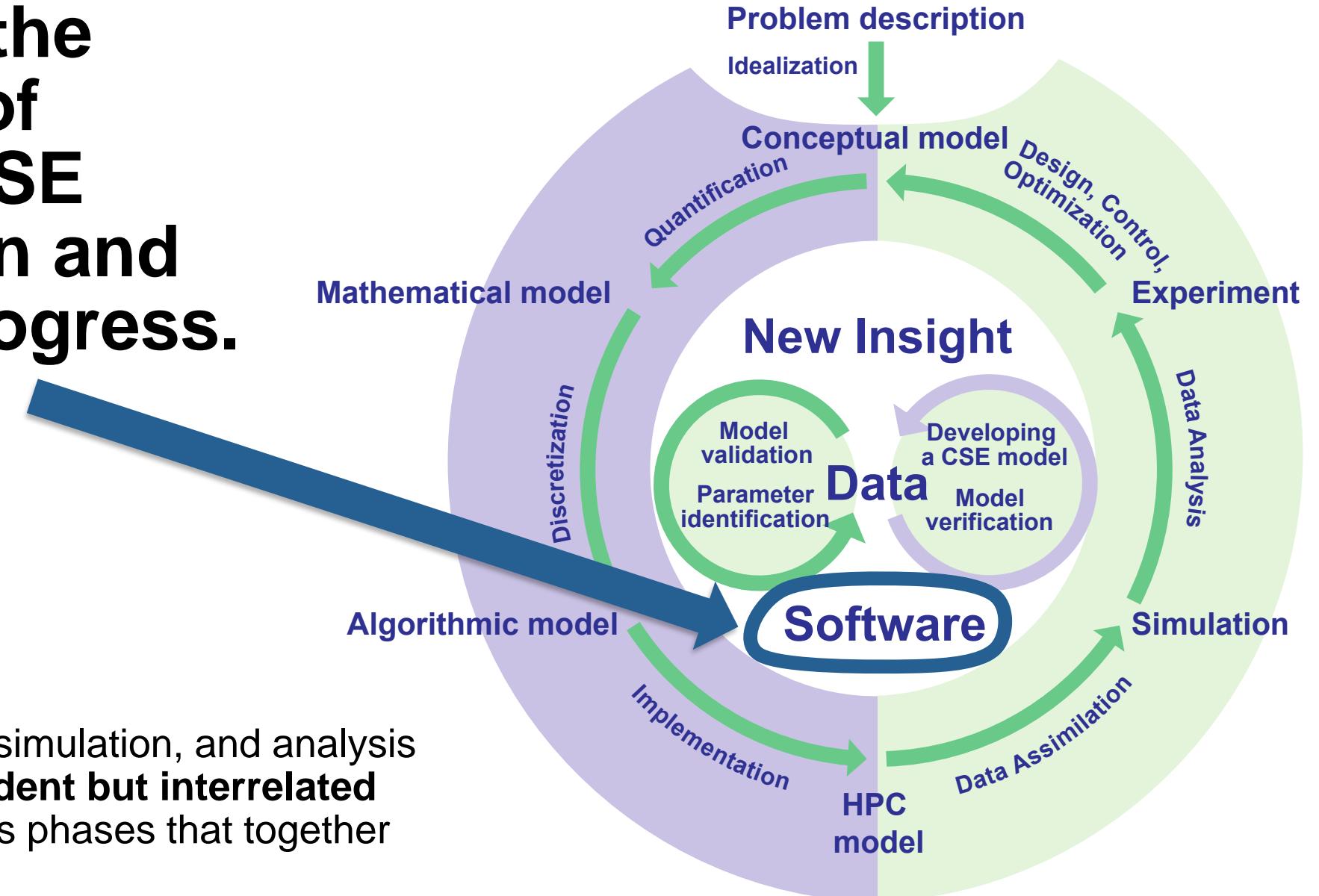
- Mathematical methods and algorithms
- CSE and HPC: Ubiquitous parallelism
- CSE and the data revolution
- CSE software
- CSE education & workforce development



Research and Education in Computational Science & Engineering

U. Rüde, K. Willcox, L.C. McInnes, H. De Sterck, G. Biros, H. Bungartz, J. Coronas, E. Cramer, J. Crowley, O. Ghattas, M. Gunzburger, M. Hanke, R. Harrison, M. Heroux, J. Hesthaven, P. Jimack, C. Johnson, K. Jordan, D. Keyes, R. Krause, V. Kumar, S. Mayer, J. Meza, K.M. Mørken, J.T. Oden, L. Petzold, P. Raghavan, S. Shontz, A. Trefethen, P. Turner, V. Voevodin, B. Wohlmuth, C.S. Woodward, **SIAM Review**, 60(3), Aug 2018, <https://doi.org/10.1137/16M1096840>.

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



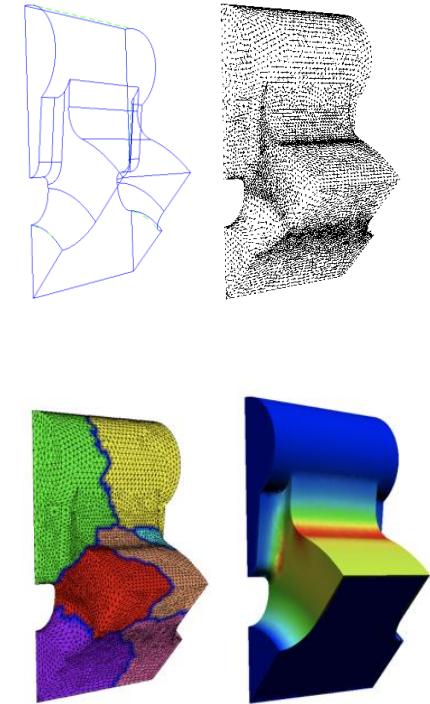
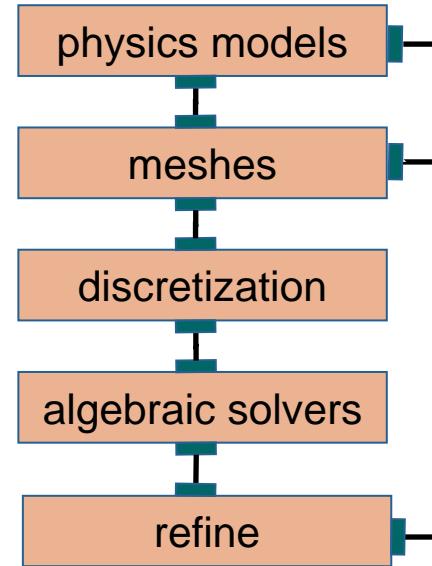
CSE cycle: Modeling, simulation, and analysis

- **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

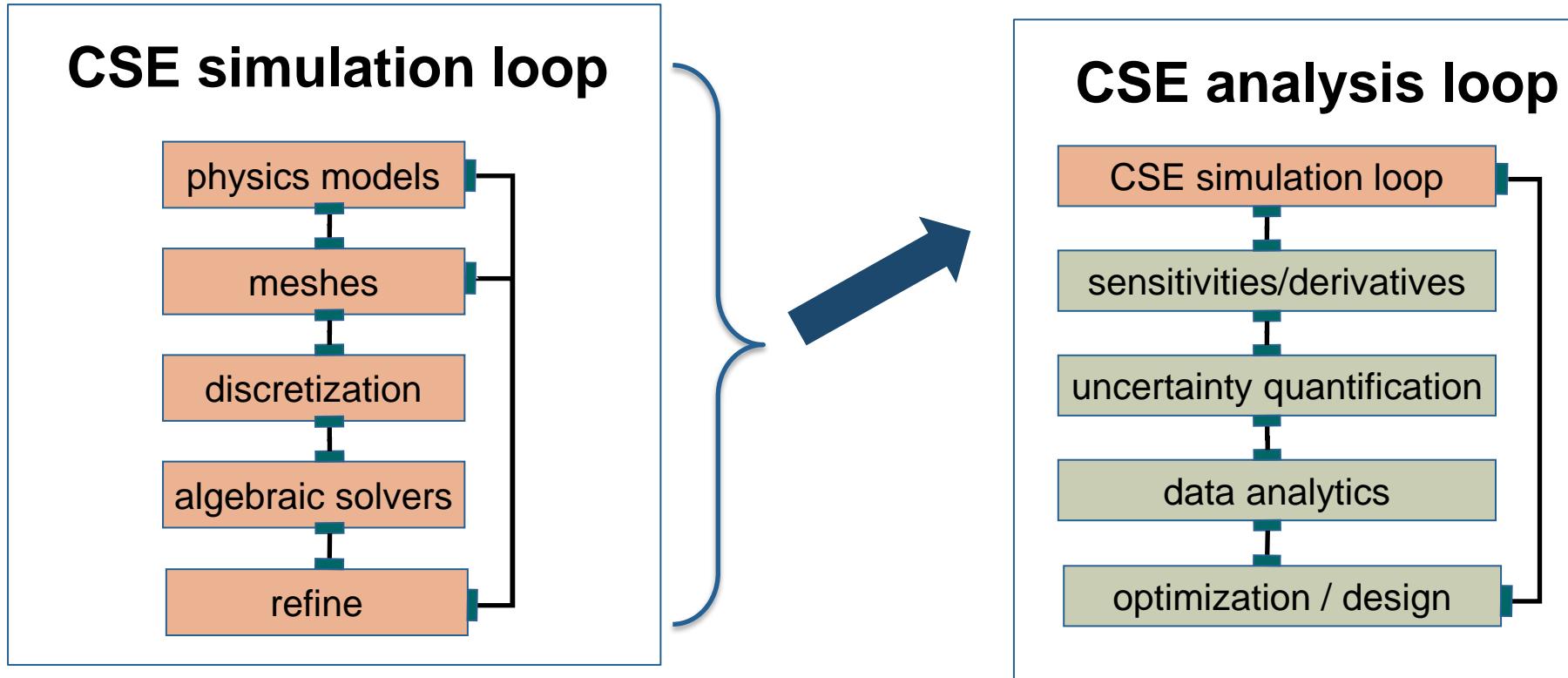
- Develop a mathematical model of the phenomenon of interest
- Approximate the model using a discrete representation
- Solve the discrete representation
- Adapt and refine the mesh or model
- Incorporate different physics, scales

CSE simulation loop



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



*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

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

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

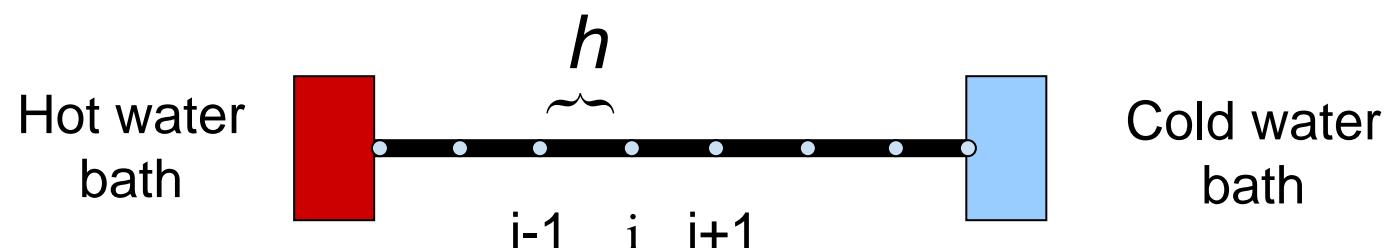


The first step is to discretize the equations

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

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

$$T_0 = 180^\circ \quad T_n = 0^\circ$$



Then you can solve for the unknowns T_i

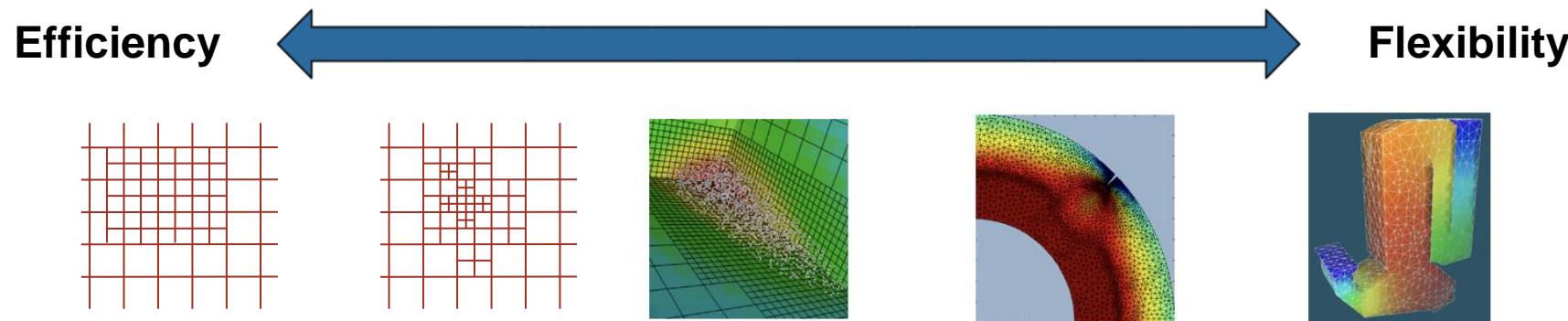
- Set up a matrix of the unknown coefficients
 - include the known boundary conditions
- Solve the linear system for T_i

$$\begin{pmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \dots & & & & & & \\ 0 & \dots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{n-1} \end{pmatrix} = \begin{pmatrix} 180 h^2 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- Visualize and analyze the results

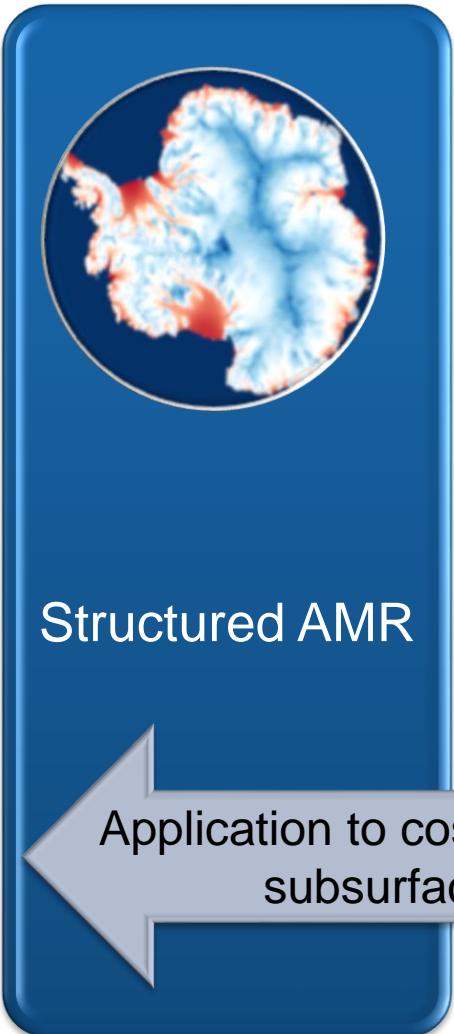
As problems get more complicated, so do the steps in the process

- Different discretization strategies exist for differing needs

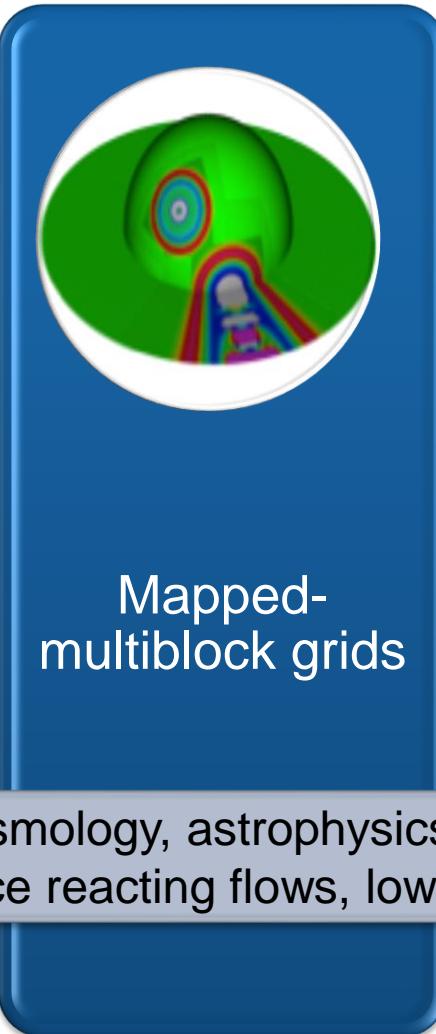


- Most problems are time dependent and nonlinear
 - Need higher algorithmic levels than linear solvers
- Increasingly combining multiple physical processes
 - Interactions require careful handling
- Goal-oriented problem solving requires optimization, uncertainty quantification

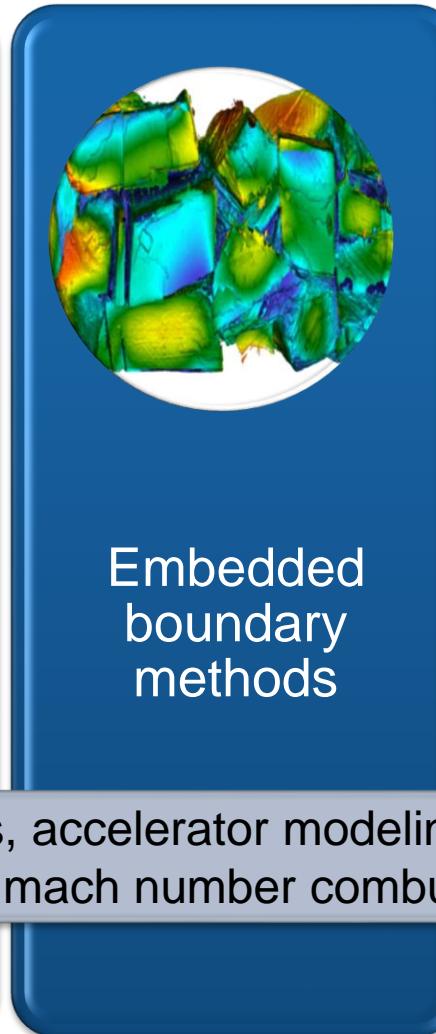
Structured grid efforts focus on high-order, mapped grids, embedded boundaries, AMR, and particles



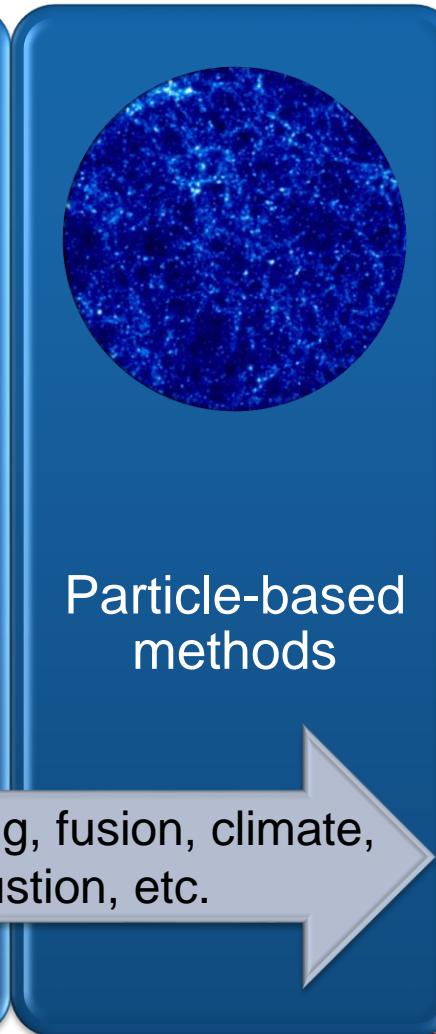
Structured AMR



Mapped-
multiblock grids



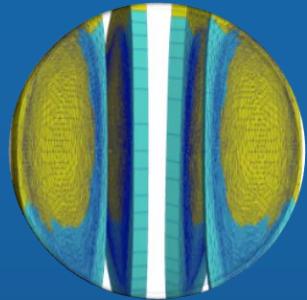
Embedded
boundary
methods



Particle-based
methods

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

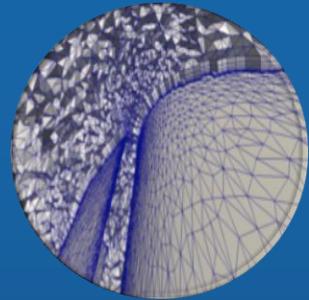
Unstructured grid capabilities focus on adaptivity, high-order, and the tools needed for extreme scaling



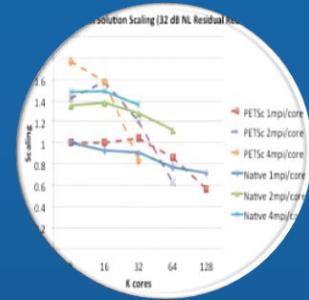
Parallel mesh
infrastructures



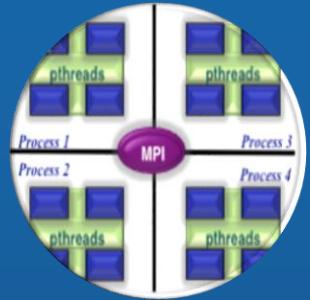
Dynamic load
balancing



Mesh adaptation
and quality
control



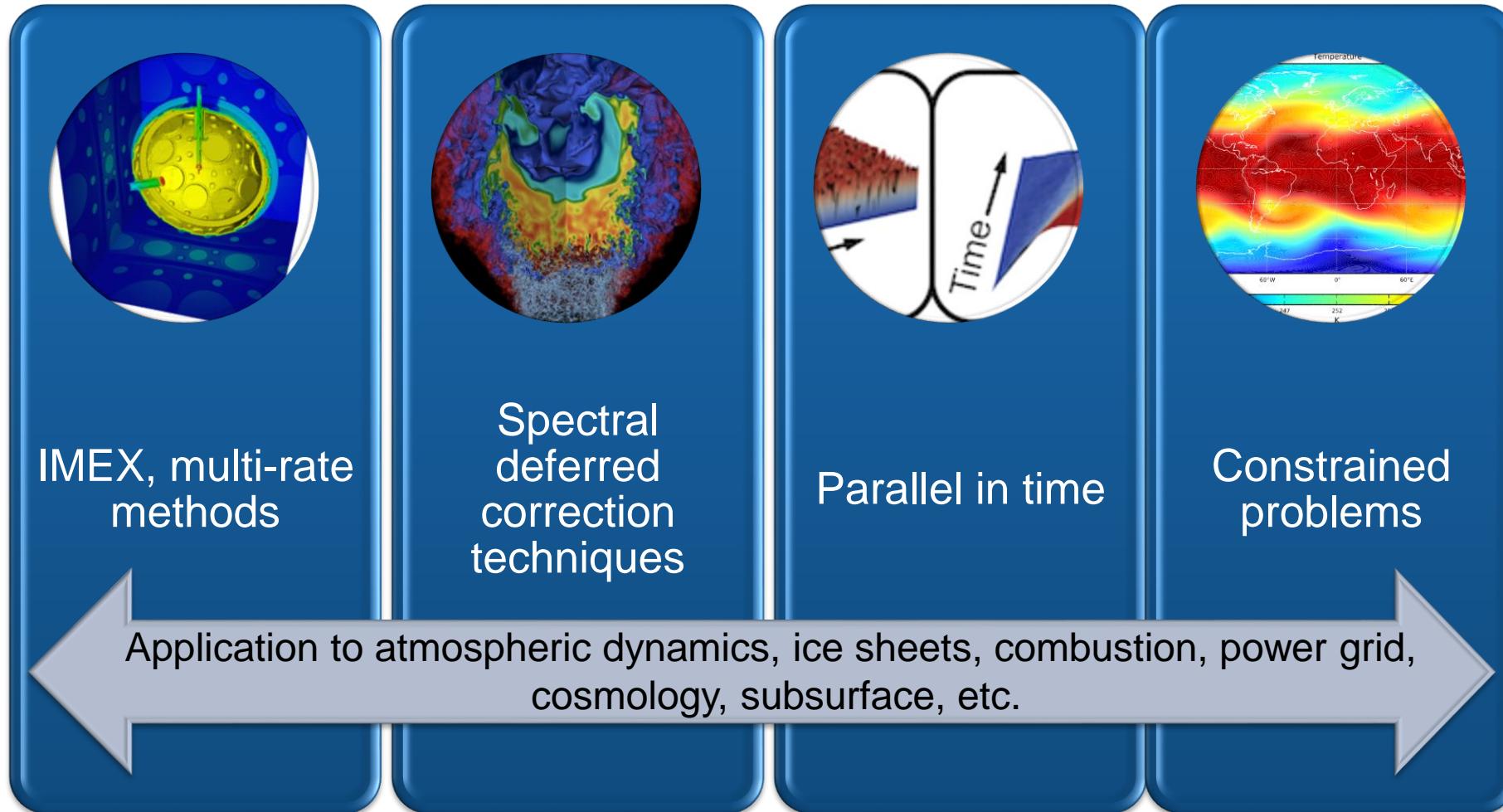
Parallel
performance on
unstructured
meshes



Architecture
aware
implementations

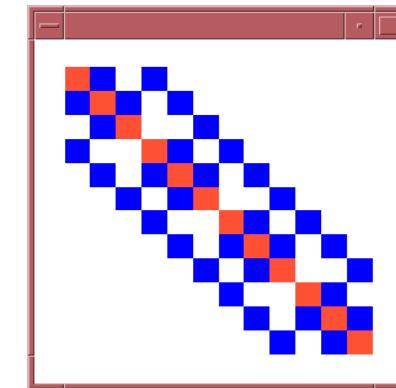
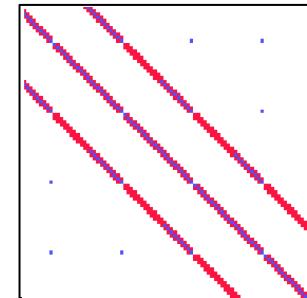
Application to fusion, climate, accelerator modeling, NNSA applications,
nuclear energy, manufacturing processes, etc.

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

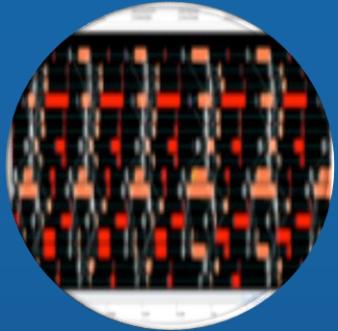


As problems grow in size, so do corresponding discrete systems

- Targeting applications with billions grid points and unknowns
- Most linear systems resulting from these techniques are **LARGE** and sparse
- Often most expensive solution step
- Solvers:
 - Direct methods (e.g., Gaussian Elimination)
 - Iterative methods (e.g., Krylov Methods)
 - Preconditioning is typically critical
 - Mesh quality affects convergence rate
- Many software tools deliver this functionality as numerical libraries
 - hypre, PETSc, SuperLU, Trilinos, etc.



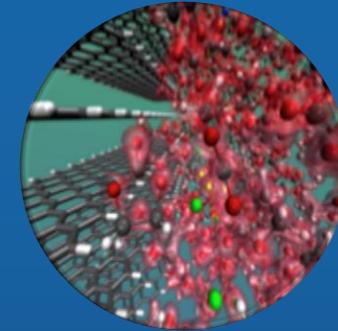
Research on algebraic systems provides key solution technologies to applications



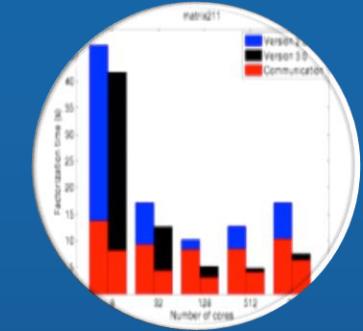
Linear system
solution using direct
and iterative solvers



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,

DOE HPC Roadmap to Exascale Systems

FY 2012



Titan
ORNL
Cray/AMD/NVIDIA



Mira
ANL
IBM BG/Q

FY 2016



Summit
ORNL
IBM/NVIDIA



Theta
ANL
Cray/Intel KNL



Cori
LBNL
Cray/Intel Xeon/KNL



Sequoia
LLNL
IBM BG/Q



Trinity
LANL/SNL
Cray/Intel Xeon/KNL



Sierra
LLNL
IBM/NVIDIA

FY 2018

FY 2021

FY 2022

FY 2023



FRONTIER
ORNL
HPE/AMD



Aurora
ANL
HPE/Intel



Perlmutter
LBNL
HPE/AMD/NVIDIA



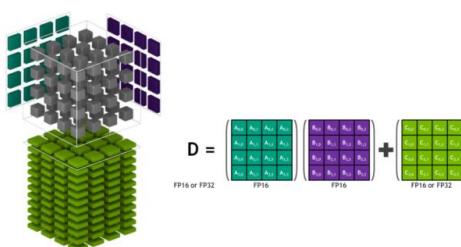
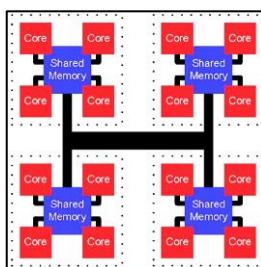
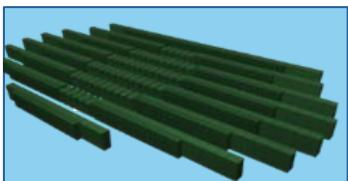
CROSSROADS
LANL/SNL
HPE/TBD



EL CAPITAN
LLNL
HPE/AMD

Disruptive changes in HPC architectures

- **Extreme levels of concurrency**
 - Increasingly deep memory hierarchies
 - Very high node and core counts
- **Additional complexities**
 - Hybrid architectures
 - GPUs, multithreading, manycore
 - Relatively poor memory latency and bandwidth
 - Challenges with fault resilience
 - Must conserve power – limit data movement
 - New (not yet stabilized) programming models
 - Etc.
- **Research advances: On-node and inter-node capabilities**
 - Reduce communication and synchronization
 - Increase concurrency
 - Address memory footprint
 - Enable large communication/computation overlap
 - Use GPUs and multithreading
 - Compare task and data parallelism
 - Low-level kernels for vector operations that support hybrid programming models
 - Mixed precision (leverage compute power available in low-precision tensor cores)
 - Etc.



$$D = \begin{bmatrix} A_{00} & A_{01} & A_{02} & A_{03} \\ A_{10} & A_{11} & A_{12} & A_{13} \\ A_{20} & A_{21} & A_{22} & A_{23} \\ A_{30} & A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} B_{00} & B_{01} & B_{02} \\ B_{10} & B_{11} & B_{12} \\ B_{20} & B_{21} & B_{22} \end{bmatrix} + \begin{bmatrix} C_{00} & C_{01} & C_{02} \\ C_{10} & C_{11} & C_{12} \\ C_{20} & C_{21} & C_{22} \end{bmatrix}$$

Software libraries facilitate progress in computational science and engineering

- **Software library:** a high-quality, encapsulated, documented, tested, and multiuse software collection that provides functionality commonly needed by application developers
 - Organized for the purpose of being reused by independent (sub)programs
 - User needs to know only
 - Library interface (not internal details)
 - When and how to use library functionality appropriately
- **Key advantages** of software libraries
 - Contain complexity
 - Leverage library developer expertise
 - Reduce application coding effort
 - Encourage sharing of code, ease distribution of code
- **References:**
 - [https://en.wikipedia.org/wiki/Library_\(computing\)](https://en.wikipedia.org/wiki/Library_(computing))
 - [What are Interoperable Software Libraries? Introducing the xSDK](#)

Broad range of HPC numerical software

Some packages with general-purpose, reusable algorithmic infrastructure in support of high-performance CSE:

- ★ • **AMReX** – <https://github.com/AMReX-codes/amrex>
- ★ • **Chombo** - <https://commons.lbl.gov/display/chombo>
- **Clawpack** - <http://www.clawpack.org>
- ★ • **Deal.II** - <https://www.dealii.org>
- **FEniCS** - <https://fenicsproject.org>
- ★ • **hypre** - <http://www.llnl.gov/CASC/hypre>
- **libMesh** - <https://libmesh.github.io>
- ★ • **MAGMA** - <http://icl.cs.utk.edu/magma>
- ★ • **MFEM** - <http://mfem.org/>
- ★ • **PETSc/TAO** – <http://www.mcs.anl.gov/petsc>
- ★ • **PUMI** - <https://github.com/SCOREC/core>
- ★ • **SUNDIALS** - <http://computation.llnl.gov/casc/sundials>
- ★ • **SuperLU** - <http://crd-legacy.lbl.gov/~xiaoye/SuperLU>
- ★ • **Trilinos** - <https://trilinos.github.io/>
- **Uintah** - <http://www.uintah.utah.edu>
- **waLBerla** - <http://www.walberla.net>



See info about scope, performance, usage, and design, including:

- tutorials
- demos
- examples
- how to contribute

★ Discussed today:
Gallery of highlights

... and many, many more ... Explore, use, contribute!

ECP applications need sustainable coordination among math libraries

ECP AD Teams

Combustion-Pele, EXAALT, ExaAM, ExaFEL, ExaSGD, ExaSky, ExaStar, ExaWind, GAMESS, MFIX-Exa, NWChemEx, Subsurface, WarpX, WDMApp, WarpX, ExaAM, ATDM (LANL, LLNL, SNL) apps, AMReX, CEED, CODAR, CoPA, ExaLearn

Examples:

- **ExaAM**: DTK, hypre, PETSc, Sundials, Tasmanian, Trilinos, FFT, etc.
- **ExaWind**: hypre, KokkosKernels, SuperLU, Trilinos, FFT, etc.
- **WDMApp**: PETSc, hypre, SuperLU, STRUMPACK, FFT, etc.
- **CEED**: MFEM, MAGMA, hypre, PETSc, SuperLU, Sundials, etc.
- And many more ...

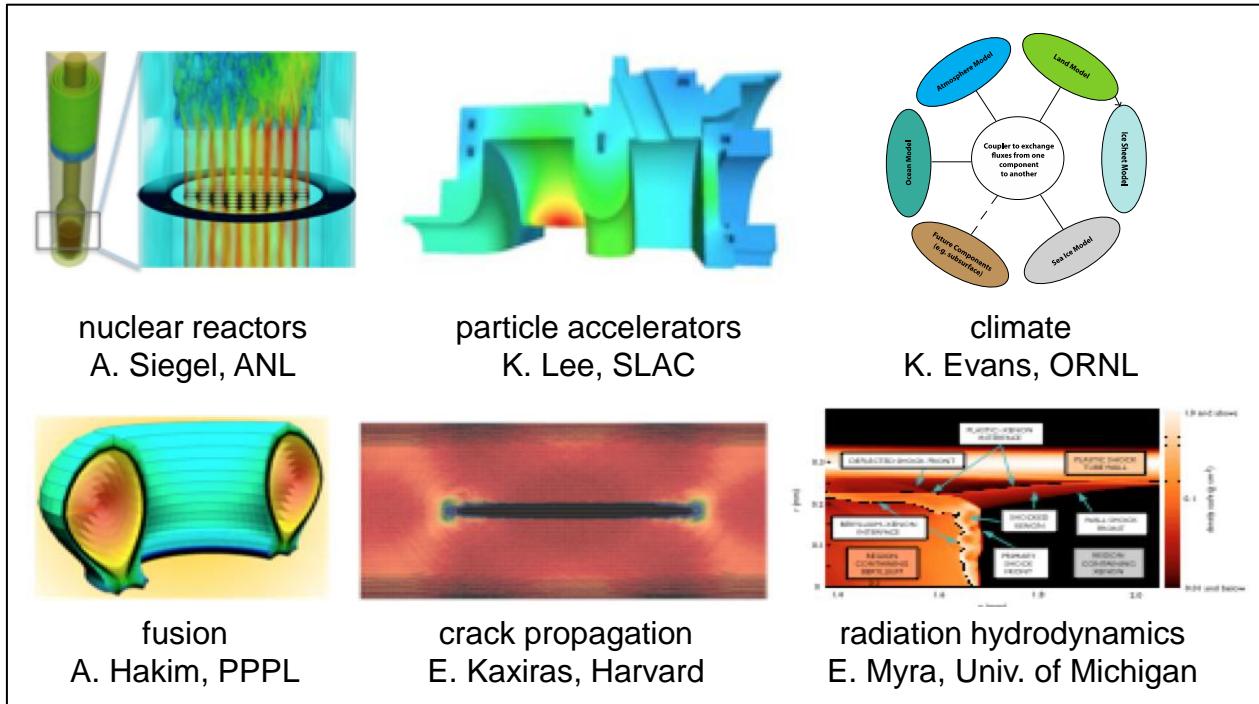
ECP Math Libraries



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



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



The International Journal of High Performance Computing Applications
27(1) 4-83
© The Author(s) 2012
Reprints and permissions:
sagepub.co.uk/journalsPermissions.nav
DOI: [10.1177/1094342012468181](https://doi.org/10.1177/1094342012468181)
hpc.sagepub.com



Multiphysics simulations: Challenges and opportunities

David E Keyes^{1,2}, Lois C McInnes³, Carol Woodward⁴,
William Gropp⁵, Eric Myra⁶, Michael Pernice⁷, John Bell⁸,
Jed Brown³, Alain Clo¹, Jeffrey Connors⁴, Emil Constantinescu³, Don Estep⁹,
Kate Evans¹⁰, Charbel Farhat¹¹, Ammar Hakim¹², Glenn Hammond¹³, Glen Hansen¹⁴,
Judith Hill¹⁰, Tobin Isaac¹⁵, Xiangmin Jiao¹⁶, Kirk Jordan¹⁷, Dinesh Kaushik³,
Eftimios Kaxiras¹⁸, Alice Koniges⁸, Kihwan Lee¹⁹, Aaron Lott⁴, Qiming Lu²⁰,
John Magerlein¹⁷, Reed Maxwell²¹, Michael McCourt²², Miriam Mehl²³,
Roger Pawlowski¹⁴, Amanda P Randles¹⁸, Daniel Reynolds²⁴, Beatrice Rivière²⁵,
Ulrich Rüde²⁶, Tim Scheibe¹³, John Shadid¹⁴, Brendan Sheehan⁹, Mark Shephard²⁷,
Andrew Siegel³, Barry Smith³, Xianzhu Tang²⁸, Cian Wilson² and Barbara Wohlmuth²³

[doi:10.1177/1094342012468181](https://doi.org/10.1177/1094342012468181)

Software libraries are not enough

Apps need to use software packages **in combination**

The way you get programmer productivity is by eliminating lines of code you have to write.

– Steve Jobs, Apple World Wide Developers Conference, Closing Keynote, 1997

- **Need consistency** of compiler (+version, options), 3rd-party packages, etc.
- **Namespace and version conflicts** make simultaneous build/link of packages difficult
- **Multilayer interoperability** requires careful design and sustainable coordination

Need software ecosystem perspective

Ecosystem: A group of independent but interrelated elements comprising a unified whole

Ecosystems are challenging!

“We often think that when we have completed our study of one we know all about two, because ‘two’ is ‘one and one.’ We forget that we still have to make a study of ‘and.’ ”



– Sir Arthur Stanley Eddington (1892–1944), British astrophysicist

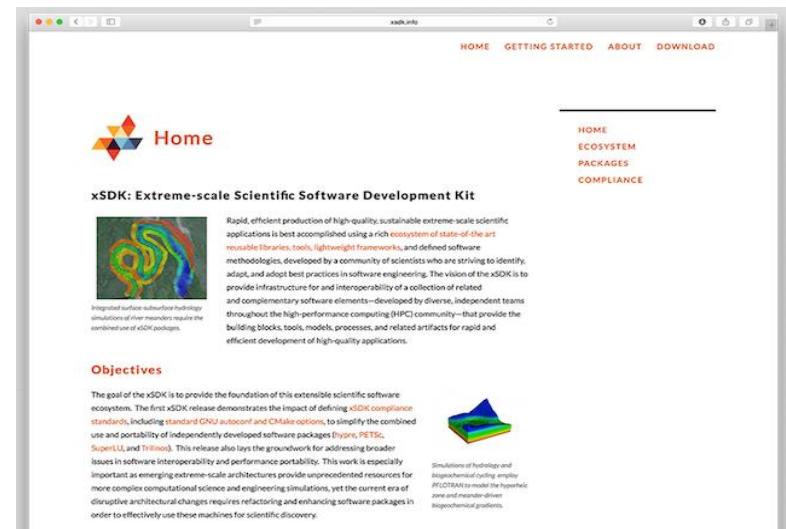


Building the foundation of a highly effective extreme-scale scientific software ecosystem

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



website: xSDK.info

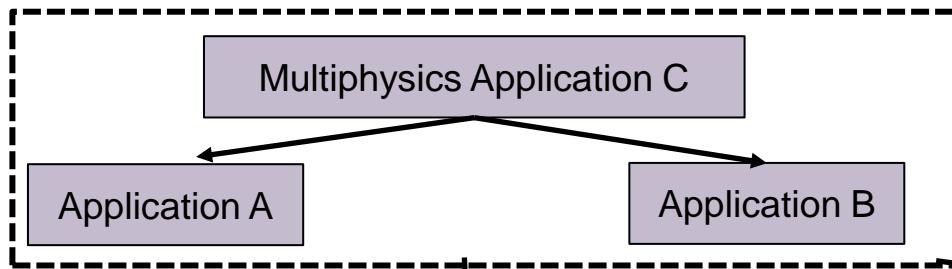


xSDK Version 0.5.0: November 2019

<https://xsdk.info>

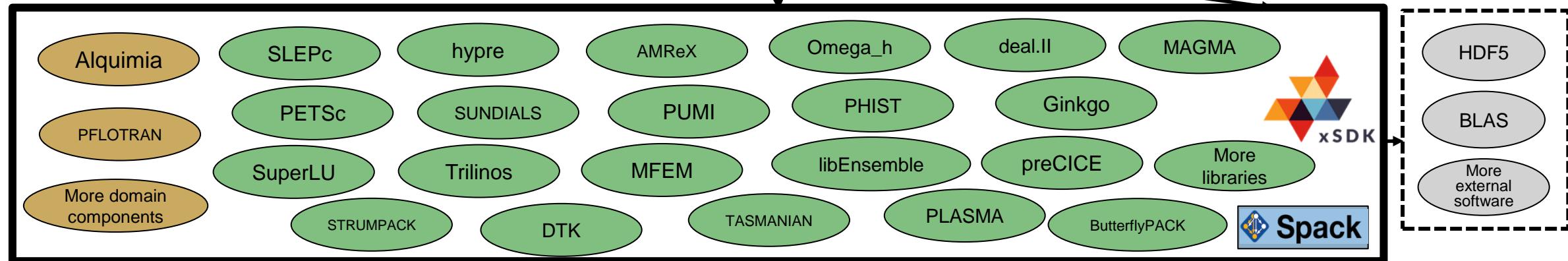
<https://xsdk.info>

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 2019

Tested on key machines at ALCF, NERSC, OLCF, also Linux, Mac OS X



November 2019

- 21 math libraries
- 2 domain components
- 16 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 collaborators



Lawrence Livermore
National Laboratory



xSDK Release 0.5.0, Nov 2019

- **xSDK release lead:** Jim Willenbring (SNL)
- **xSDK planning**
 - Ulrike Meier Yang (LLNL)
- **Leads for xSDK testing**
 - Satish Balay (ANL): ALCF testing
 - Piotr Luszczek (UTK): OLCF testing
 - Aaron Fisher (LLNL): general testing
 - Cody Balos (LLNL): general testing
 - Keita Teranishi (SNL): general testing
- **Spack liaison:** Todd Gamblin (LLNL)

and many more ...

- **Package compatibility with xSDK community policies and software testing:**

- **AMReX:** Ann Almgren, Michele Rosso (LBNL)
- **DTK:** Stuart Slattery, Bruno Turcksin (ORNL)
- **deal.II:** Wolfgang Bangerth (Colorado State University)
- **Ginkgo:** Hartwig Anzt (Karlsruhe Institute of Technology)
- **hypre:** Ulrike Meier Yang, Sarah Osborn, Rob Falgout (LLNL)
- **libEnsemble:** Stefan Wild, Steve Hudson (ANL)
- **MAGMA** and **PLASMA:** Piotr Luszczek (UTK)
- **MFEM:** Aaron Fisher, Tzanio Kolev (LLNL)
- **Omega_h:** Dan Ibanez (SNL)
- **PETSc/TAO:** Satish Balay, Alp Denner, Barry Smith (ANL)
- **preCICE:** Frederic Simonis (Technical University Munich)
- **PUMI:** Cameron Smith (RPI)
- **SUNDIALS:** Cody Balos, David Gardner, Carol Woodward (LLNL)
- **SuperLU, STRUMPACK, ButterflyPACK:** Sherry Li, Pieter Ghysels, Yang Liu (LBNL)
- **TASMANIAN:** Miroslav Stoyanov, Damien Lebrun Grandie (ORNL)
- **Trilinos:** Keita Teranishi, Jim Willenbring, Sam Knight (SNL)
- **PHIST:** Jonas Thies (DLR, German Aerospace Center)
- **SLEPc:** José Roman (Universitat Politècnica de València)
- **Alquimia:** Sergi Mollins (LBNL)
- **PFLOTRAN:** Glenn Hammond (PNNL)

xSDK community policies

<https://x sdk.info/policies>



Version 0.5.0,
July 2019

xSDK compatible package: Must satisfy mandatory xSDK policies:

- M1.** Support xSDK community GNU Autoconf or CMake options.
- M2.** Provide a comprehensive test suite.
- M3.** Employ user-provided MPI communicator.
- M4.** Give best effort at portability to key architectures.
- M5.** Provide a documented, reliable way to contact the development team.
- M6.** Respect system resources and settings made by other previously called packages.
- M7.** Come with an open source license.
- M8.** Provide a runtime API to return the current version number of the software.
- M9.** Use a limited and well-defined symbol, macro, library, and include file name space.
- M10.** Provide an accessible repository (not necessarily publicly available).
- M11.** Have no hardwired print or IO statements.
- M12.** Allow installing, building, and linking against an outside copy of external software.
- M13.** Install headers and libraries under <prefix>/include/ and <prefix>/lib/.
- M14.** Be buildable using 64 bit pointers. 32 bit is optional.
- M15.** All xSDK compatibility changes should be sustainable.
- M16.** The package must support production-quality installation compatible with the xSDK install tool and xSDK metapackage.

Also **recommended policies**, which currently are encouraged but not required:

- R1.** Have a public repository.
- R2.** Possible to run test suite under valgrind in order to test for memory corruption issues.
- R3.** Adopt and document consistent system for error conditions/exceptions.
- R4.** Free all system resources it has acquired as soon as they are no longer needed.
- R5.** Provide a mechanism to export ordered list of library dependencies.
- R6.** Provide versions of dependencies.
- R7.** Have README, SUPPORT, LICENSE, and CHANGELOG file in top directory.

xSDK member package: Must be an xSDK-compatible package, and it uses or can be used by another package in the xSDK, and the connecting interface is regularly tested for regressions.

We welcome feedback.
What policies make sense
for your software?

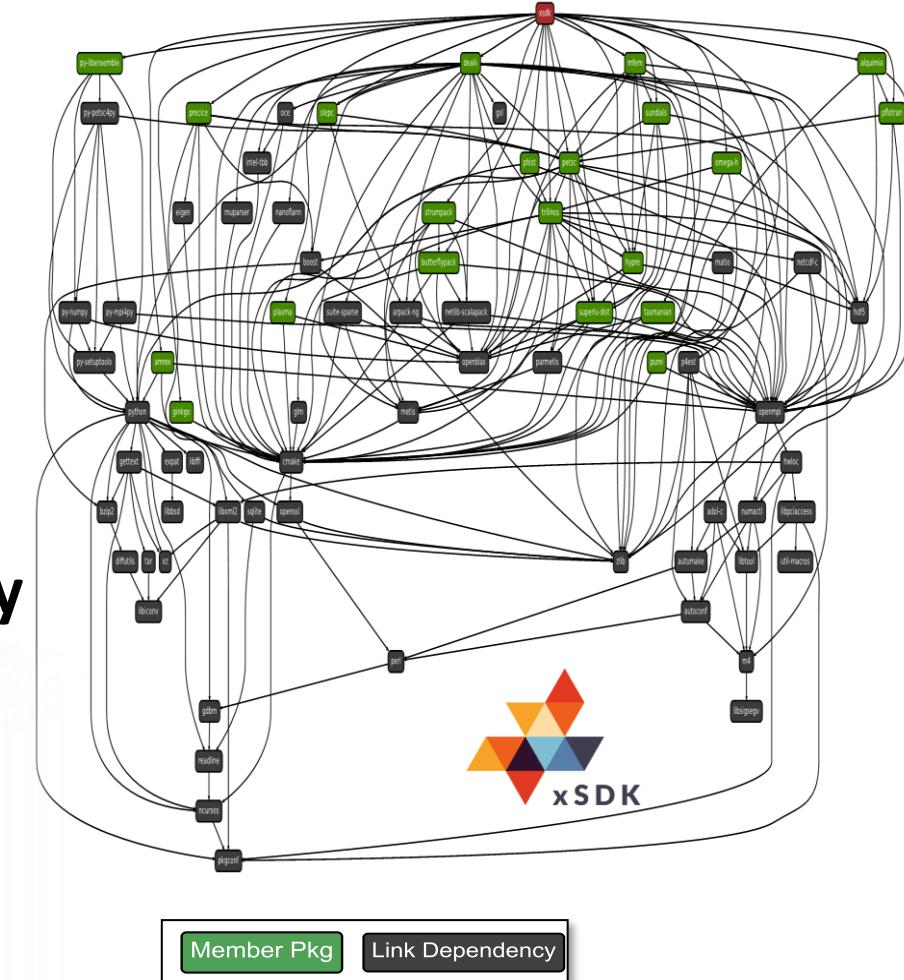
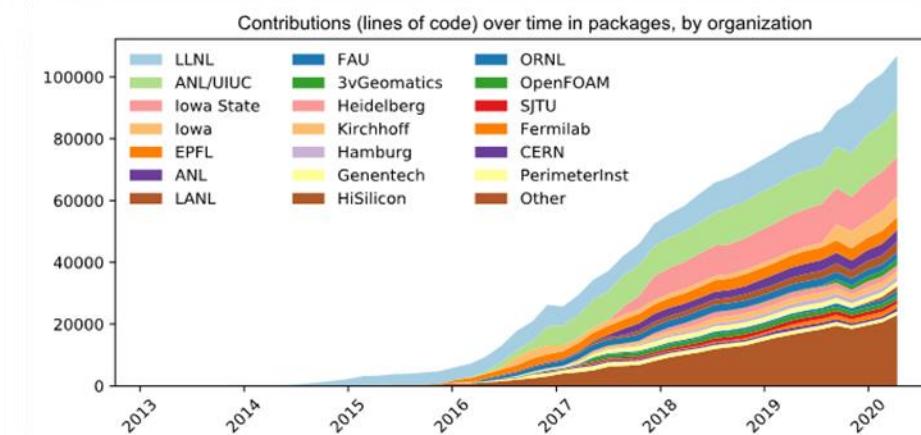
The xSDK is using Spack to deploy its software

- The xSDK packages depend on a number of open source libraries
- Spack is a flexible package manager for HPC
- Spack allows the xSDK to be deployed with a single command
 - User can optionally choose compilers, build options, etc.
 - Will soon support combinatorial test dashboards for xSDK packages



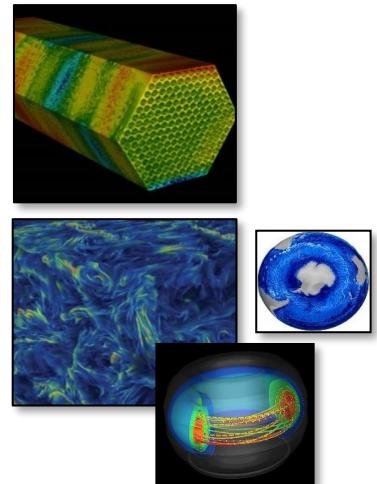
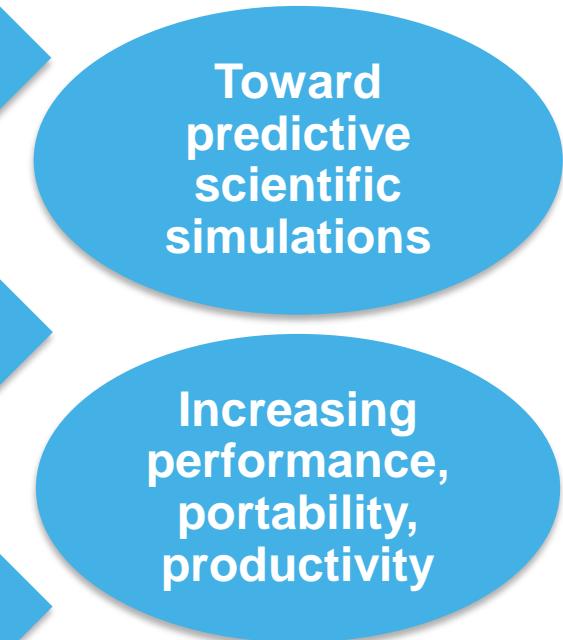
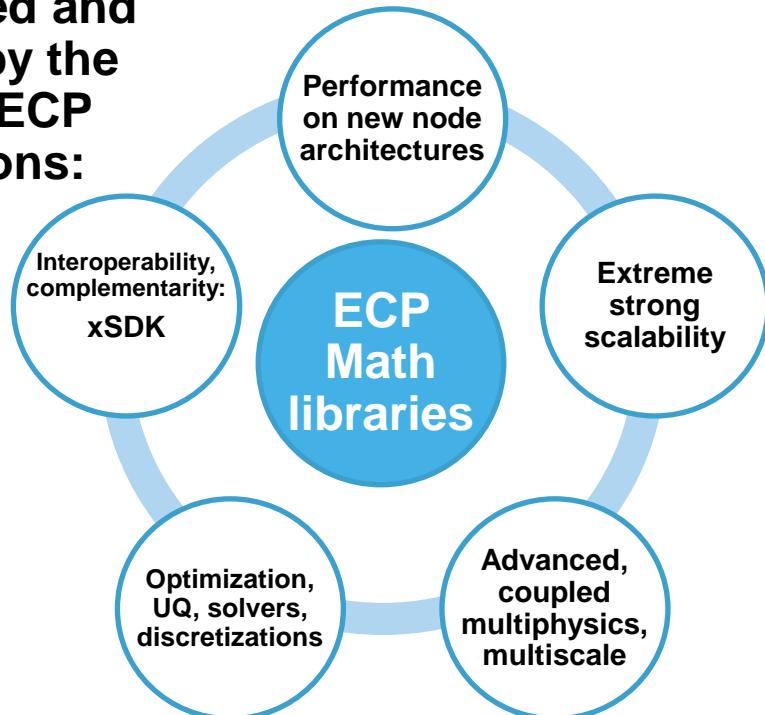
Spack has grown into a thriving open source community

- Over 600 contributors
- Over 4,300 software packages
- Used world-wide
- Key component of ECP strategy for software deployment



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

As motivated and validated by the needs of ECP applications:



Timeline:

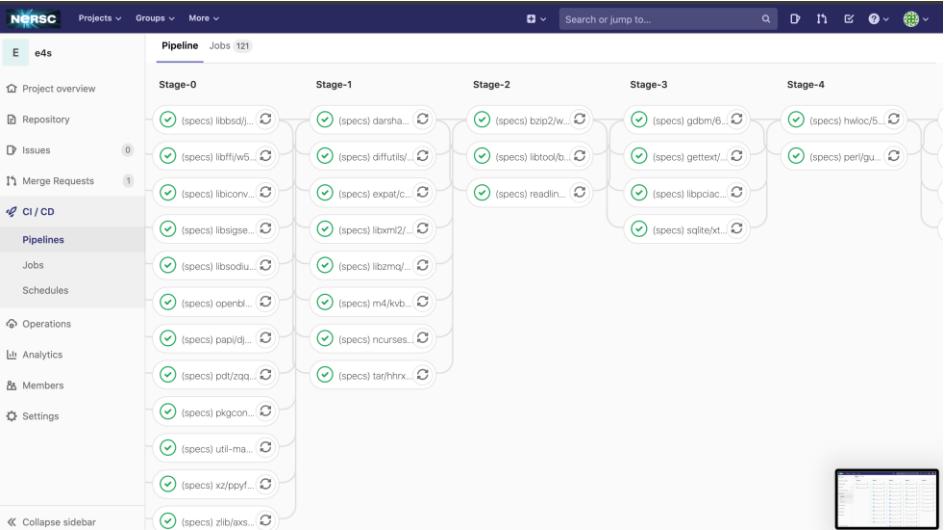
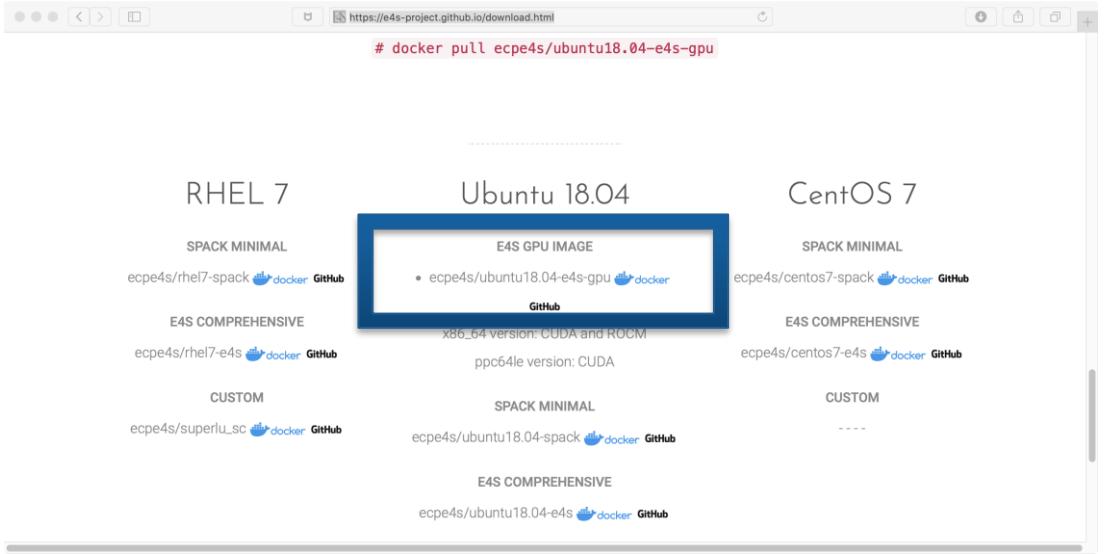
Extreme-scale Scientific Software Stack (E4S)

<https://e4s.io>



- As our software gets more complex, it is getting harder to install tools and libraries correctly in an integrated and interoperable software stack.
- E4S is a community effort to provide open source software packages for developing, deploying, and running scientific applications on HPC platforms.
 - Delivering a modular, interoperable, and deployable software stack based on Spack [spack.io].
 - E4S provides both source builds and containers of a broad collection of HPC software packages.
 - E4S exists to accelerate the development, deployment and use of HPC software, lowering the barriers.
- E4S provides containers and turn-key, from-source builds of 50+ popular HPC software packages:
 - MPI: MPICH and OpenMPI
 - Development tools: TAU, HPCToolkit, and PAPI
 - Math libraries: hypre, PETSc, SUNDIALS, SuperLU, Trilinos
 - Data and Viz tools: Adios, HDF5, and Paraview
- E4S containers support Docker, Singularity, Shifter, and Charliecloud HPC container runtimes.
- E4S Spack build cache has over 10,000 binaries.
- Platforms: x86_64, ppc64le, and aarch64. GPUs runtimes: NVIDIA (CUDA) and AMD (ROCm).
- E4S DocPortal provide a single online location for *accurate* product descriptions for software products.
- E4S helps applications reduce the burden to install dependencies:
 - WDMapp installation speeds up from hours to minutes on Rhea at OLCF [<https://wdmapp.readthedocs.io/en/latest/machines/rhea.html>]

Download E4S v1.1 GPU image

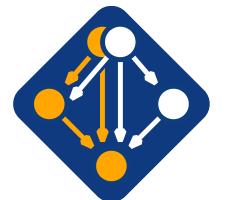


E4S build pipeline
• Cori, NERSC

- 50 ECP ST products
 - CUDA
 - ROCm
 - Tensorflow
 - PyTorch

E4S

<https://e4s.io>



<https://spack.io>



E4S Summary



What E4S is not

A closed system taking contributions only from DOE software development teams.

A monolithic, take-it-or-leave-it software behemoth.

A commercial product.

A simple packaging of existing software.

What E4S is

Extensible, open architecture software ecosystem accepting contributions from US and international teams.
Framework for collaborative open-source product integration.

A full collection if compatible software capabilities **and**
A manifest of a la carte selectable software capabilities.

Vehicle for delivering high-quality reusable software products in collaboration with others.

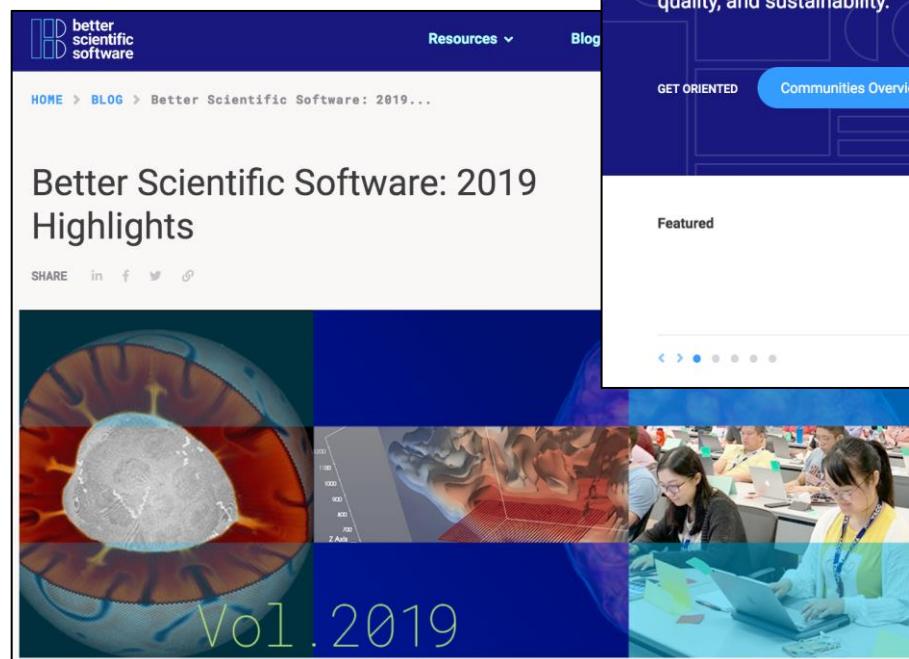
The conduit for future leading edge HPC software targeting scalable next-generation computing platforms.
A hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations.

Further reading

- [Building community through software policies](#), Piotr Luszczek and Ulrike Yang
- [SuperLU: How advances in software practices are increasing sustainability and collaboration](#), Sherry Li
- [Porting the Ginkgo package to AMD's HIP ecosystem](#), Hartwig Anzt
- [Scientific software packages and their communities](#), Rene Gassmoeller
- [Leading a scientific software project: It's all personal](#), Wolfgang Bangerth
- [The art of writing scientific software in an academic environment](#), Hartwig Anzt
- [Working Remotely: The Exascale Computing Project \(ECP\) panel series](#), Elaine Raybourn et al.
- [Better Scientific Software: 2019 highlights](#), Rinku Gupta
- And many more ...



A screenshot of the Better Scientific Software (BSSw) website. The header includes the BSSw logo, navigation links for 'Information For', 'Contribute to BSSw', 'Receive Our Email Digest', and 'Contact BSSw'. A yellow banner at the top right contains a message about the 2021 Fellowship Program. The main content area features a section titled 'Better Scientific Software (BSSw)' with a sub-section about software complexity and a central hub. Below this are buttons for 'GET ORIENTED', 'Communities Overview', 'Site Overview', 'Intro to CSE', and 'Intro to HPC'. A 'Featured' section on the left shows a thumbnail for a blog post about working remotely for the Exascale Computing Project (ECP). The right side of the page shows a preview of the ECP panel series video.



See also Track 7:
Software Productivity & Sustainability (Aug 6)



Gallery of highlights

- Overview of some HPC numerical software packages
- 1 slide per package, emphasizing key capabilities, highlights, and where to go for more info
 - Listed first
 - Packages featured in ATPESC 2020 lectures and hands-on lessons
 - Developers are available for optional discussions
 - Listed next
 - Additional highlighted packages (not a comprehensive list)

Block-structured adaptive mesh refinement framework. Support for hierarchical mesh and particle data with embedded boundary capability.

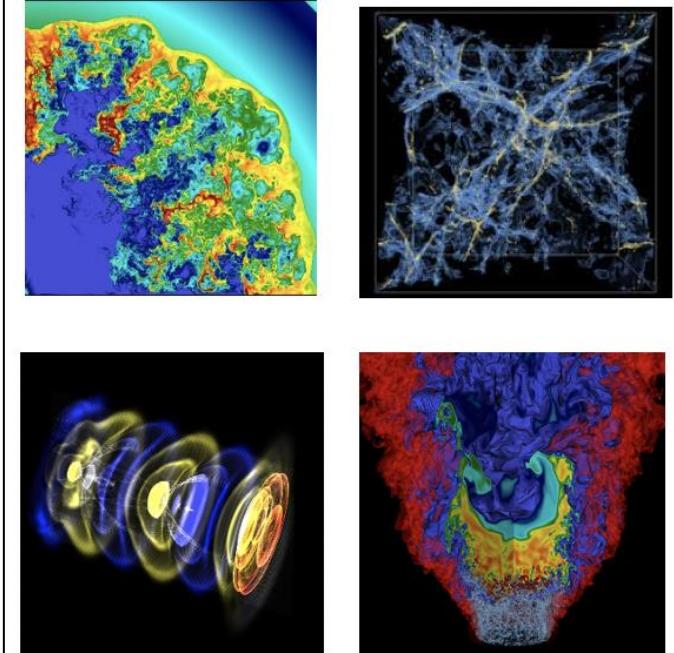
■ Capabilities

- Support for solution of PDEs on hierarchical adaptive mesh with particles and embedded boundary representation 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 (CUDA and beyond)
- 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
- Tutorial examples available in repository

■ Open source software

- Used for divers apps, including accelerator modeling, adaptive manufacturing, astrophysics, combustion, cosmology, multiphase flow, phase field modeling, ...
- Freely available on github with extensive documentation

Examples of AMReX applications

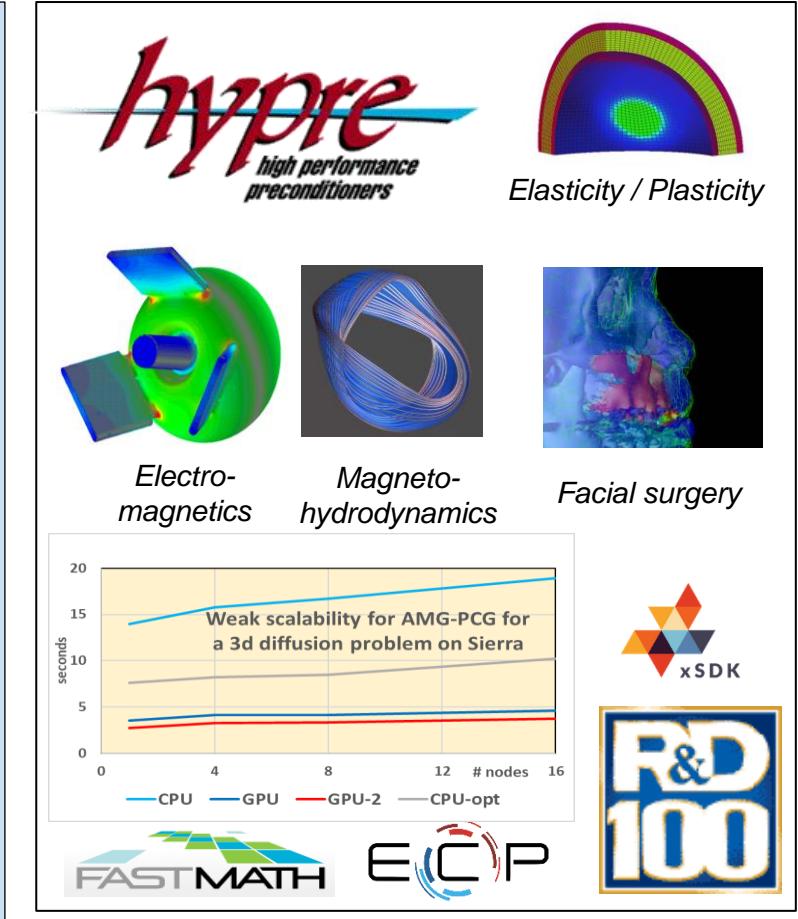


<https://www.github.com/AMReX-Codes/amrex>



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 more efficient (scalable) linear solvers through more effective data storage schemes and more efficient computational kernels
- **Scalable preconditioners and solvers**
 - Structured and unstructured algebraic multigrid solvers
 - Maxwell solvers, H-div solvers
 - Multigrid solvers for nonsymmetric systems: pAIR, MGR
 - Matrix-free Krylov solvers
- **Open source software**
 - Used worldwide in a vast range of applications
 - Can be used through PETSc and Trilinos
 - Provide CPU and GPU support
 - Available on github: <https://www.github.com/LLNL/hypre>

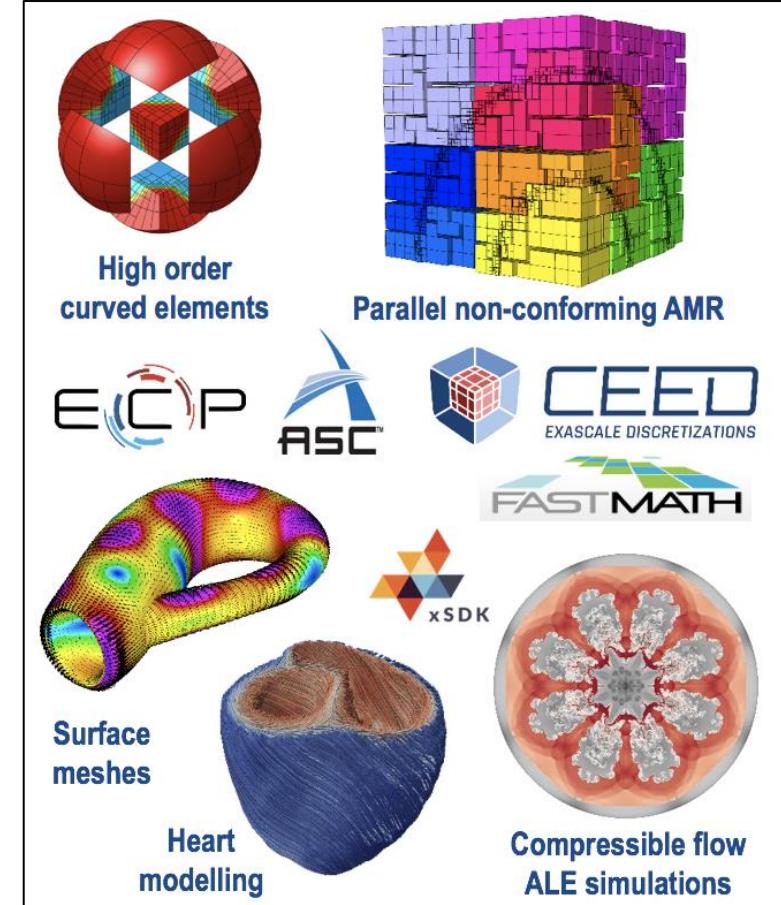


<http://www.llnl.gov/CASC/hypre>

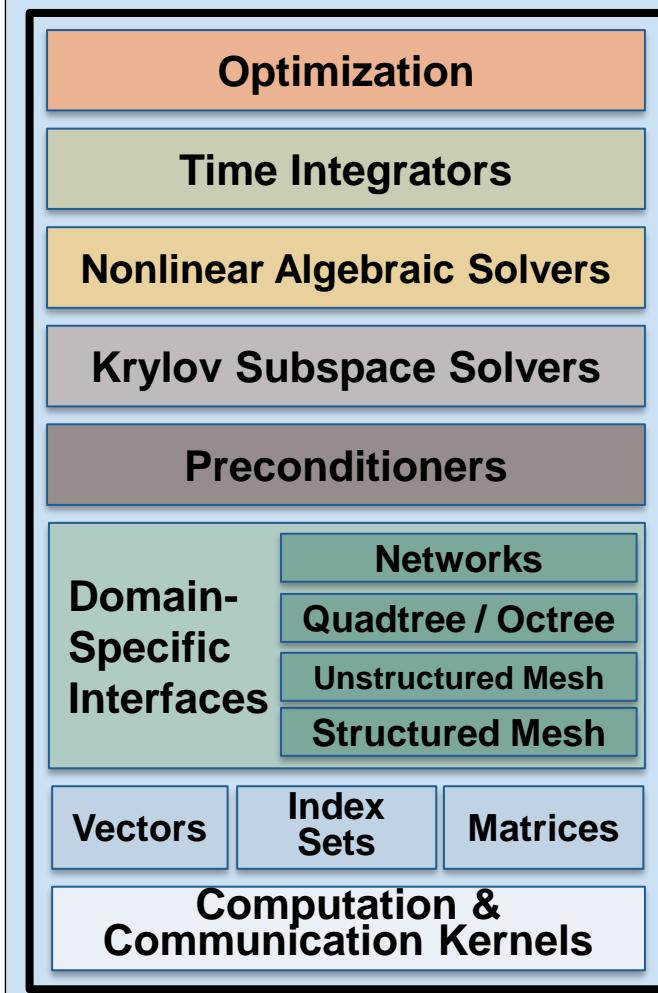


Free, lightweight, scalable C++ library for finite element methods. Supports arbitrary high order discretizations and meshes for wide variety of applications.

- **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**
 - LGPL-2.1 with thousands of downloads/year worldwide.
 - Available on GitHub, also via OpenHPC, Spack. Part of ECP's CEED co-design center.



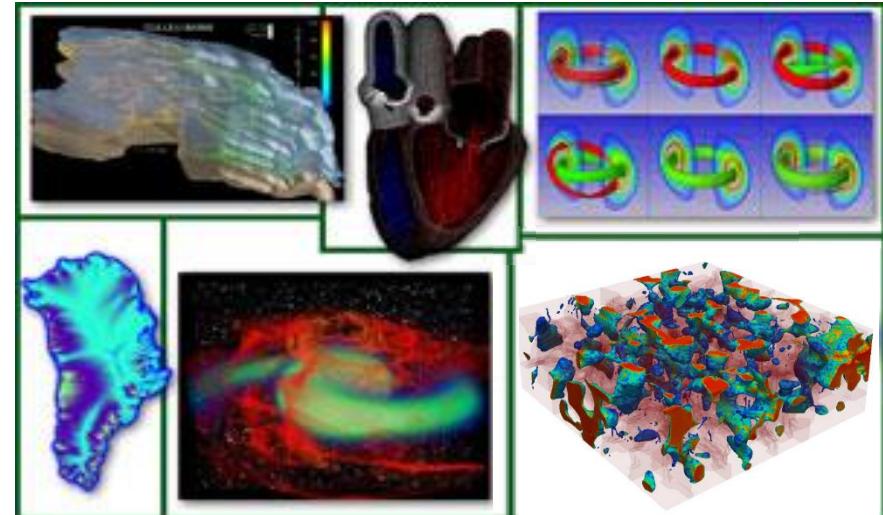
<http://mfem.org>



- **Easy customization and compositability of solvers at runtime**
 - 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
 - Thousands of users worldwide



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



PETSc provides the backbone of diverse scientific applications.

clockwise from upper left: hydrology, cardiology, fusion, multiphase steel, relativistic matter, ice sheet modeling



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

Parallel Unstructured Mesh Infrastructure

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

Core functionality

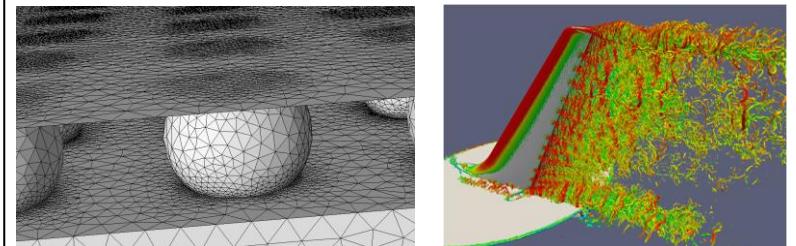
- Distributed, conformant mesh with entity migration, remote read only copies, fields and their operations
- Link to the geometry and attributes
- Mesh adaptation (straight and curved), mesh motion
- Multi-criteria partition improvement
- Distributed mesh support for Particle In Cell methods

Designed for integration into existing codes

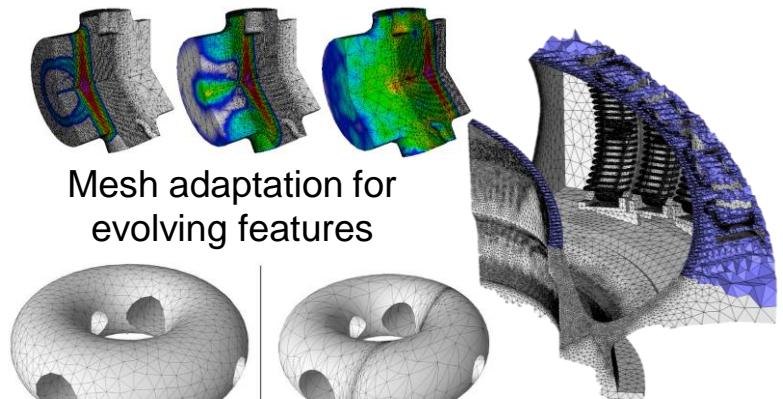
- Conformant with XSDK
- Permissive license enables integration with open and closed-source codes

In-memory integrations developed

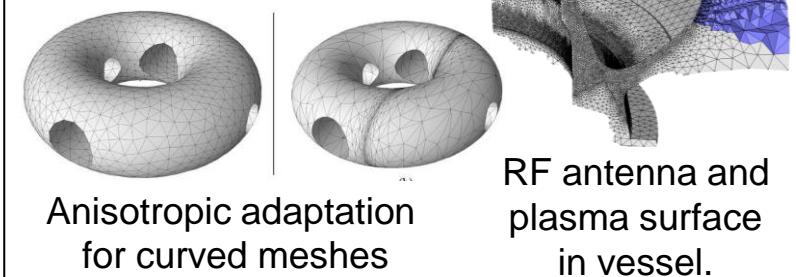
- MFEM: High order FE framework
- PetraM: Adaptive RF fusion
- PHASTA: FE for turbulent flows
- FUN3D: FV CFD
- Proteus: Multiphase FE
- ACE3P: High order FE for EM
- M3D-C1: FE based MHD
- Nektar++: High order FE for flow
- Albany/Trilinos: Multi-physics FE



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



Mesh adaptation for evolving features



Anisotropic adaptation for curved meshes

Source Code: github.com/SCOREC/core
Paper: www.scorec.rpi.edu/REPORTS/2014-9.pdf

PUMIPic Parallel Unstructured Mesh Infrastructure for Particle-in-Cell

Parallel management of unstructured meshes with particles.
Framework for GPU accelerated particle-in-cell applications using unstructured meshes.

Core functionality

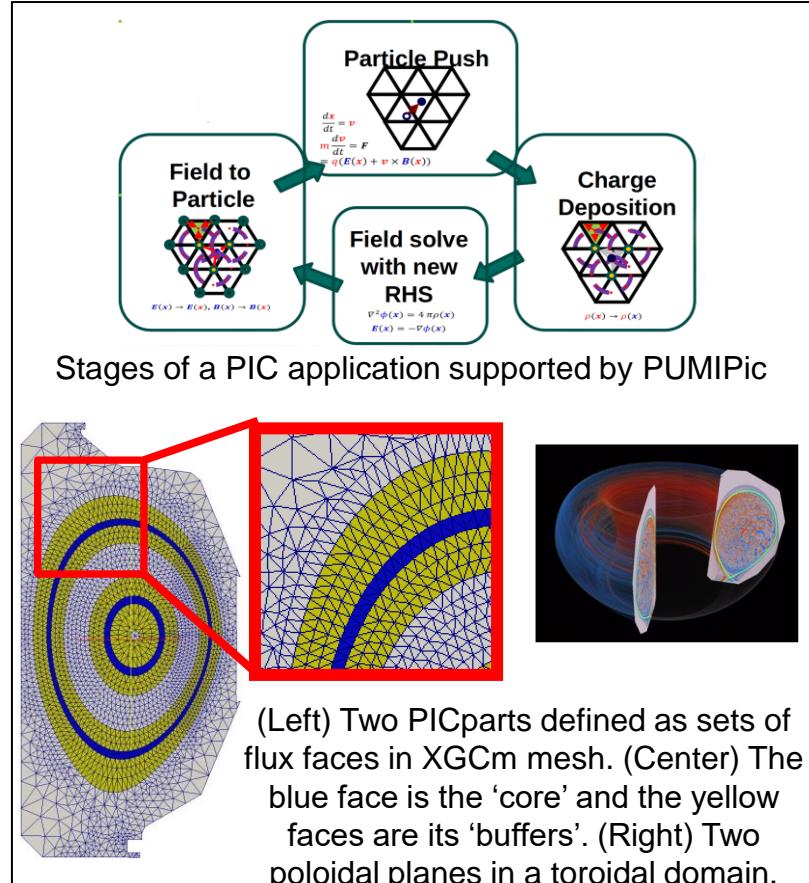
- Unstructured mesh-based approach
 - Particles accessed through mesh
 - Particle search through mesh adjacencies
 - Effective coupling to PDE solvers
 - Partitioning using bounding flux surfaces, graph, or geometric methods
 - PICpart: owned elements (defined by partition) + copied elements from topologically or spatially neighboring processes
 - Stored on GPU using Omega_h library: github.com/SNLComputation/omega_h
- Particles
 - Supports multiple species each with distinct combinations of ‘Plain Old Data’ per particle
 - Group particles by the mesh element that they are spatially located within
 - Stored on GPU using Sell-C-Sigma structure [Kreutzer 2014] that provides coalesced accesses for ‘warp’ sized blocks of work
 - Parallel kernel launch function abstracts underlying particle and mesh storage

Applications Supported

- GITRm: impurity transport
- XGCr: core+edge fusion plasma physics
- Weak scaling on up to 24,000 GPUs of Summit with 1.15 trillion particles running push, particle-to-mesh, and mesh-to-particle operations with an XGCr tokamak mesh and domain decomposition



Rensselaer



Source Code: github.com/SCOREC/pumi-pic
Paper: www.scorec.rpi.edu/REPORTS/2019-2.pdf

PUMIPic Applications

Unstructured mesh particle-in-cell fusion applications using PUMIPic. Supporting the analysis of tokamak plasma physics and impurity transport using extensions to the PUMIPic framework.

XGCM

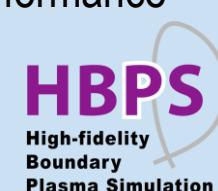
- Core and edge fusion plasma physics with ions and kinetic electrons
- Tokamak: 2D mesh partitioned into PICParts (see PUMIPic slide) based on bounding flux surfaces
- A group of processes is assigned to a PICPart and $1/P^{\text{th}}$ of the torus in the toroidal direction – group size controls particle load on each GPU
- Initial focus on performance and scaling with pseudo operations
- Weak scaling on up to 24,000 GPUs of Summit with 1.15 trillion particles running push, particle-to-mesh, and mesh-to-particle operations
- Current focus on implementing physically correct operations

GITRm

- Impurity transport
- 3D meshes PICParts formed using graph based partitions
- Tracking wall collisions and multiple species
- Initial focus on verifying implementation of all physics model terms
- Statistical and numerical verification complete
- Current focus on performance and scalability

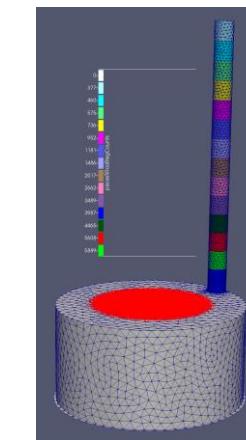
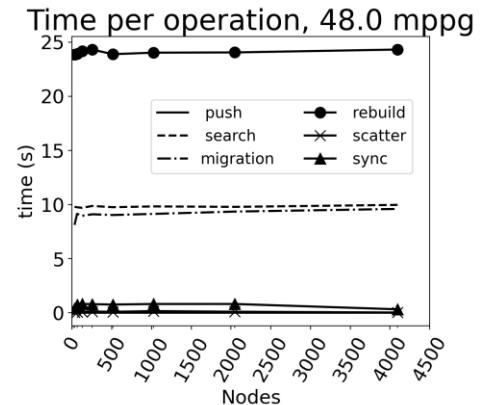


Rensselaer

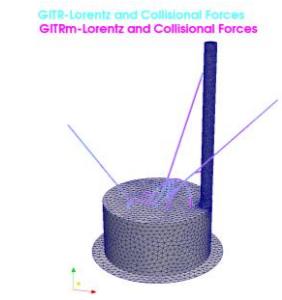


XGCM weak scaling on Summit

D3D, 2M elm. mesh,
192 PICParts/plane,
1 to 128 planes,
48M ptcls/GPU,
6 GPUs/node



Counts of impacting particles



Particle paths match

GITRm PISCES initial test case

Contact: Mark S. Shephard
shephard@rpi.edu

SUNDIALS

Suite of Nonlinear and Differential
/Algebraic Equation Solvers

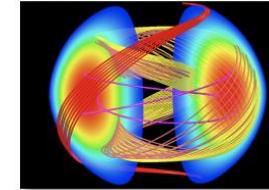


Adaptive time integrators for ODEs and DAEs and efficient nonlinear solvers
Used in a variety of applications. Freely available. Encapsulated solvers & parallelism.

- **ODE integrators:**
 - CVODE: adaptive order and step BDF (stiff) & Adams (non-stiff) methods
 - ARKode: adaptive step implicit, explicit, IMEX, and multirate Runge-Kutta methods
- **DAE integrators:** IDA – adaptive order and step BDF integrators
- **Sensitivity Analysis:** CVODES and IDAS provide forward and adjoint sensitivity analysis capabilities for ODEs and DAEs respectively
- **Nonlinear Solvers:** KINSOL – Newton-Krylov, Picard, and accelerated fixed point
- **Modular Design:** Users can supply own data structures and solvers or use SUNDIALS provided modules
 - Written in C with interfaces to Fortran
 - Vectors modules: serial, MPI, OpenMP, CUDA, RAJA, hypre, PETSc, & Trilinos
- **Open Source:** Freely available (BSD License) from LLNL site, GitHub, and Spack. Can be used from MFEM, PETSc, and deal.II



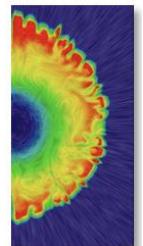
SUNDIALS is used by thousands worldwide in applications from research and industry



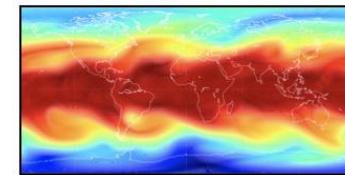
Magnetic Reconnection



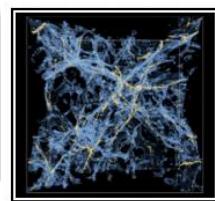
Dislocation Dynamics



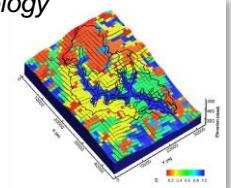
Core Collapse Supernova



Atmospheric Dynamics



Cosmology



Subsurface Flow

SUNDIALS is supported by extensive documentation, a user email list, and an active user community

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

SuperLU



Supernodal Sparse LU Direct Solver. Unique user-friendly interfaces. Flexible software design. Used in a variety of applications. Freely available.

■ Capabilities

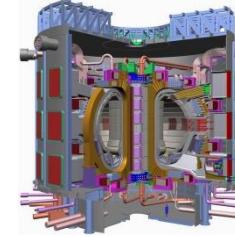
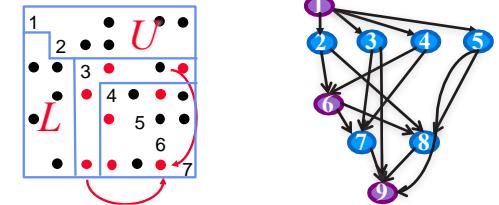
- Serial (thread-safe), shared-memory (SuperLU_MT, OpenMP or Pthreads), distributed-memory (SuperLU_DIST, hybrid MPI+ OpenM + CUDA).
 - Implemented in C, with Fortran interface
- Sparse LU decomposition, triangular solution with multiple right-hand sides
- Incomplete LU (ILU) preconditioner in serial SuperLU
- Sparsity-preserving ordering:
 - Minimum degree ordering applied to $A^T A$ or A^T+A
 - Nested dissection ordering applied to $A^T A$ or A^T+A [(Par)METIS, (PT)-Scotch]
- User-controllable pivoting: partial pivoting, threshold pivoting, static pivoting
- Condition number estimation, iterative refinement.
- Componentwise error bounds

■ Performance

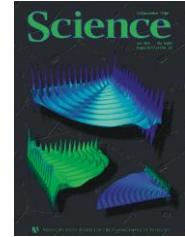
- Factorization strong scales to 24,000 cores (IPDPS'18)
- Triangular solve strong scales to 4000 cores (CSC'18)

■ Open source software

- Used worldwide 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.



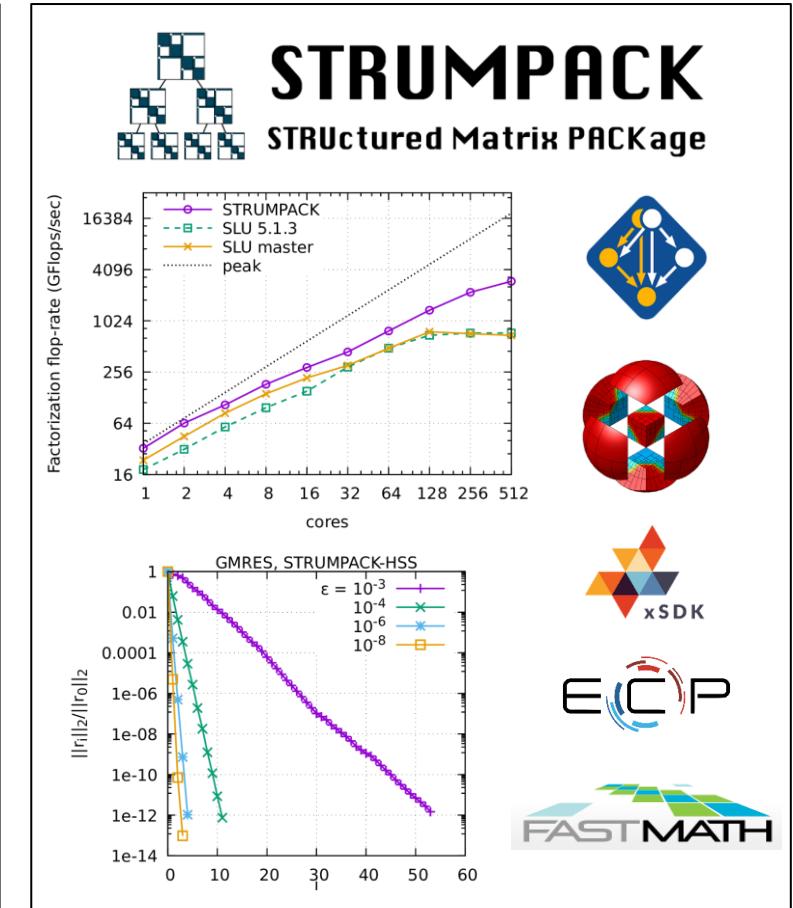
<http://crd-legacy.lbl.gov/~xiaoye/SuperLU>

STRUMPACK



STRUctured Matrix PACKage. Hierarchical solvers for dense rank-structured matrices; fast sparse solver and robust and scalable preconditioners.

- **Dense Matrix Solvers, Hierarchical Approximations**
 - Hierarchical partitioning, low-rank approximations
 - Formats: Hierarchically Semi-Separable (HSS), Hierarchically Off-Diagonal Block Low-Rank (HODLR), Block Low-Rank (BLR)
 - Applicable to integral equations discretized with boundary element methods, structured matrices such as Cauchy or Toeplitz, kernel matrices, covariance matrices, ...
 - Algorithms with much lower asymptotic complexity than corresponding ScaLAPACK routines
- **Sparse Direct Solver**
 - Multifrontal algorithm, Fill-reducing orderings: Par-METIS, PT-Scotch, RCM, spectral
 - Good scalability, fully distributed, parallel symbolic phase
- **Sparse Preconditioners**
 - Sparse direct solver with dense hierarchical (low-rank) approximations
 - Scalable and robust, aimed at PDE discretizations, indefinite systems, ...
 - Iterative solvers: GMRES, BiCGStab, iterative refinement
- **Software**
 - BSD License, MPI+OpenMP, scalable to 10K+ cores
 - Interfaces from PETSc, MFEM (Trilinos coming), available in Spack
 - Under very active development



github.com/pghysels/STRUMPACK

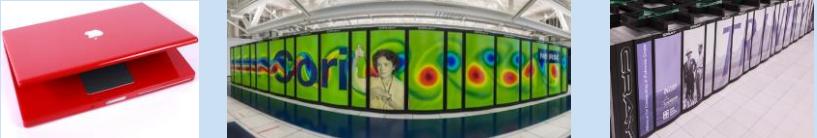
Trilinos



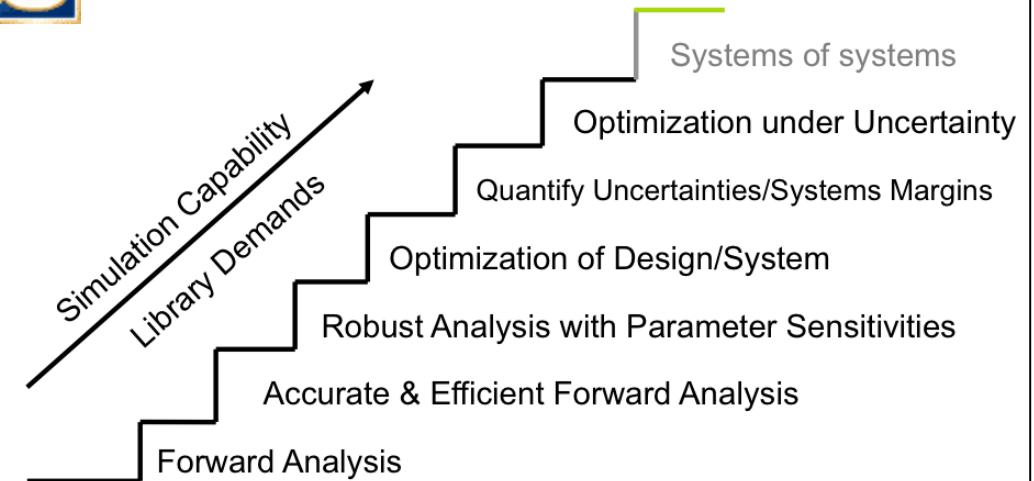
Sandia
National
Laboratories

Optimal kernels to optimal solutions. Over 60 packages. Laptops to leadership systems. Next-gen systems, multiscale/multiphysics, large-scale graph analysis.

- **Optimal kernels to optimal solutions**
 - Scalable linear, nonlinear, eigen, transient, optimization, UQ solvers
 - Discretization, geometry, meshing
 - Load balancing
 - ***Performance Portability across multiple platforms (GPU, multicore) provided by Kokkos***
- **60+ packages**
 - Other distributions: Cray LIBSCI, Github repo
 - Thousands of users, worldwide distribution
 - Laptops to leadership systems: MPI, GPU, multicore



Transforming Computational Analysis To Support High Consequence Decisions



Each stage requires *greater performance and error control* of prior stages:
**Always will need: more accurate and scalable methods.
more sophisticated tools.**

<https://trilinos.github.io/>

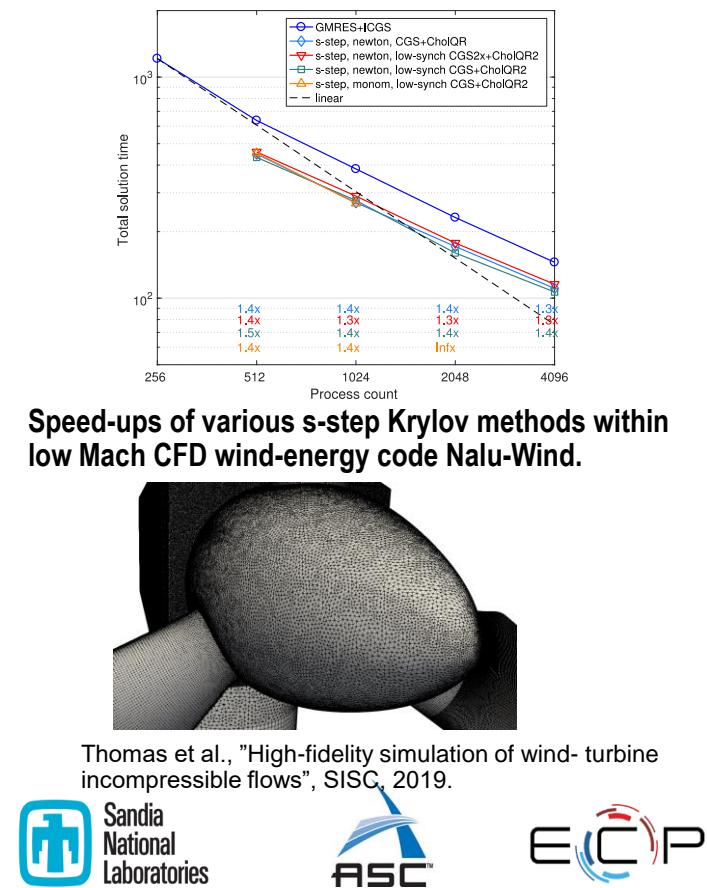


Trilinos/Belos

Iterative Krylov-based solvers. Templatized 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: $AX_i = B_i, i=1,\dots,t$
 - Sequences of multiple-RHS systems: $A_iX_i = B_i, i=1,\dots,t$
- **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.



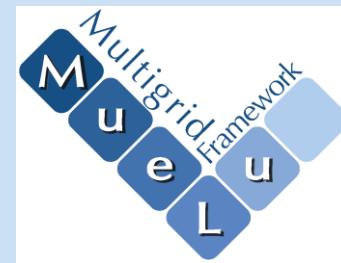
<https://trilinos.github.io/belos.html>

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)



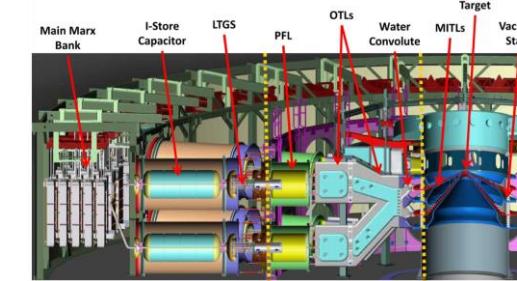
▪ Capabilities

- Aggregation-based coarsening
- **Smoothers**: Jacobi, GS, $\sqrt{1}$ 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

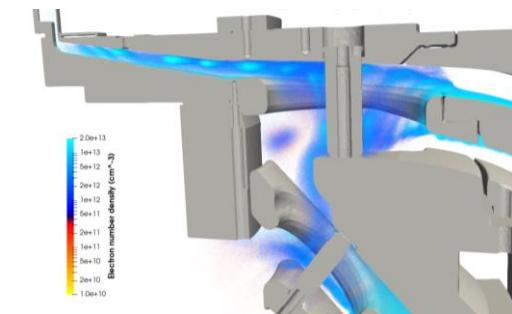
- AMG for multiphysics
- Multigrid for coupled structured/unstructured meshes
- Algorithm selection via machine learning

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.



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

AMG preconditioning for $H(\text{curl})$ 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).



Sandia
National
Laboratories



SciDAC
Scientific Discovery
through Advanced Computing



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

Gallery of highlights

- Overview of HPC numerical software packages
- 1 slide per package, emphasizing key capabilities, highlights, and where to go for more info
 - Listed first (alphabetically)
 - Packages featured in ATPESC 2020 lectures and hands-on lessons
 - Listed next (alphabetically)
 - Additional highlighted packages (not a comprehensive list)

ButterflyPACK



Fast direct solvers. Low-rank and butterfly compression. Distributed-memory parallel. Particularly for highly-oscillatory wave equations.

■ Capabilities

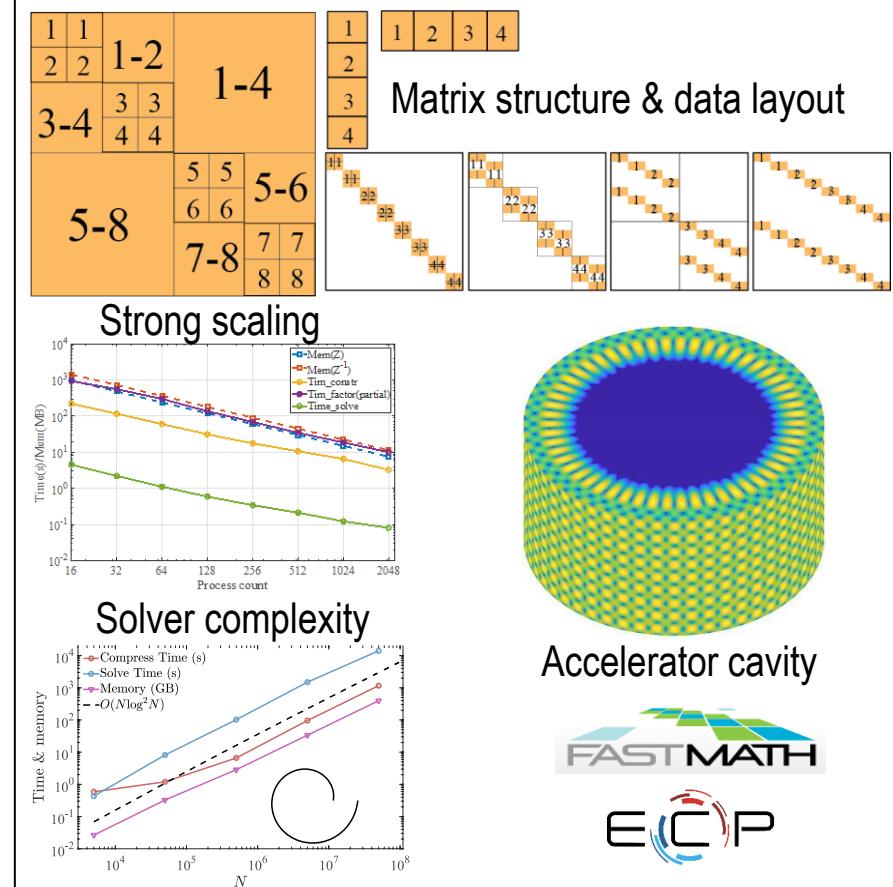
- Fast algebraic operations for rank-structured dense and sparse matrices, including matrix compression, multiplication, factorization and solution
- Support distributed-memory H-matrix, HODLR formats with low-rank and butterflies
- Particularly targeted at high-frequency electromagnetic, acoustic and elastic applications

■ Conceptual interfaces

- User input: a function to compute arbitrary matrix entries or to multiply the matrix with arbitrary vectors
- Both Fortran2008 and C++ interface available
- Highly interoperable with STRUMPACK

■ Open source software

- Software dependence: BLAS, LAPACK, SCALAPACK, ARPACK
- Newly released on github with tutorial examples available:
<https://github.com/liuyangzhan/ButterflyPACK/tree/master/EXAMPLE>



<https://github.com/liuyangzhan/ButterflyPACK>

Chombo



Scalable adaptive mesh refinement framework. Enables implementing scalable AMR applications with support for complex geometries.

■ Adaptive Mesh Refinement (AMR)

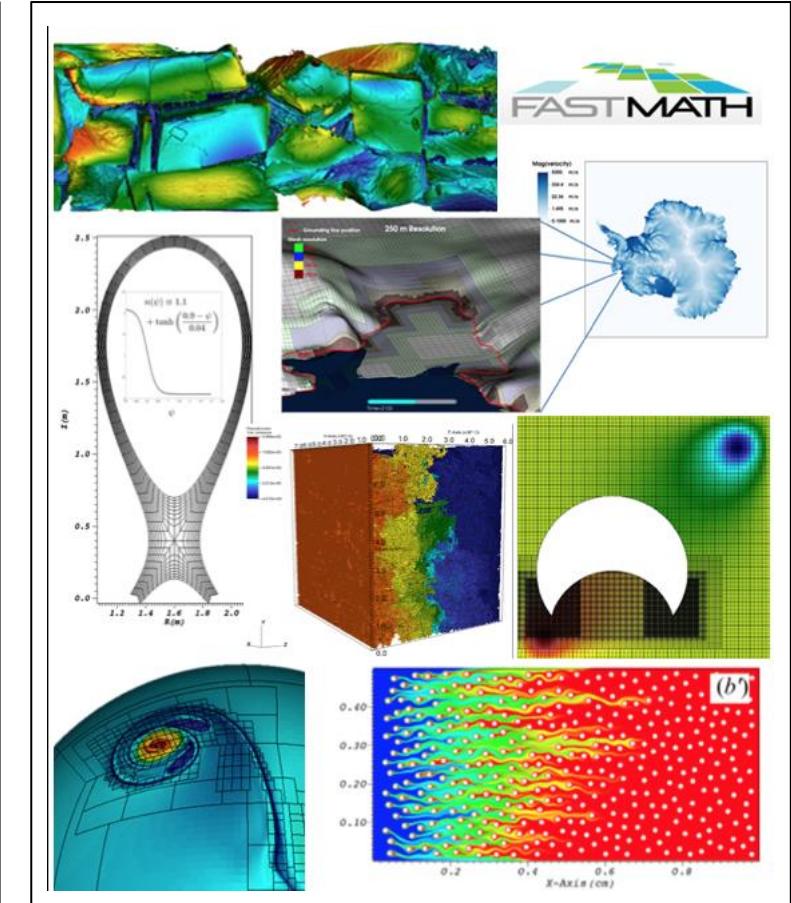
- Block structured AMR dynamically focuses computational effort where needed to improve solution accuracy
- Designed as a developers' toolbox for implementing scalable AMR applications
- Implemented in C++/Fortran
- Solvers for hyperbolic, parabolic, and elliptic systems of PDEs

■ Complex Geometries

- Embedded-boundary (EB) methods use a cut-cell approach to embed complex geometries in a regular Cartesian mesh
- EB mesh generation is extremely efficient
- Structured EB meshes make high performance easier to attain

■ Higher-order finite-volume

- Higher (4th)-order schemes reduce memory footprint & improve arithmetic intensity
- Good fit for emerging architectures
- Both EB and mapped-multiblock approaches to complex geometry



<http://Chombo.lbl.gov>

DataTransferKit



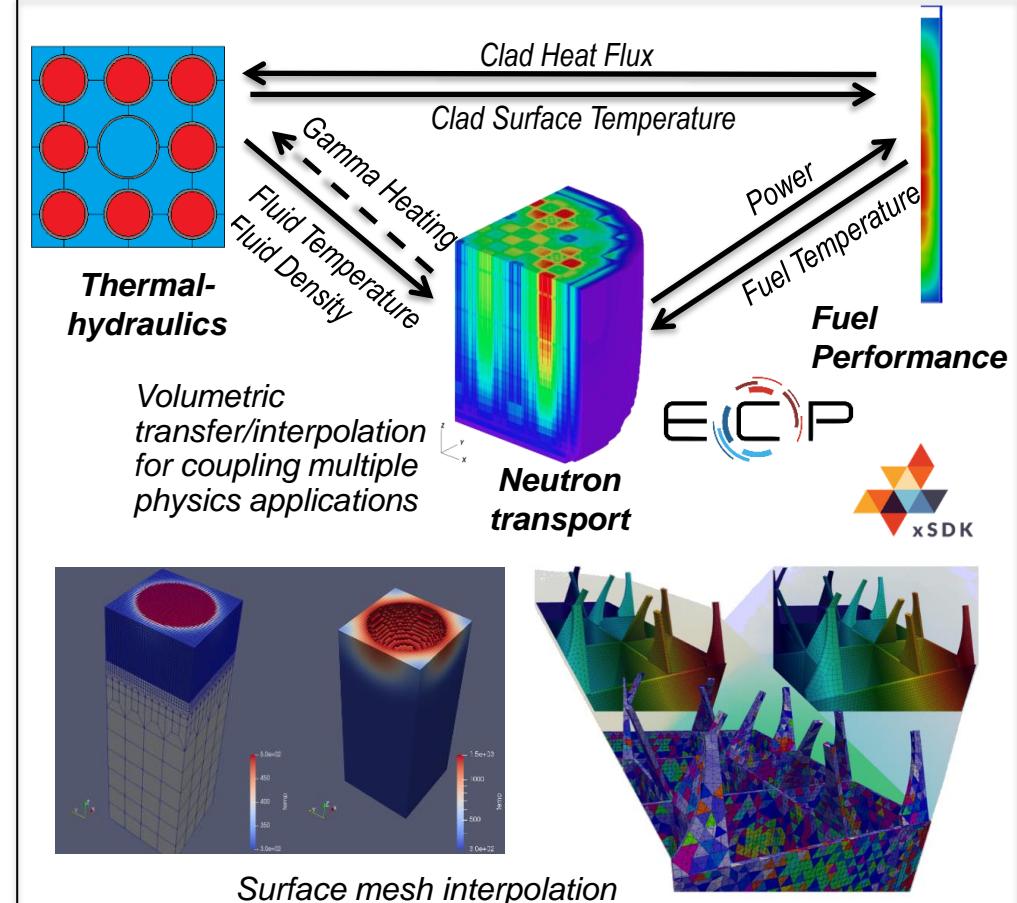
Open source library for parallel solution transfer.
Support for grid-based and mesh-free applications.

Overview

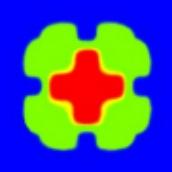
- Transfers application solutions between grids with differing layouts on parallel accelerated architectures
- Coupled applications frequently have different grids with different parallel distributions; DTK is able to transfer solution values between these grids efficiently and accurately
- Used for a variety of applications including conjugate heat transfer, fluid structure interaction, computational mechanics, and reactor analysis

Capabilities

- Support for DOE leadership class machines through MPI+Kokkos programming model
- Algorithms demonstrated scalable to billions of degrees of freedom
- General geometric search algorithms
 - Comparable serial performance to Boost r-Tree and NanoFlann
 - Also thread scalable on many core CPU and GPUs and distributed via MPI
- Grid interpolation operators and mesh-free transfer operators

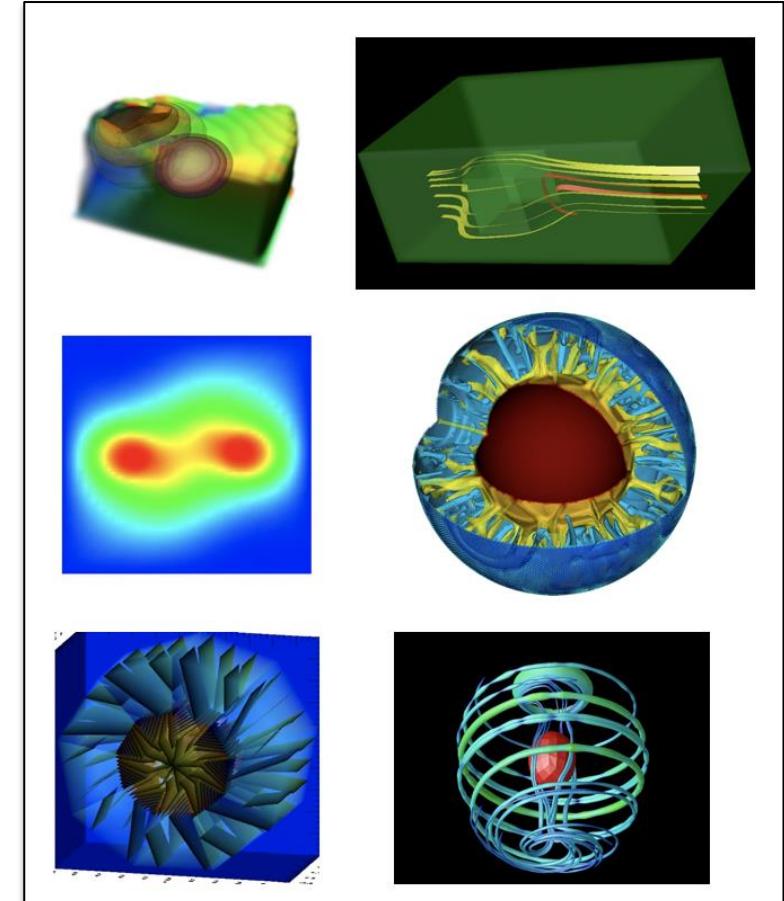


<https://github.com/ORNL-CEES/DataTransferKit>



deal.II — an open source finite element library. Modern interface to the complex data structures and algorithms required for solving partial differential equations computationally using state-of-the-art programming techniques.

- **Meshes and elements:**
 - Supports h- and p-adaptive meshes in 1d, 2d, and 3d
 - Easy ways to adapt meshes: Standard refinement indicators already built in
 - Many standard finite element types (continuous, discontinuous, mixed, Raviart-Thomas, Nedelec, ABF, BDM,...)
 - Full support for coupled, multi-component, multi-physics problems
- **Linear algebra:**
 - Has its own sub-library for dense and sparse linear algebra
 - Interfaces to PETSc, Trilinos, UMFPACK, ScalAPACK, ARPACK
- **Pre- and postprocessing:**
 - Can read most mesh formats
 - Can write almost any visualization file format
- **Parallelization:**
 - Uses threads and tasks on shared-memory machines
 - Uses up to 100,000s of MPI processes for distributed-memory machines
 - Can use CUDA
- **Open-source software:**
 - Used for a wide range of applications, including heart muscle fibers, microfluidics, oil reservoir flow, fuel cells, aerodynamics, quantum mechanics, neutron transport, numerical methods research, fracture mechanics, damage models, sedimentation, biomechanics, root growth of plants, solidification of alloys, glacier mechanics, and many others.
 - Freely available on GitHub



<https://www.dealii.org>

libEnsemble



A Python library to coordinate the evaluation of dynamic ensembles of calculations. Use massively parallel resources to accelerate the solution of design, decision, and inference problems.

libEnsemble aims for:

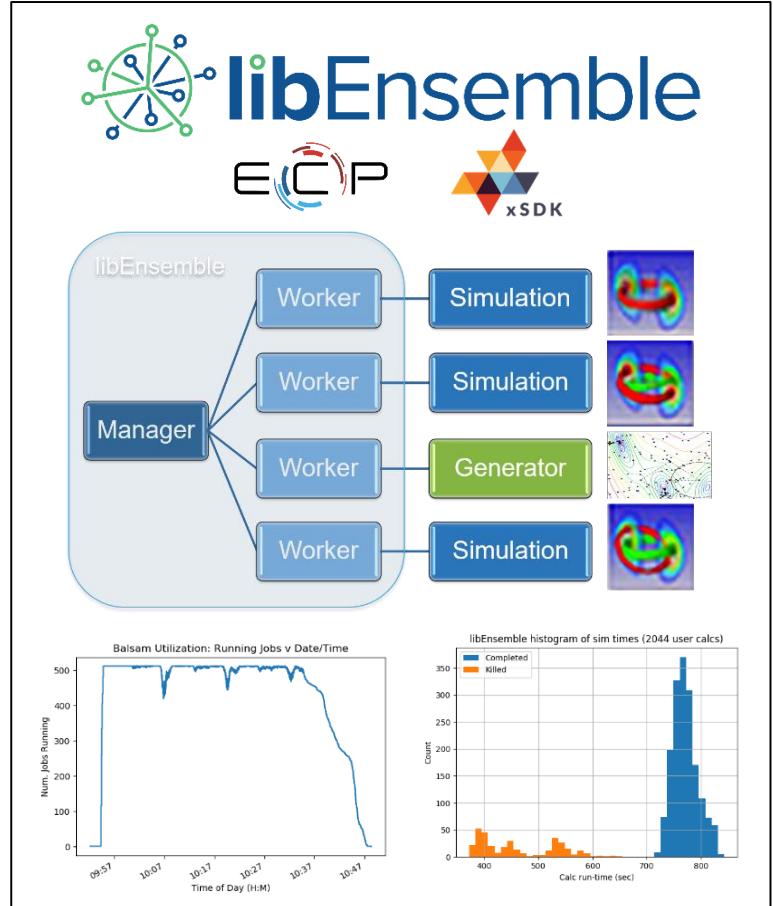
- Extreme scaling
- Resilience and fault tolerance
- Monitoring and killing tasks and recovering resources
- Portability and flexibility

■ libEnsemble features:

- Communications using MPI, multiprocessing, or TCP
- Support for calculations using parallel resources, including user-provided executables
- Executor auto-detects system resources and launches user executables
- Support on Summit (ORNL), Theta (ALCF), Cori (NERSC), Bridges (PSC)

■ Dynamic ensembles:

- Workers are allocated simulations or generate input for simulations
- One use case: an optimization method generates parameters to be evaluated by a computationally expensive simulation
- Example interfaces with PETSc, SciPy, and NLOpt solvers are available



<https://libensemble.readthedocs.io>

Dense Linear Algebra Solvers

- Linear systems of equations
- Linear least squares
- Singular value decomposition

Matrix spectrum methods

- Symmetric and non-symmetric eigenvalues
- Generalized eigenvalue problems
- Singular Value Decomposition

Sparse Solvers & Tensor Computations

MAGMA SPARSE

ROUTINES BiCG, BiCGSTAB, Block-Asynchronous Jacobi, CG, CGS, GMRES, IDR, Iterative refinement, LOBPCG, LSQR, QMR, TFQMR

PRECONDITIONERS ILU / IC, Jacobi, ParILU, ParILUT, Block Jacobi, ISAI

KERNELS SpMV, SpMM

DATA FORMATS CSR, ELL, SELL-P, CSR5, HYB

FEATURES AND SUPPORT

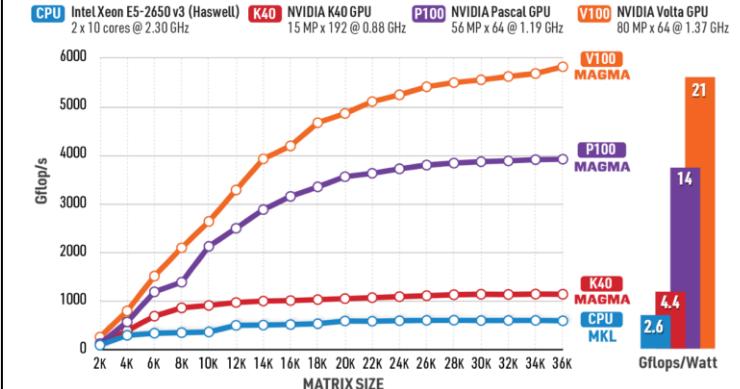
- MAGMA 2.3 FOR CUDA
- cIMAGMA 1.4 FOR OpenCL
- MAGMA MIC 1.4 FOR Intel Xeon Phi

CUDA OpenCL Intel Xeon Phi

- Linear system solvers
- Eigenvalue problem solvers
- Auxiliary BLAS
- Batched LA
- Sparse LA
- CPU/GPU Interface
- Multiple precision support
- Non-GPU-resident factorizations
- Multicore and multi-GPU support
- MAGMA Analytics/DNN
- LAPACK testing
- Linux
- Windows
- Mac OS

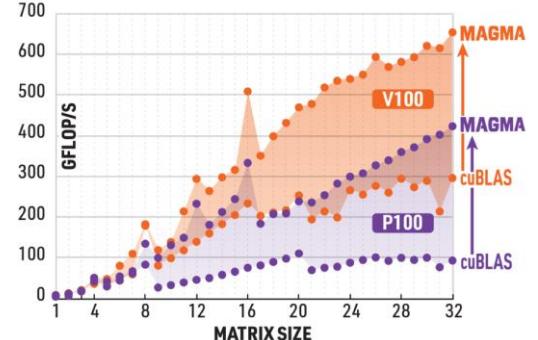
PERFORMANCE & ENERGY EFFICIENCY

MAGMA LU factorization in double precision arithmetic



PERFORMANCE OF BATCHED LU

in double precision arithmetic on 1 million matrices



<http://icl.utk.edu/magma>

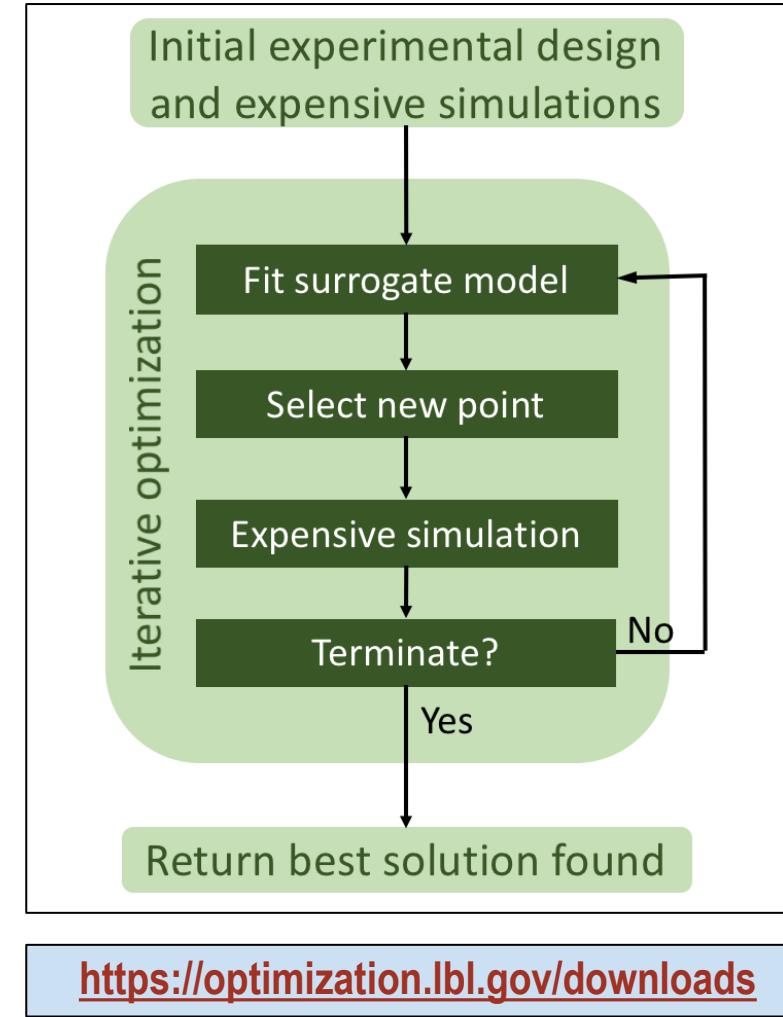
Efficient optimization of computationally-expensive black-box problems. For integer, mixed-integer, and continuous variables. Your choice of surrogate model, sampling method, and initial design strategy. Easy to use. Freely available.

- **Capabilities**

- Efficient solution of parameter optimization problems that involve time-consuming black-box HPC simulations during the objective function evaluation
- Surrogate models approximate the expensive function and aid in iterative selection of sample points
- Adaptive sampling for continuous, integer, and mixed-integer problems *without* relaxation of integer constraints

- **Available User options**

- **Surrogate model choices:** radial basis functions, polynomial regression, multivariate adaptive regression splines, surrogate model ensembles
- **Iterative sample point selection:** local perturbations, global candidate points, minimization over the surrogate model
- **Initial experimental design:** Latin hypercube, symmetric Latin hypercube, design space corners



<https://optimization.lbl.gov/downloads>

- **Sparse Eigenvalue Solver: Block Jacobi-Davidson QR**

- Hermitian or non-Hermitian matrices
- Generalized problems $\mathbf{A}x = \lambda \mathbf{B}x$ (for Hermitian pos. def. matrix \mathbf{B})
- Blocked iterative linear solvers like GMRES, BiCGStab and CGMN
- Can be accelerated by preconditioning
- Matrix-free interface
- Supported data types: D, Z, S, C

- **Algorithmic Building Blocks**

- block orthogonalization
- Eigenvalue counting (kernel polynomial method/KPM)
- Fused basic operations for better performance

- **Various interfaces**

- C, C++, Fortran 2003, Python

Can choose from several
backends at compile time



full interoperability

PHIST (builtin)

optimized (Fortran, MPI, OpenMP)
row-major block vectors
CRS format



C, MPI, OpenMP, SIMD, CUDA
SELL-C-sigma format

Funded by the DFG
project ESSEX



<https://bitbucket.org/essex/phist>

required flexibility

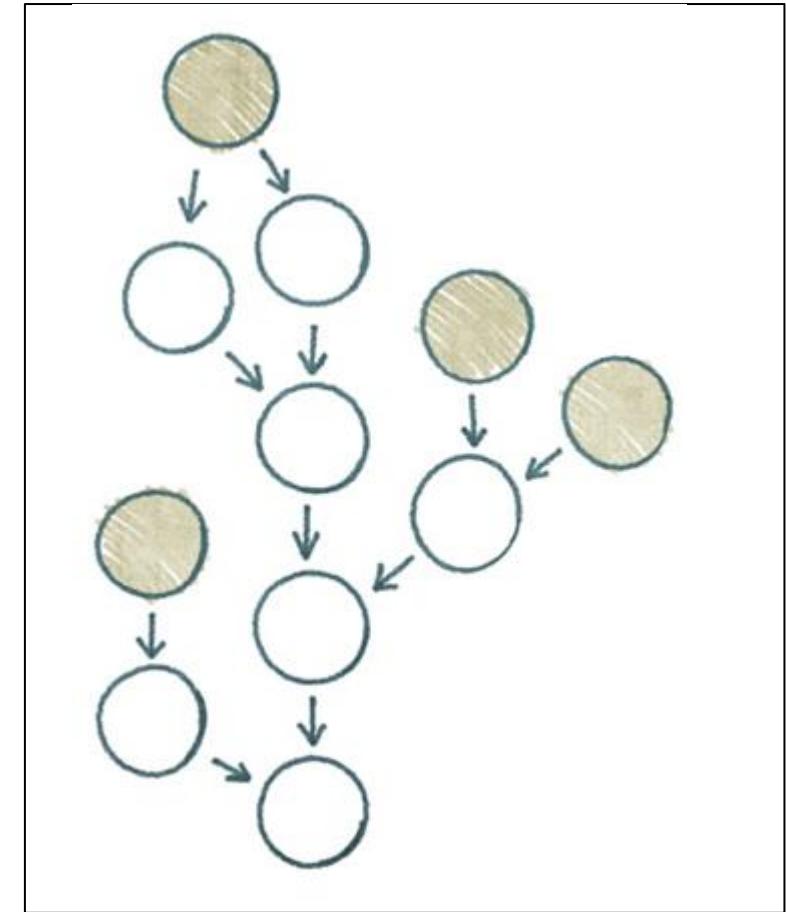
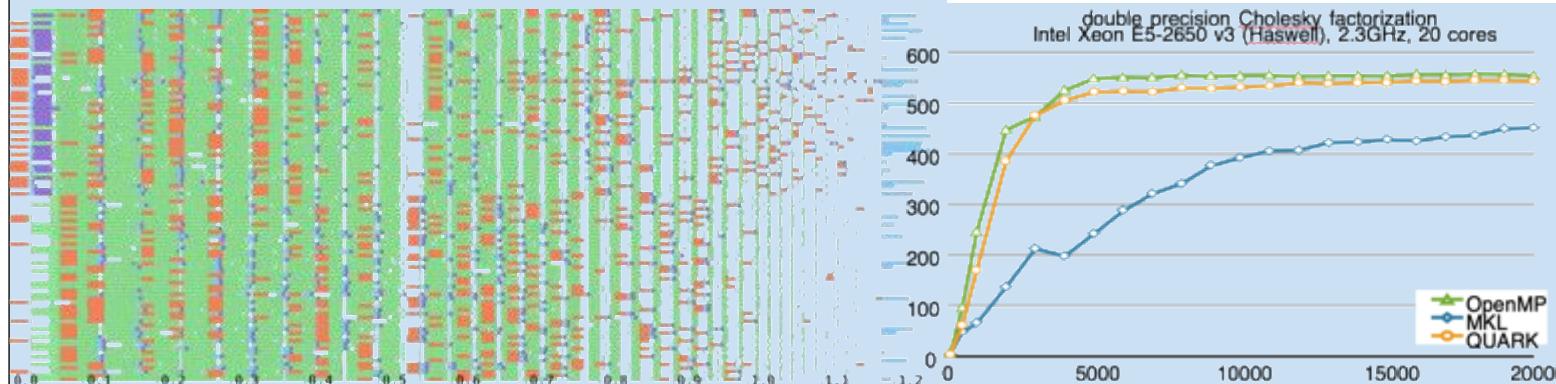
hardware awareness

PLASMA



Linear algebra solvers and spectral decompositions for multicore processors.
Portable and scalable dense solvers for large core counts.

- **Dense Linear Algebra Solvers**
 - Linear systems of equations
 - Linear least squares
 - Positive/Hermitian definitive solvers
- **Matrix spectrum methods**
 - Symmetric and non-symmetric eigenvalues
 - Generalized eigenvalue problems
 - Singular Value Decomposition
- **Data conversion and thread control**



<http://icl.utk.edu/plasma>

Scalable Library for Eigenvalue Problem Computations. Parallel solvers for linear and nonlinear eigenproblems. Also functionality for matrix functions.

■ Linear eigenvalue problems and SVD

- Standard and generalized eigenproblem, $Ax=\lambda x$, $Ax=\lambda Bx$; singular values $Au=\sigma v$
- Easy selection of target eigenvalues, shift-and-invert available for interior ones
- Many solvers: Krylov, Davidson, LOBPCG, contour integral, ...

■ Nonlinear eigenvalue problems

- Polynomial eigenproblem $P(\lambda)x=0$, for quadratic or higher-degree polynomials
- Solvers: Krylov with compact basis representation; Jacobi-Davidson
- General nonlinear eigenproblem $T(\lambda)x=0$, for any nonlinear function incl. rational

■ Matrix functions

- Parallel Krylov solver to evaluate $y=f(A)v$
- Support for matrix exponential, square root, etc. and combinations thereof

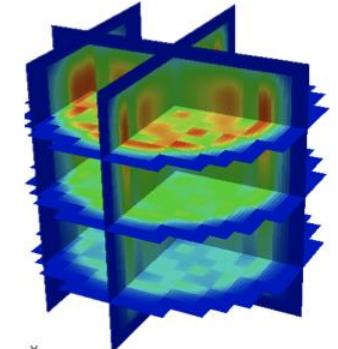
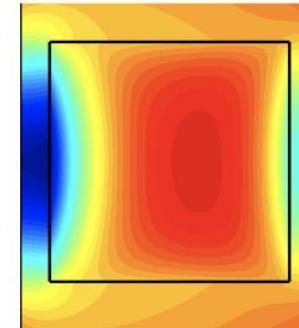
■ Extension of PETSc

- Runtime customization, portability and performance, C/C++/Fortran/python
- Can use any PETSc linear solvers and preconditioners

SLEPc



Nonlinear Eigensolver				M. Function	
SLP	RII	N-Arnoldi	Interp.	CISS	NLEIGS
Polynomial Eigensolver				SVD Solver	
TOAR	Q-Arnoldi	Linearization	JD	Cross Product	Cyclic Matrix
Linear Eigensolver				Thick R. Lanczos	
Krylov-Schur	Subspace	GD	JD	LOBPCG	CISS
				...	



<http://slepc.upv.es>

Zoltan/Zoltan2

Parallel partitioning, load balancing, task placement, graph coloring, matrix ordering, unstructured communication utilities, distributed directories

- Partitioning & load-balancing support many applications**

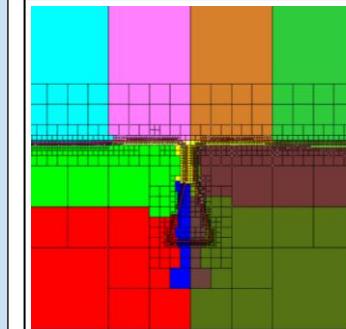
- Fast geometric methods maintain spatial locality of data (e.g., for adaptive finite element methods, particle methods, crash/contact simulations)
- Graph and hypergraph methods explicitly account for communication costs (e.g., for electrical circuits, finite element meshes, social networks)
- Single interface to popular partitioning TPLs: XtraPuLP (SNL, RPI); ParMA (RPI); PT-Scotch (U Bordeaux); ParMETIS (U Minnesota)
- MPI+X geometric partitioning using Kokkos for GPU and multicore

- Architecture-aware MPI task placement reduces application communication time**

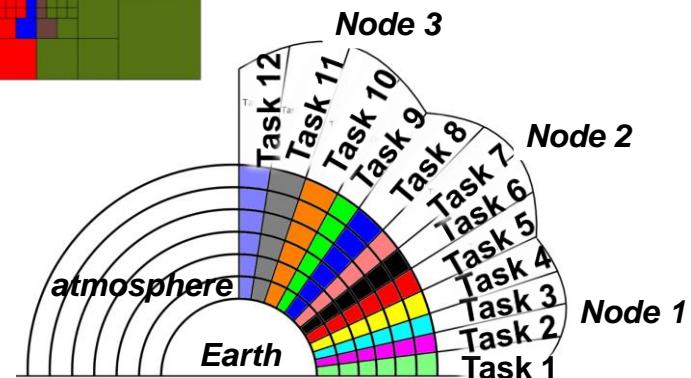
- Places interdependent MPI tasks on “nearby” nodes in network
- Reduces communication time and network congestion

- Graph algorithms for coloring, ordering, connectivity**

- Use as a stand-alone library or as a Trilinos component**



Zoltan's fast, geometric partitioner redistributes work to maintain load balance in a surface deposition simulation with adaptive meshing



Zoltan2's task placement reduced communication time in E3SM HOMME (atmospheric modeling) by up to 31% on 16K cores of IBM BG/Q



Sandia
National
Laboratories



<http://www.cs.sandia.gov/Zoltan>

HandsOn Lessons

- Hand-coded heat equation intro
- Structured meshing & discretization
- Unstructured meshing & discretization
- Krylov solvers & preconditioners
- Sparse direct solvers
- Nonlinear solvers
- Time integration
- Numerical optimization



ATPESC 2020 Hands On Lessons

[Meshing and Discretization with AMReX](#)

A Block Structured Adaptive Mesh Refinement Framework

[Hand Coded Heat](#)

Why use numerical packages...

[Krylov Solvers and Algebraic Multigrid with hypre](#)

Demonstrate utility of multigrid

And more ...

Github pages site:

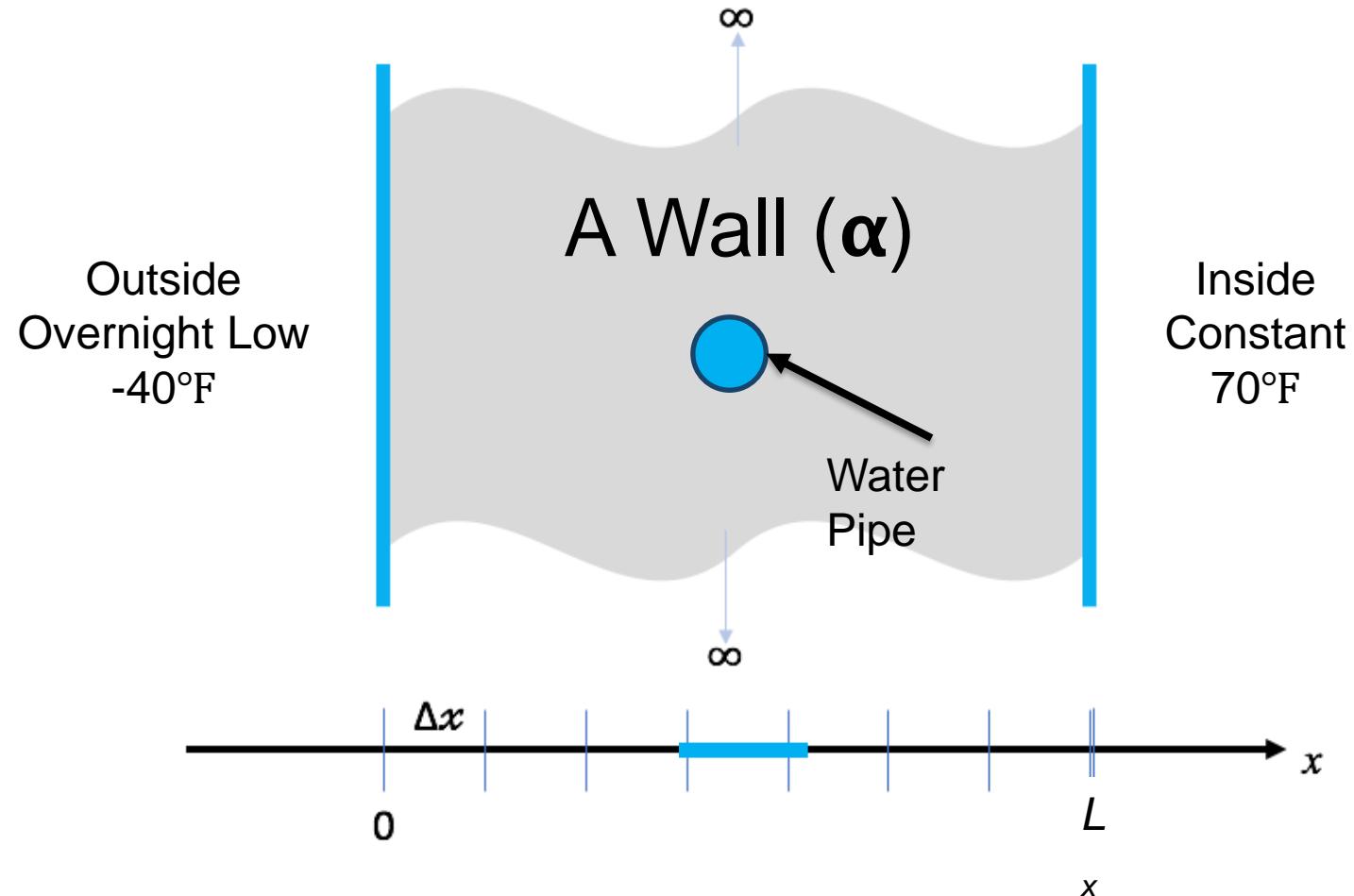
<https://xSDK-project.github.io/MathPackagesTraining2020/lessons/>

Hello World (for numerical packages)

Mark C Miller, LLNL

IDEAS-ECP/ATPESC SQE Support and Training Coordinator

A Science Problem of Interest: Will My Water Pipes Freeze?



$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

The One-Dimensional Heat Equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

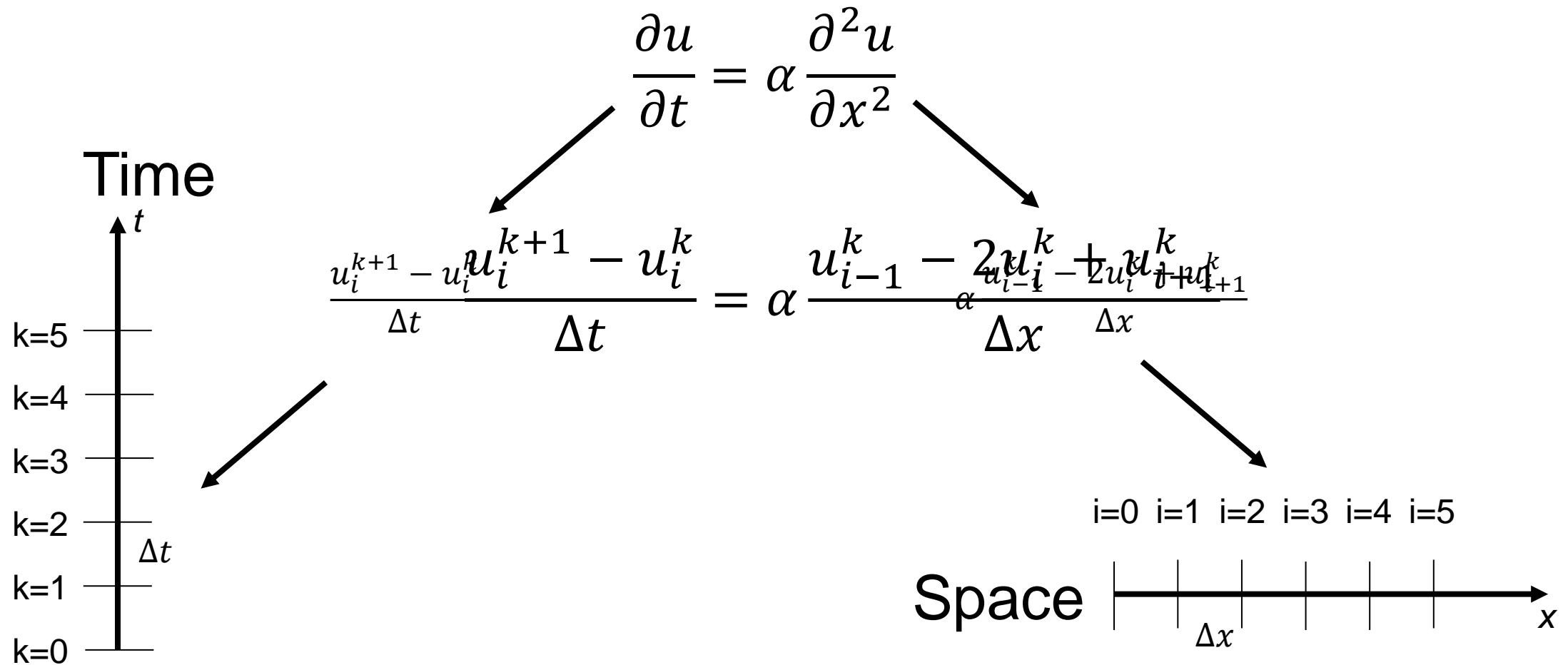
- $u(x,t)$ is temperature in Kelvin
- x is distance in meters
- t is time in seconds
- α is thermal diffusivity of the material (m^2/s)

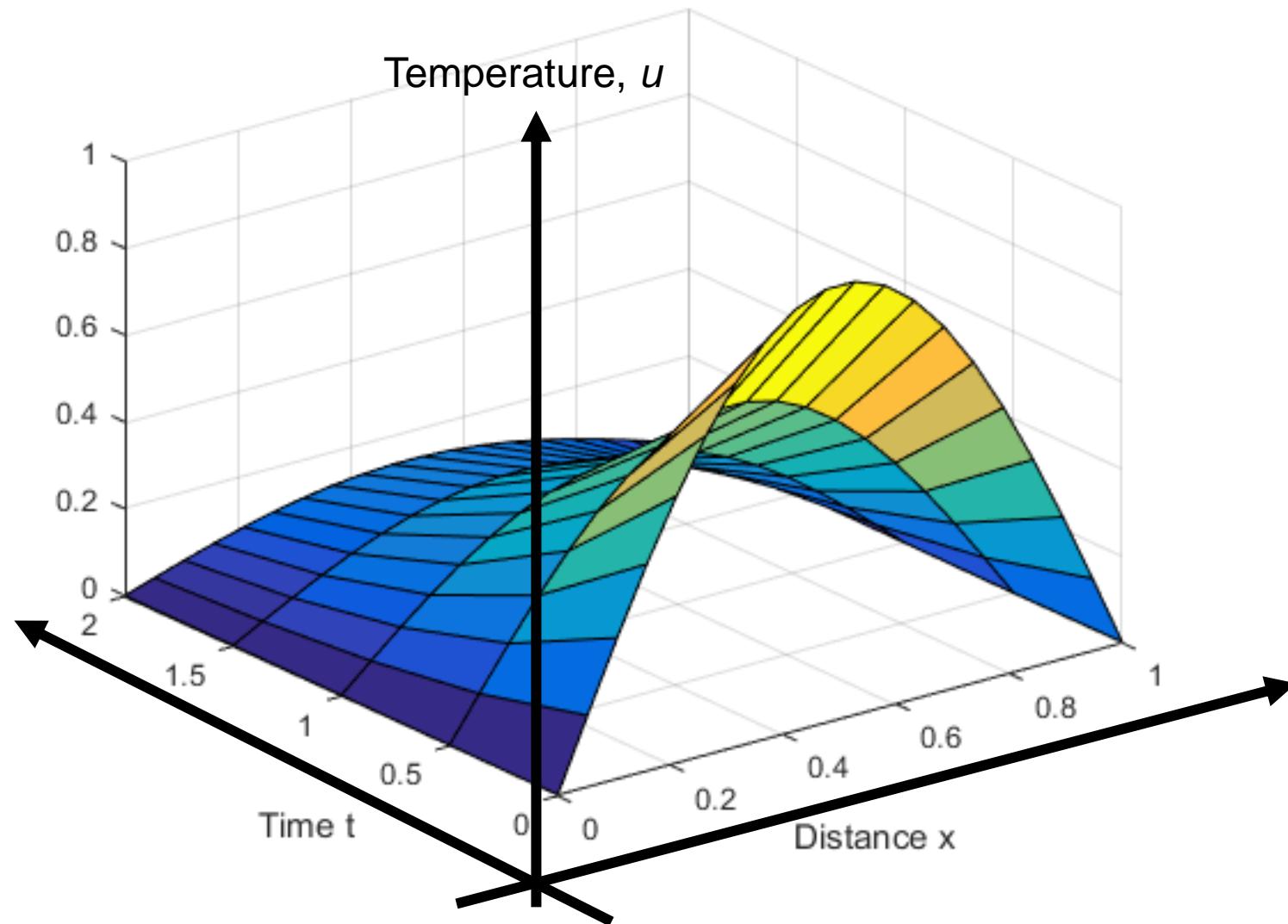
Given boundary and initial conditions

- Left end-point: $u(0,t) = U_0$
- Right end-point: $u(L_x,t) = U_L$
- Initial temperature profile: $u(x,0) = U(x)$

We seek a numerical software solution for $u(x,t)$ (all space & time)

Discretize: Continuous → Discrete





A numerical, iterative solution algorithm

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = \alpha \frac{u_{i-1}^k - 2u_i^k + u_{i+1}^k}{\Delta x}$$

$$u_i^{k+1} = ru_{i+1}^k + (1 - 2r)u_i^k + ru_{i-1}^k \quad r = \alpha \frac{\Delta t}{(\Delta x)^2}$$

- k is indexing time, t , and i is indexing distance, x
- Known as “FTCS” algorithm
- Is an *explicit* method.
 - For more sophisticated cases, need a full-fledged solver.
- Known to be **unstable** for $r > \frac{1}{2}$

Exercise #1 (3 mins)

**Open ftcs.C w/editor and write
the body of this function**

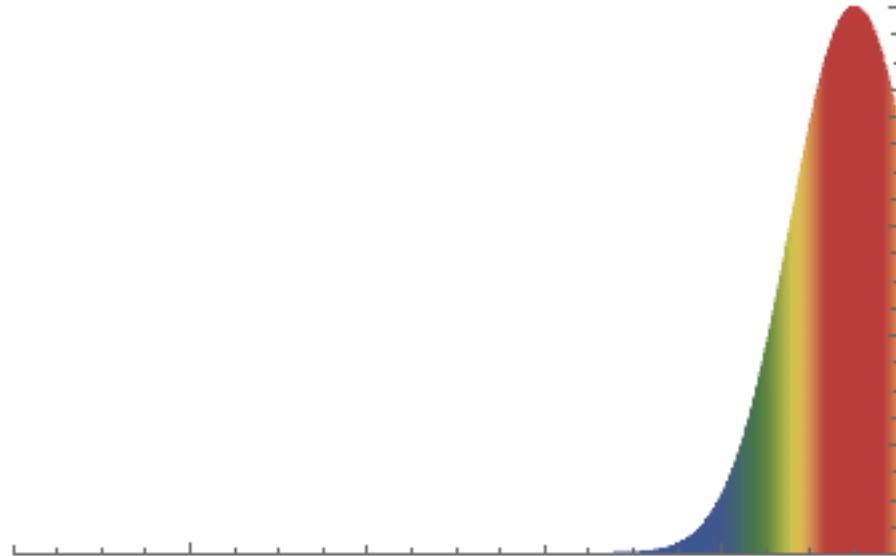
$$u_i^{k+1} = ru_{i+1}^k + (1 - 2r)u_i^k + ru_{i-1}^k$$
$$r = \alpha \frac{\Delta t}{(\Delta x)^2}$$

```
bool update_solution_ftcs(
    int n,
    Double *uk1,
    Double const *uk0,
    Double alpha,
    Double dx, Double dt,
    Double bc0, Double bc1)
{
}
```

Exercise #2 (1 min)

Build and test the application

```
% make  
c++ -c heat.C -o heat.o  
c++ -c utils.C -o utils.o  
c++ -c args.C -o args.o  
c++ -c exact.C -o exact.o  
c++ -c ftcs.C -o ftcs.o  
c++ -c upwind15.C -o upwind15.o  
c++ -c crankn.C -o crankn.o  
c++ -o heat heat.o utils.o args.o exact.o ftcs.o upwind15.o crankn.o -lm
```



- How might we test it?
 - We know steady state solution for $bc0=A$ and $bc1=B$ is line from A to B

Exercise #3 (2 mins):

Run the application to model a problem of interest

- Outside temp has been same as inside temp @ 70 °F for a long time
- Night/Storm will last 15.5 hours @ -40 °F
- Walls are 0.25 meters thick wood, pipe is 0.1 meters diameter

Material	Thermal Diffusivity, α , (m ² /s)
Wood	8.2×10^{-8}
Adobe Brick	2.7×10^{-7}
Common ("red") brick	5.2×10^{-7}

Exercise #4 (1 min)

Analyze the results

Criterion: Will conclude pipe freezes if...
...center point drops below freezing before storm passes

```
make plot PTOOL=[visit|gnuplot|pyplot] RUNAME=<run-name>
```

What if our problem was to find the optimum wall width?

Simplifications hide challenges of math package software engineering

- **Challenges in numerical algorithms**

- Discretizations: Dimensions, geometries, material interfaces, etc
- Time Integrators: Adaptive, faster convergence, efficiencies, etc.
- Solvers: Implicit, explicit, iterative, direct, preconditioners, etc.
- Optimization: Outer loops, nonintrusive, reduced-order models, etc.
- Validation & verification: Vetted, trusted results, community accepted

- **Challenges in software development**

- Time and space performance
- Scalability & performance portability
- Encapsulation, interfaces & interoperability
- Documentation, ease of installation, ease of use
- Sustainable open source, supported with regular updates, bug tracking/fixing
- Support for user-defined customization and extensibility

Next steps

- **Attend parallel sessions**
 - 10:30 CDT and 11:45 CDT
 - Access Zoom rooms via
 - <https://xSDK-project.github.io/MathPackagesTraining2020/agenda>
- **During breaks and lunch**
 - Submit questions for panelists (optional)
 - Sign up for discussions with numerical software developers (optional)
 - Your email address
 - Select 1st, 2nd, and 3rd priorities
 - Brief description of interests
 - Complete by 3:30 pm CDT
- **Panel session: Main Room @ 1:45 pm CDT**

The screenshot shows the ATPESC 2020 agenda page. On the left, there's a sidebar with links like 'SETUP INSTRUCTIONS', 'TODAY'S AGENDA', 'VIP TALKS', 'VIRTUAL MEETING ROOMS', 'GETTING HELP', 'PANEL QUESTION SUBMISSIONS', 'SME SPEED DATING SELECTIONS' (which is highlighted in blue), 'COMPUTING HISTORY GAME (OPENS 11:40AM)', 'WOMEN IN COMPUTING GAME (OPENS 3:35PM)', 'SUBMIT A SHOW YOUR WORK', and 'ATPESC 2020 AGENDA PAGE'. Two red arrows point from the 'SME SPEED DATING SELECTIONS' link to the list of developer names below. The main content area features logos for IDEAS orcale Science, ECP, FAST MATH, and Spack. To the right, there are sections for 'Interoperability & Ease of Use' and 'Enhanced Productivity' with their respective bullet points.

IDEAS orcale Science
So my code will see the future

ECP

FAST MATH

xSDK

Spack

better scientific software

Interoperability & Ease of Use

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

Enhanced Productivity

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

How can I get involved?

Today's agenda

<https://xsdk-project.github.io/MathPackagesTraining2020/agenda>

Unstructured Discretization (with MFEM/PUMI)

Slides

Unstructured meshes can yield required levels of accuracy using fewer degrees of freedom at the cost of more complex parallel data structures and algorithms. To support the ability of application code developers to take advantage of unstructured meshes, FASTMath develops core tools to support the development of unstructured mesh simulation capabilities. This lecture will first introduce the highly extendible MFEM high order finite element solver library and then overview the PUMI unstructured mesh tools developed to support mesh adaptation, load balancing and PIC calculations.

Direct Solvers (with SuperLU/Strumpack)

Slides

Direct Solvers are presented in three different time slots, each with a slightly different emphasis...

- Session 1 (10:30am-11:30am):
 - Sparse direct solvers (both SuperLU and Strumpack), 30 minutes (Sherry)
 - Low rank approximation techniques in Strumpack, 15 minutes (Pieter)
 - SuperLU hands-on demo, 15 minutes (Sherry)
- Session 2 (11:45am-12:45pm):
 - Sparse direct solvers (both SuperLU and Strumpack), 30 minutes (Sherry)
 - Low rank approximation techniques in Strumpack, 15 minutes (Pieter)
 - Strumpack hands-on demo, 15 minutes (Pieter)
- Session 4 (3:40pm - 4:30pm):
 - Sparse direct solvers (both SuperLU and Strumpack), 30 minutes (Sherry)
 - Low rank approximation techniques in Strumpack, 15 minutes (Pieter)
 - Q&A. (Sherry, Pieter)

Mix-n-Match topics
to your interests
See Synopses from Agenda

CDT Start	Mins	Topic	Speaker(s)	Virtual Venue
09:30	55	Intro. to Numerical Libraries	Lois Curfman McInnes Mark Miller	Main-Room
10:25	5	Telecon Transition		
10:30	60	Parallel Session One		
		Structured Discretization (with AMReX)	Ann Almgren Don Willcox	Frontier
		Unstructured Discretization (with MFEM/PUMI)	Aaron Fisher Mark Shephard	Aurora
		Iterative Solvers & Preconditioners (with MueLu)	Jonathan Hu Christian Glusa	Perlmutter
		Direct Solvers (with SuperLU/Strumpack)	Sherry Li Pieter Ghysels	El-Capitan