

Introduction to Numerical Software

Presented to
ATPESC 2021 Participants

Ulrike Meier Yang
Lawrence Livermore National Laboratory

Alp Dener
Argonne National Laboratory

Date 08/10/2021

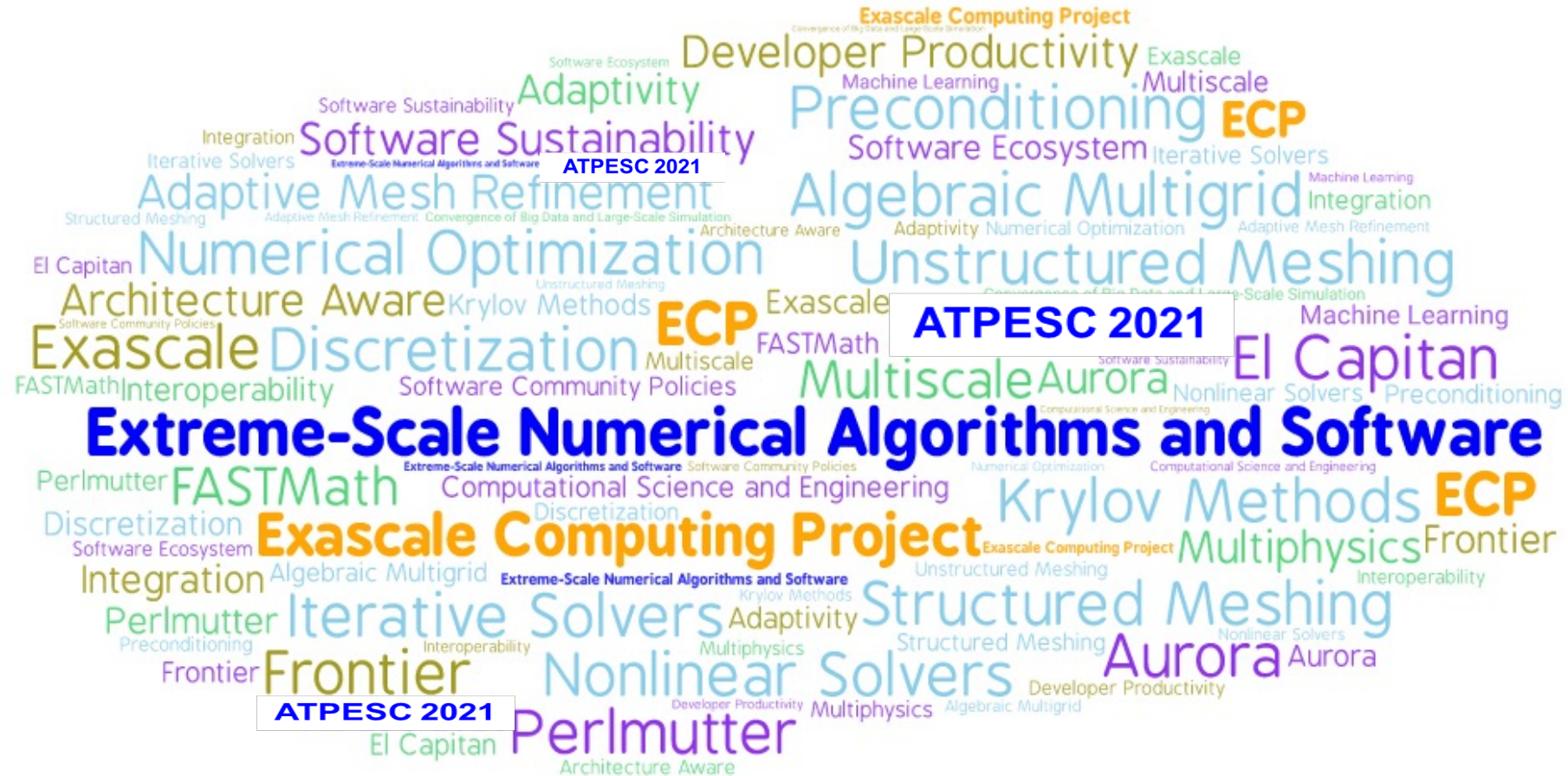


ATPESC Numerical Software Track



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-2021/#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/MathPackagesTraining2021/agenda/>

Agenda (Time Zone: CDT)

<https://extremecomputingtraining.anl.gov/agenda-2021/#Track-5>

9:00 *Speaker check-in*

9:30 Introduction to Numerical Software

Ulrike Yang, LLNL
Alp Dener, ANL

10:30 Parallel Session 1

- **ROOM FRONTIER:** Structured Discretization (with AMReX) Ann Almgren, LBL
Don Willcox, LBL
- **ROOM AURORA:** Unstructured Discretization (with MFEM/PUMI) Aaron Fisher, LLNL
Cameron Smith, RPI
- **ROOM PERLMUTTER:** Iterative Solvers & Algebraic Multigrid (with HYPRE) Sarah Osborn, LLNL
Ulrike Yang, LLNL
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack) Sherry Li, LBL
Pieter Ghysels, LBL

11:30 *Break*

11:45 Parallel Session 2

- **ROOM FRONTIER:** Structured Discretization (with AMReX) Ann Almgren, LBL
Don Willcox, LBL
- **ROOM AURORA:** Unstructured Discretization (with MFEM/PUMI) Aaron Fisher, LLNL
Cameron Smith, RPI
- **ROOM PERLMUTTER:** Iterative Solvers & Preconditioners (with MueLu) Christian Glusa, SNL
Graham Harper, SNL
Peter Ohm, SNL
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack) Sherry Li, LBL
Pieter Ghysels, LBL

12:45 p.m. *Lunch*

1:45 **MAIN ROOM:**

Panel *Discussion:* Contributing to the Numerical Package Community

Ann Almgren, LBL
Aaron Fisher, LLNL
Christian Glusa, SNL
Richard Tran Mills, ANL
Dan Reynolds, SMU
Cameron Smith, RPI
Alp Dener, ANL

2:35 Parallel Session 3

- **ROOM FRONTIER:** Nonlinear Solvers (with PETSc)
- **ROOM AURORA:** Optimization (with TAO)
- **ROOM PERLMUTTER:** Time Integration (with SUNDIALS)
- **ROOM EL CAPITAN:** Iterative Solvers & Algebraic Multigrid (with HYPRE)

Richard Tran Mills, ANL

Alp Dener, ANL

Dan Reynolds, SMU

Sarah Osborn, LLNL
Ulrike Yang, LLNL

3:25 *Break*

3:40 Parallel 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 Tran Mills, ANL

Alp Dener, ANL

Dan Reynolds, SMU

Sherry Li, LBL
Pieter Ghysels, LBL

4:35 Working with Numerical Packages in Practice

Ann Almgren, LBL

5:00 Adjourn

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

Agenda Overview (Time Zone: CDT)

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

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

#1

- **Structured Discretization** (AMReX)
- **Unstructured Discretization** (MFEM/PUMI)
- **Iterative Solvers & Preconditioners** (hypre)
- **Direct Solvers** (SuperLU/Strumpack)

#2

- **Structured Discretization** (AMReX)
- **Unstructured Discretization** (MFEM/PUMI)
- **Iterative Solvers & Preconditioners** (Trilinos/MueLU)
- **Direct Solvers** (SuperLU/Strumpack)

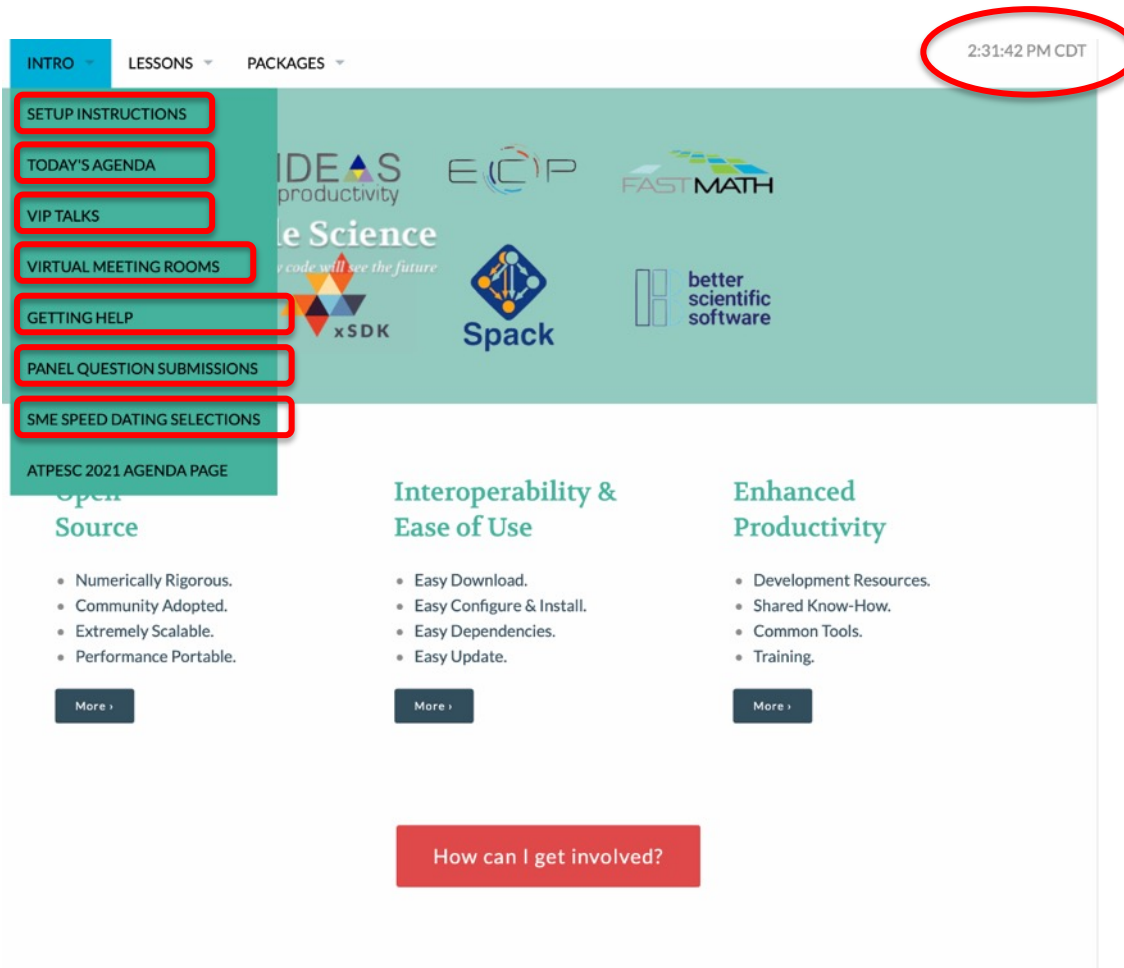
#3

- **Nonlinear Solvers** (PETSc)
- **Optimization** (TAO)
- **Time Integration** (SUNDIALS)
- **Iterative Solvers & Preconditioners** (hypre)

#4

- **Nonlinear Solvers** (PETSc)
- **Optimization** (TAO)
- **Time Integration** (SUNDIALS)
- **Direct Solvers** (SuperLU/Strumpack)

<https://xsdk-project.github.io/MathPackagesTraining2021/>



- Clock
- Setup instructions
- Today's agenda
- VIP talks
- Virtual meeting rooms
- Getting help
- Panel question submission
- SME speed dating selections

Today's agenda

<https://xsdk-project.github.io/MathPackagesTraining2021/agenda/>

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

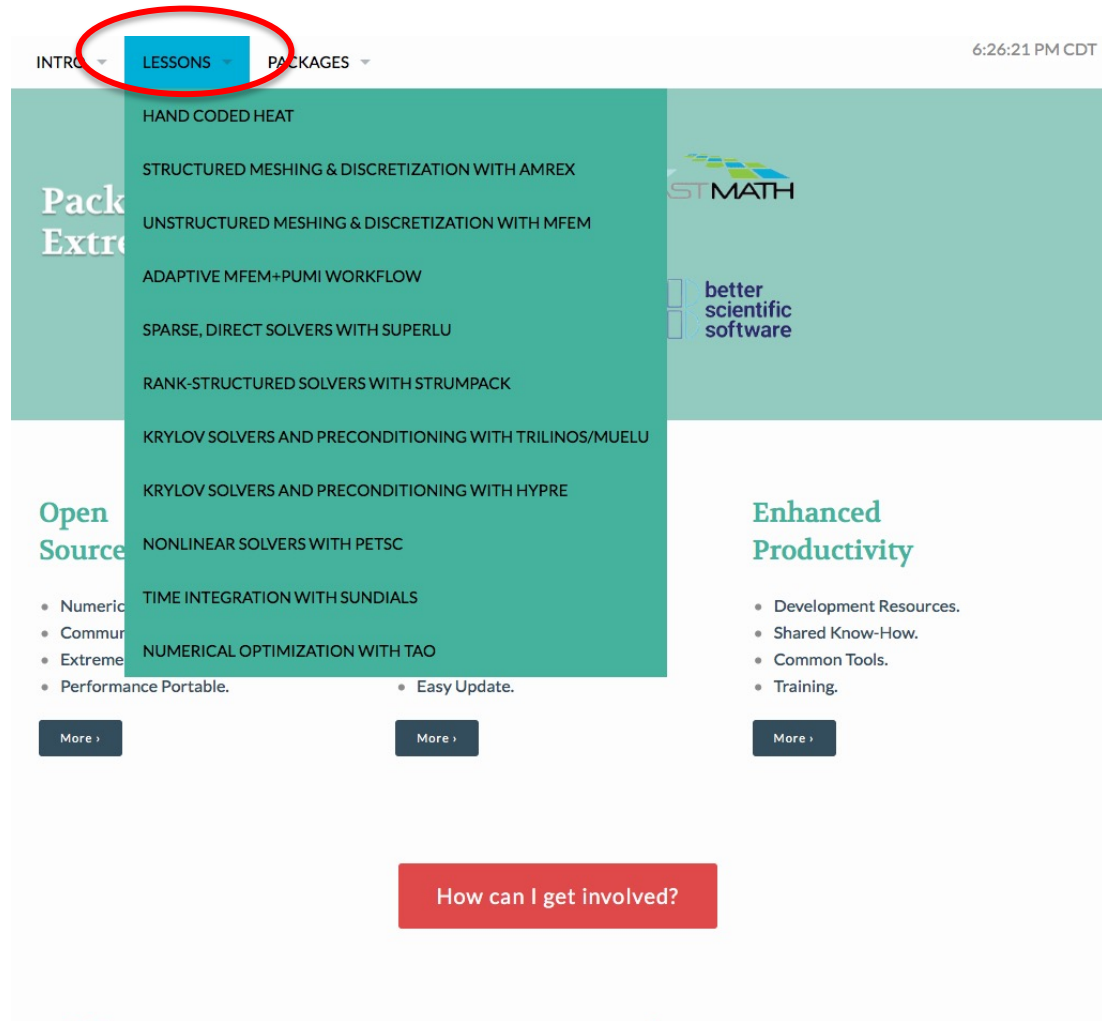
Iterative Solvers & Algebraic Multigrid (with HYPRE)

Slides

This session will present the basic concepts of iterative linear solvers with focus on Krylov solvers, including the generalized minimum residual method (GMRES), preconditioning and algebraic multigrid (AMG) methods. We will provide a brief description of the high performance linear solvers library HYPRE, its interfaces, and its most used multigrid solvers, BoomerAMG and PFMG, including a brief discussion of the effect of their data structures on performance. The lesson includes hands-on examples with structured and unstructured solvers from the HYPRE library applied to several test problems.

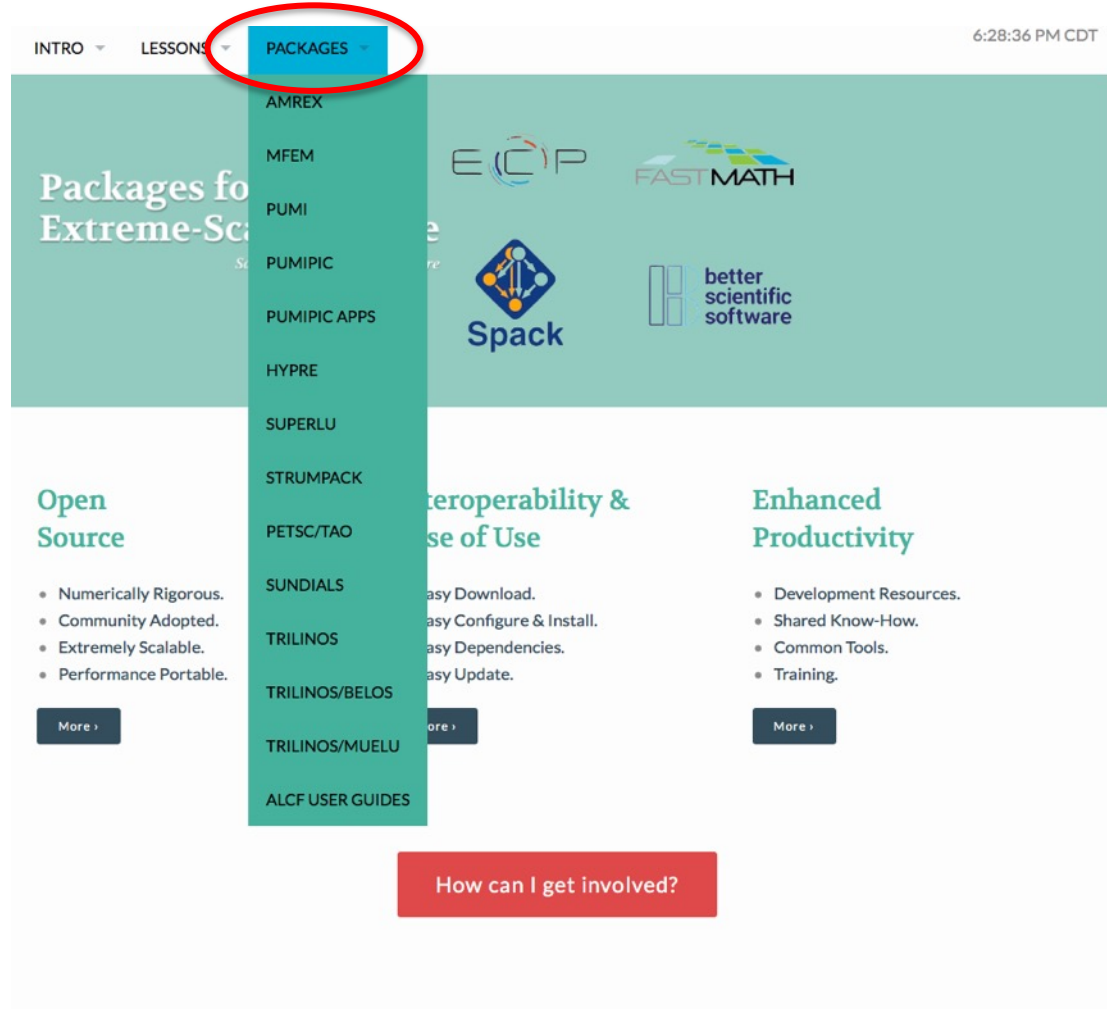
CDT Start	Mins	Topic	Speaker(s)	Virtual Venue
09:30	55	Introduction to Numerical Software	Ulrike Yang Alp Dener	Main-room
10:25	5	Telecon Transition		
10:30	60	Parallel Session One		
		Structured Discretization (with AMReX)	Ann Almgren Don Willcox	Frontier
		Unstructured Discretization (with MFEM/PUMI)	Aaron Fisher Mark Shephard Cameron Smith	Aurora
		Iterative Solvers & Algebraic Multigrid (with HYPRE)	Ulrike Yang Sarah Osborn	Perlmutter
		Direct Solvers (with SuperLU/Strumpack)	Sherry Li Pieter Ghysels	El-Capitan

<https://xsdk-project.github.io/MathPackagesTraining2021/>



- Hands-on Lessons

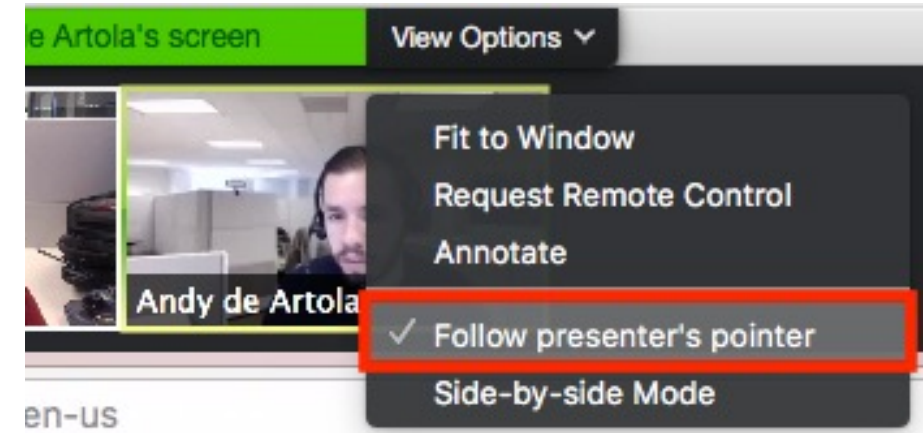
<https://xsdk-project.github.io/MathPackagesTraining2021/>



- Hands-on Lessons
- Packages

Using Zoom

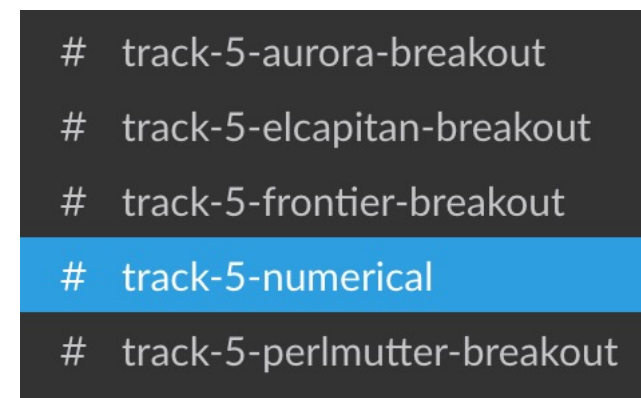
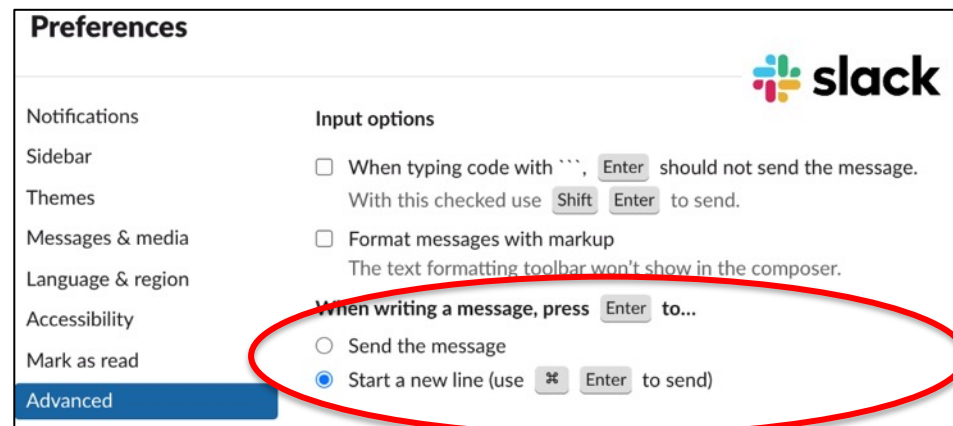
- Please stay muted unless asked to un-mute
- We're using Slack for chat, not Zoom's chat
- "Follow presenter's pointer" might be helpful
 - Available only if NOT in "Fit to Window" mode
- Download slide PDFs from ATPESC web site (agenda page) ahead of presentation as a backup
- Other useful tips
 -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



Using Slack

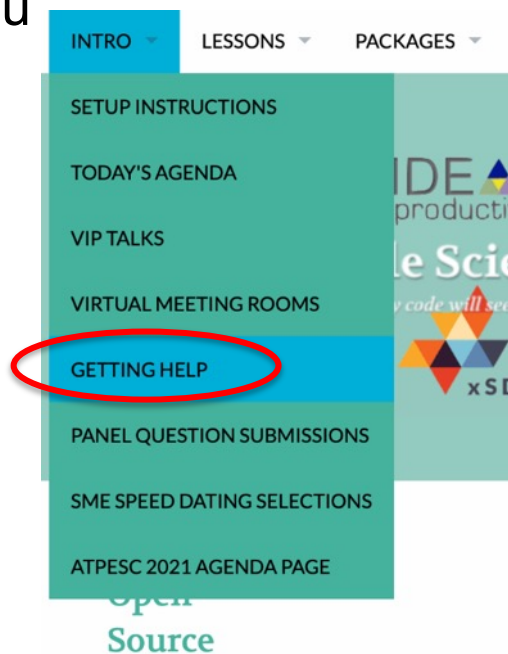
- Recommend using the desktop app, but browser ok too
- **#track-5-numerical** channel
 - For all chat during presentations in “Main room”
 - For all chat outside any specific parallel session
 - For general help
 - Recommend using the thread option to help keep track of discussions on subtopics
- **#track-5-<room-name>-breakout**
 - 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 **#track-5-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)

- **#track-5-numerical** Slack channel
- IT Support Rooms under the “Getting Help” menu



Getting help

Use the *#track-5-numerical* slack channel for general help and it support.

Launch *#track-5-numerical* Slack in
new browser window or desktop app

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

- Satish Balay,
- Cameron Smith
- Alp Dener

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.

The ATPESC Team 2021 on Zoom



Row 1:

- Dan Reynolds
- Alp Dener
- Cameron Smith
- Graham Harper

Row 2:

- Sarah Osborn
- Ulrike Yang
- Satish Balay
- Christian Glusa

Row 3:

- Peter Ohm
- Lois McInnes
- Sherry Li
- Mark Shephard

Row 4:

- David Gardner
- Pieter Ghysels
- Don Willcox

Not shown:

- Ann Almgren
- Aaron Fisher
- Richard Mills



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?

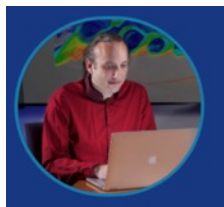
- Libraries enable users to focus on their primary interests
 - Reuse algorithms and data structures developed by experts
 - Customize and extend to exploit application-specific knowledge
 - Cope with complexity and changes over time
- More efficient, robust, reliable, scalable, sustainable scientific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

The ATPESC Team 2021

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



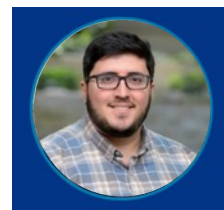
Ann Almgren, LBL



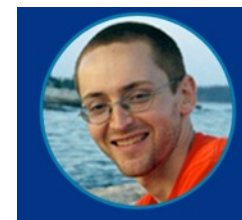
Aaron Fisher, LLNL



Christian Glusa, SNL



Alp Dener, ANL



Cameron Smith, RPI



David Gardner, LLNL



Satish Balay, ANL



Pieter Ghysels, LBL



Sherry Li, LBL



Dan Reynolds, SMU

Thank you to Peter Ohm and Graham Harper, SNL



Sarah Osborn, LLNL



Mark Shephard, RPI



Lois Curfman McInnes, ANL



**Additional contributors to
gallery of highlights:**

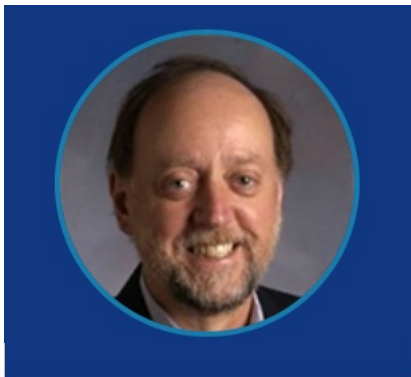
Various HPC package developers

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](#)]
 - GaMM-SIAM E-NLA Seminar, June 2020 [[video](#)]



Jack Dongarra, University of Tennessee [[bio](#)]

- An Accidental Benchmark, ATPESC 2021 [[slides](#)]
- Adaptive Linear Solvers and Eigensolvers, ATPESC 2019 [[slides](#), [video](#)]



David Keyes, KAUST [[bio](#)]

- Adaptive Nonlinear Preconditioning for PDEs with Error Bounds on Output Functionals, Univ. of Manchester 2021 [[slides](#), [video](#)]
- Data-sparse Linear Algebra for Large-scale Applications on Emerging Architectures, GaMM-SIAM E-NLA Seminar, September 2020 [[slides](#), [video](#)]

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



- 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 12)

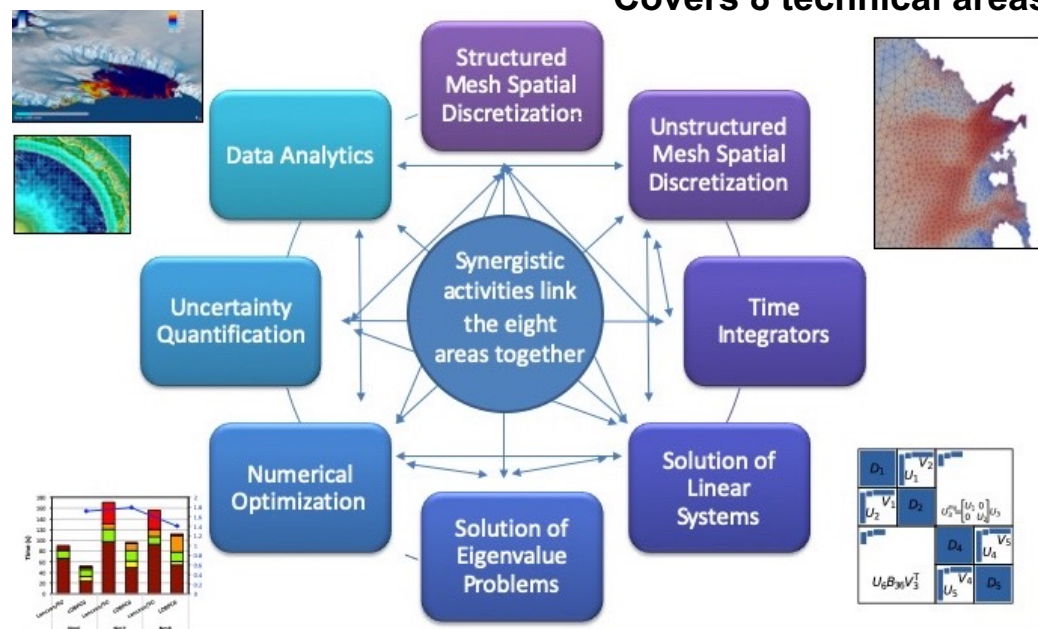
Community efforts:
Join us!



FASTMath: Frameworks, Algorithms & Scalable Technologies for Mathematics

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

Covers 8 technical areas



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

50+ researchers from 5 DOE labs and 5 universities



Argonne
NATIONAL LABORATORY



OAK
RIDGE
National Laboratory

Sandia
National
Laboratories

SuperLU

AMReX



ZOLTAN



PETSc

symPACK

hypre
high performance preconditioners



USC

MIT



Rensselaer



SMU

PUMI
Parallel Unstructured Mesh Infrastructure

UQTK

Trilinos

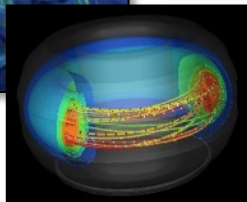
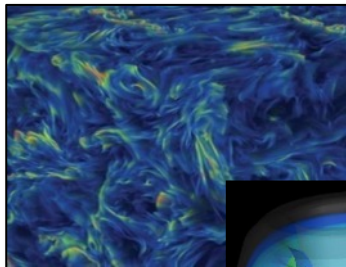
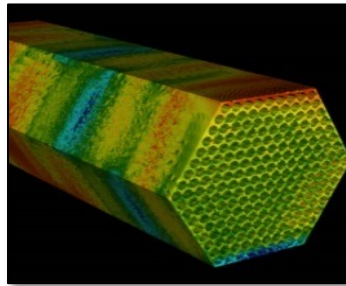
Albany



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

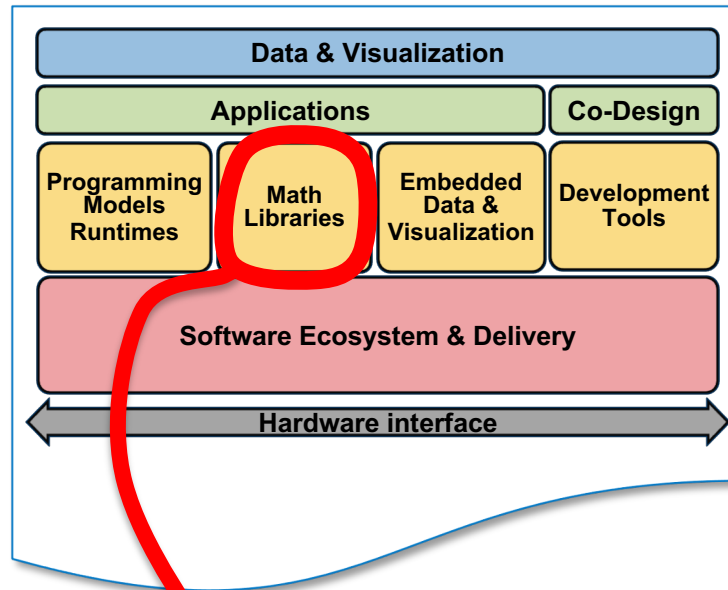
Application Development

Science and mission applications



Software Technology

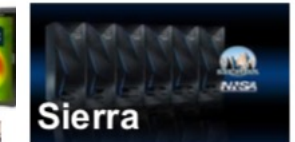
Scalable software stack



Emphasis for this presentation

Hardware and Integration

Relationships: facilities with AD/ST, with vendors

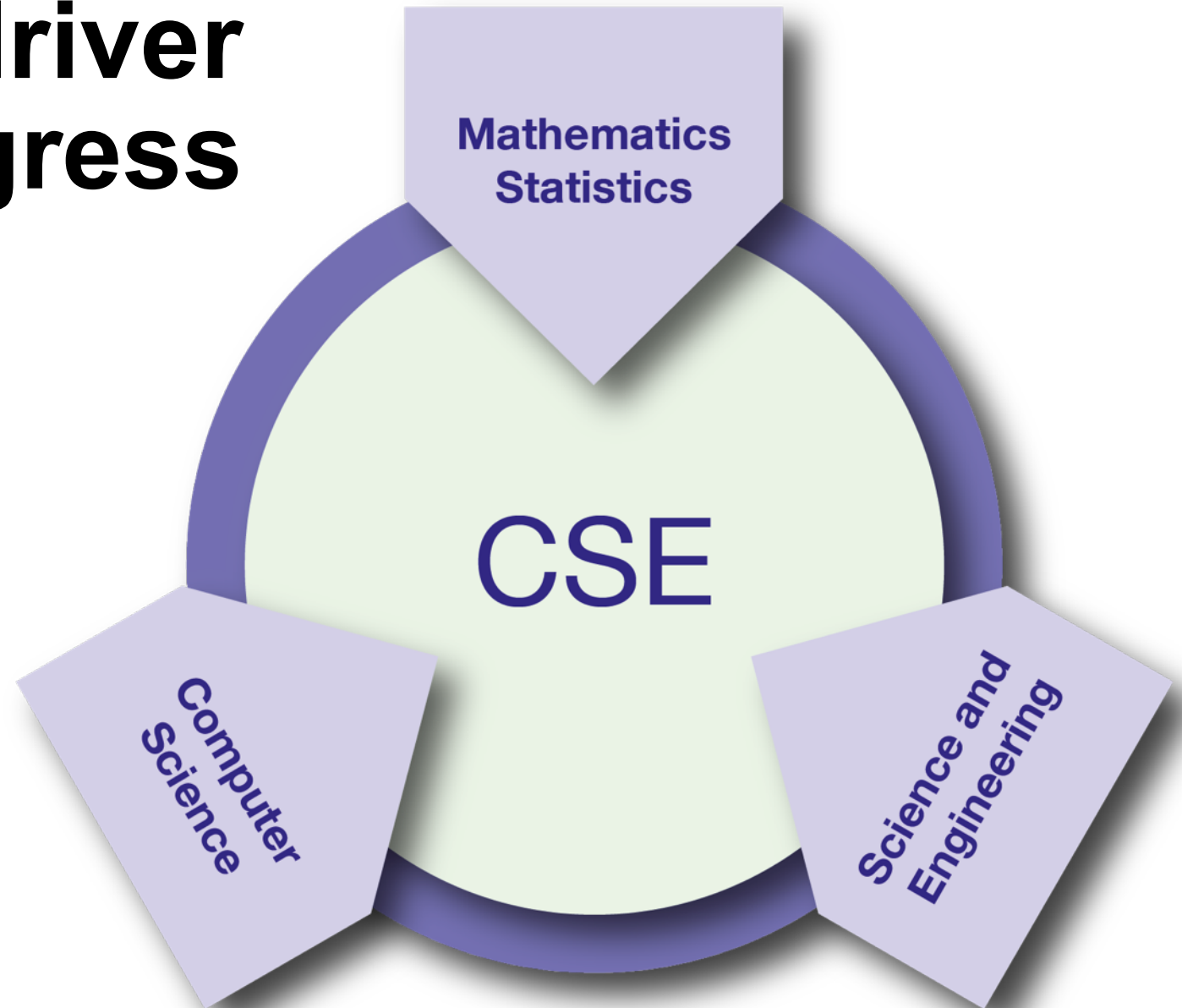


CSE: Essential driver of scientific progress

CSE = Computational Science & Engineering

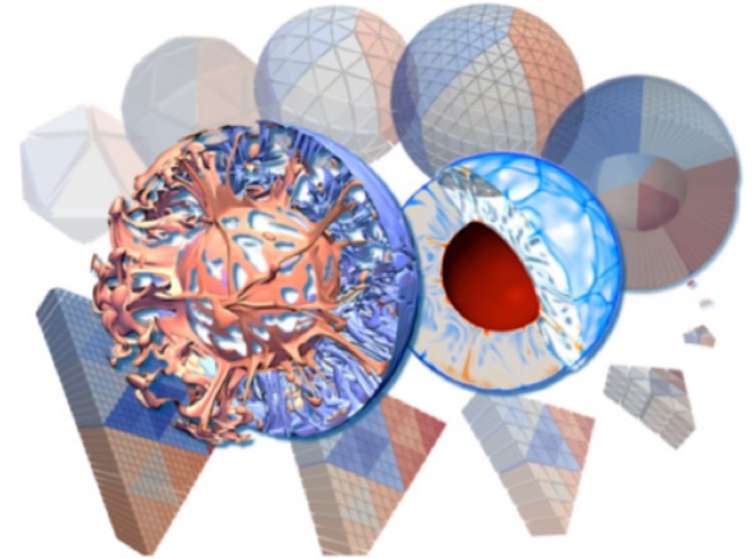
Development and use of computational methods for scientific discovery

- 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

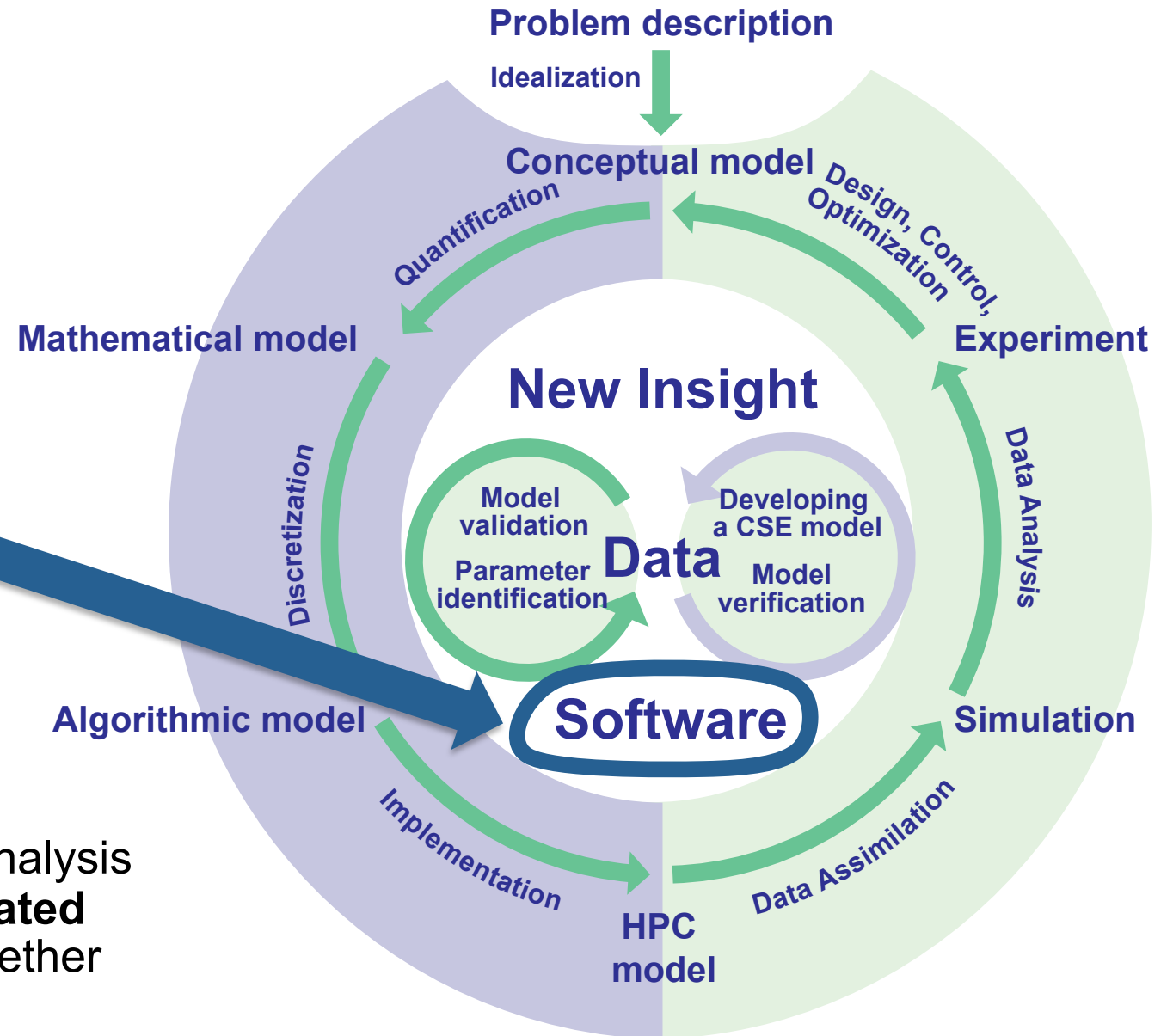
- Mathematical methods and algorithms
- CSE and HPC: Ubiquitous parallelism
- CSE and the data revolution
- CSE software
- CSE education & workforce development



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.



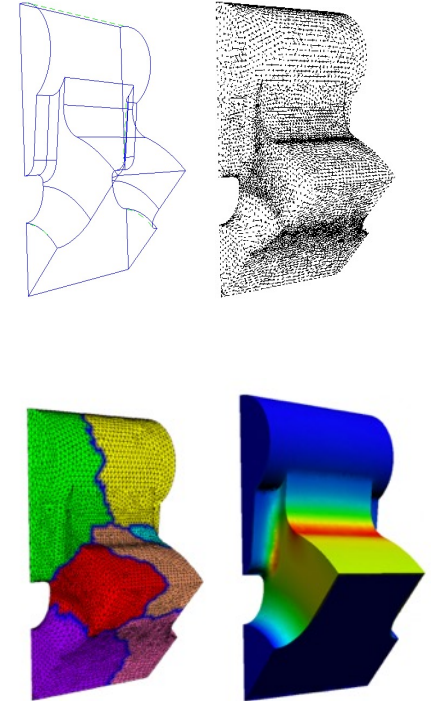
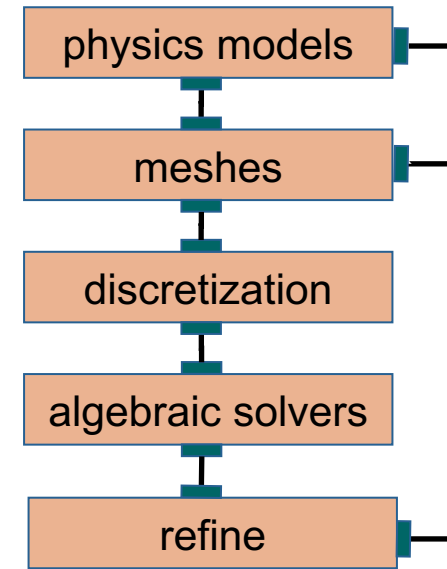
CSE cycle: Modeling, simulation, and analysis

- **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

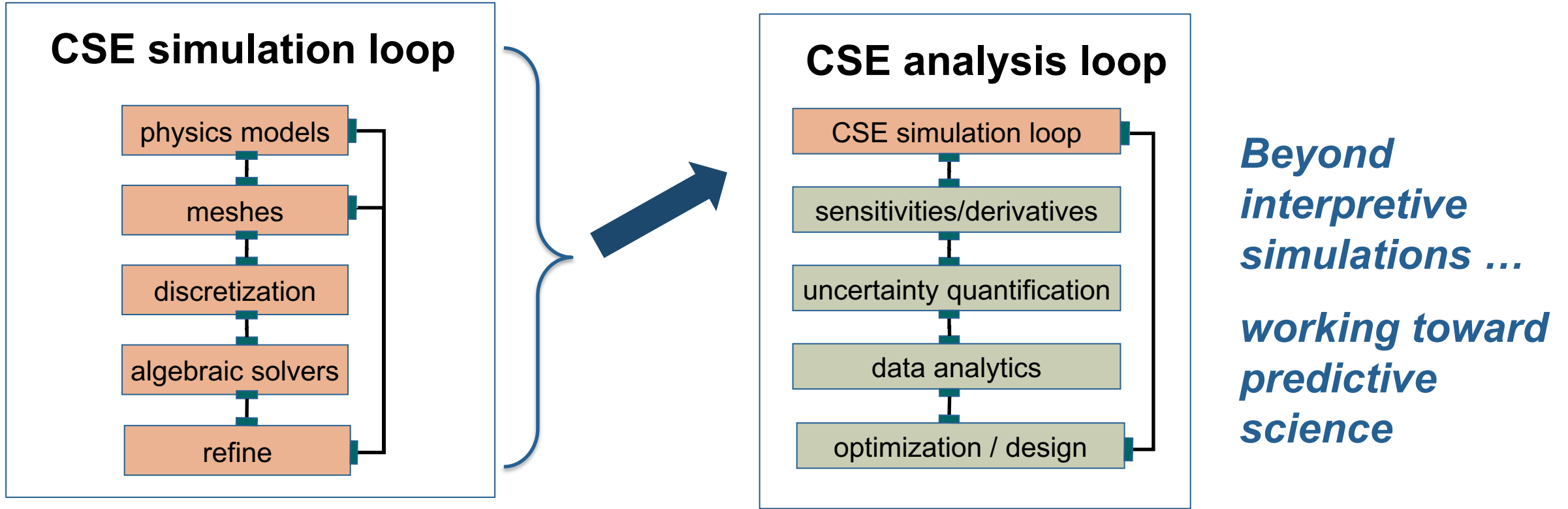
- Develop a mathematical model of the phenomenon of interest
- Approximate the model using a discrete representation
- Solve the discrete representation
- Adapt and refine the mesh or model
- Incorporate different physics, scales

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



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

$$\nabla^2 T = 0 \in \Omega$$
$$T(0) = 180^\circ \quad T(1) = 0^\circ$$

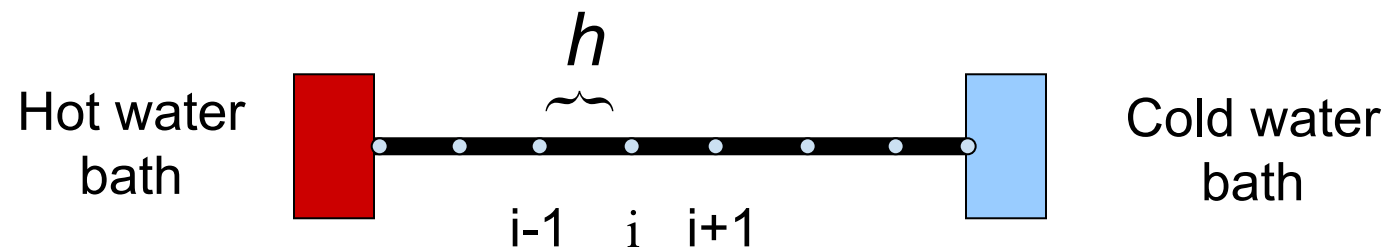


The first step is to discretize the equations

- 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

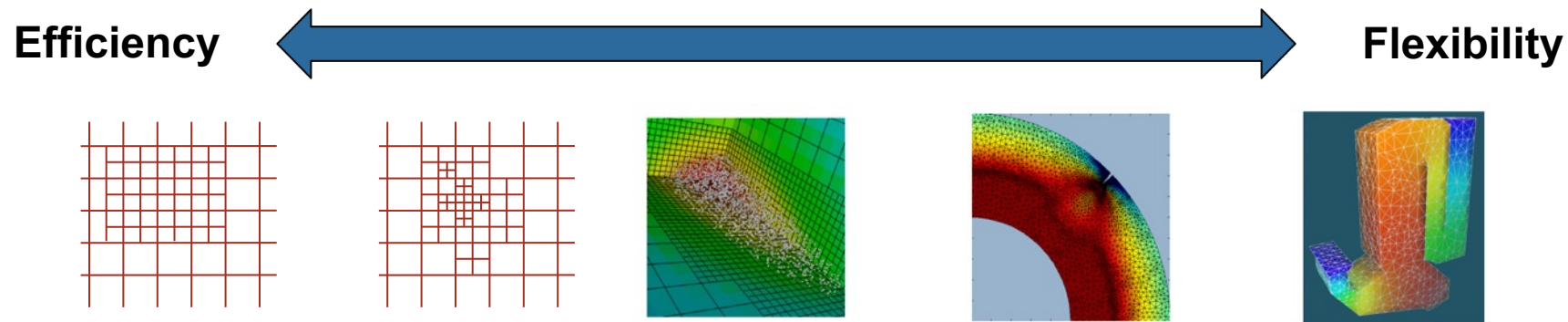
- Set up a matrix of the unknown coefficients
 - include the known boundary conditions
- Solve the linear system for T_i

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

- Visualize and analyze the results

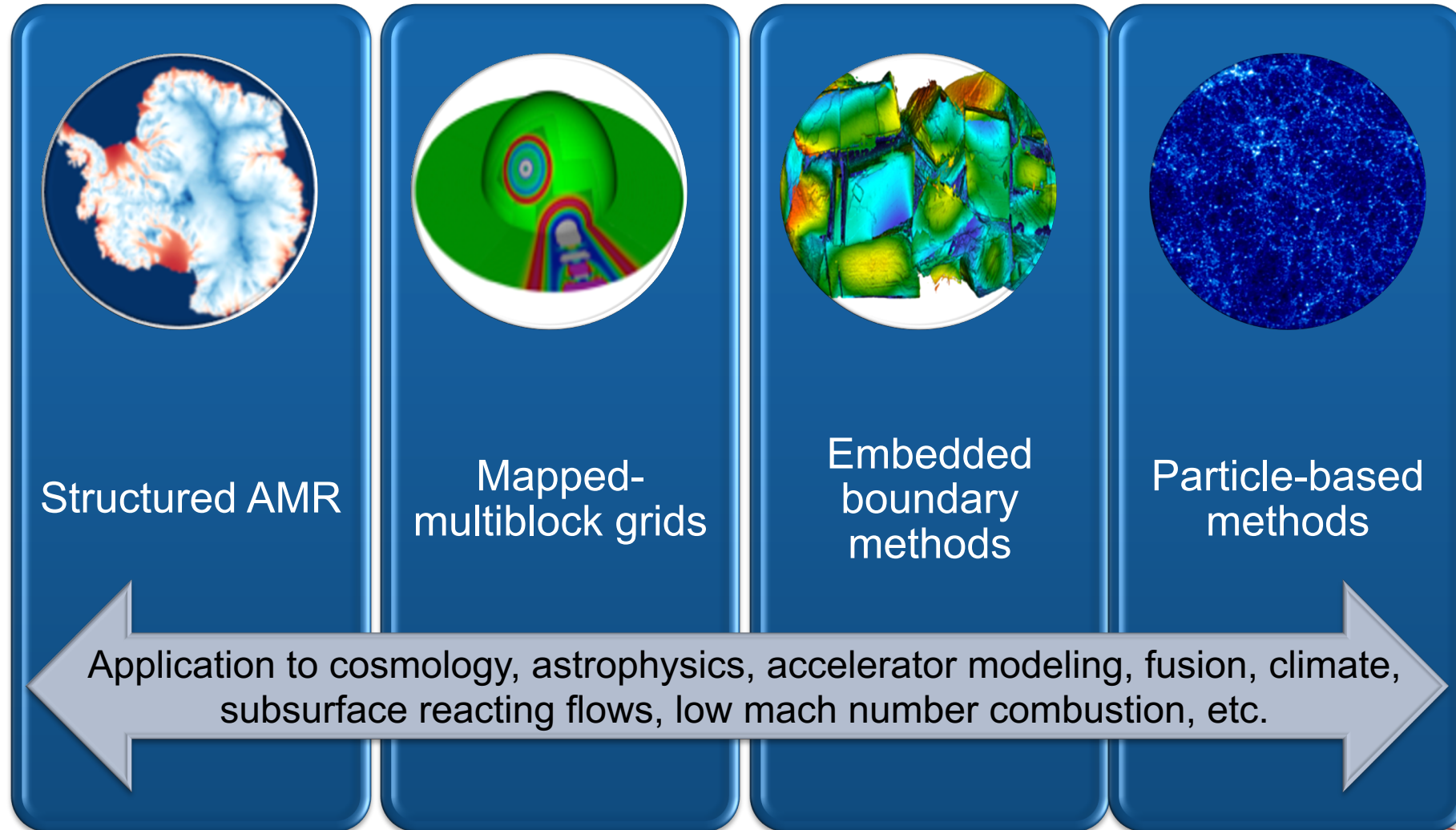
As problems get more complicated, so do the steps in the process

- Different discretization strategies exist for differing needs

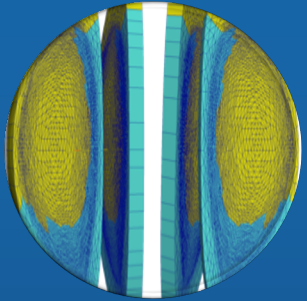


- Most problems are time dependent and nonlinear
 - Need higher algorithmic levels than linear solvers
- Increasingly combining multiple physical processes
 - Interactions require careful handling
- Goal-oriented problem solving requires optimization, uncertainty quantification

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



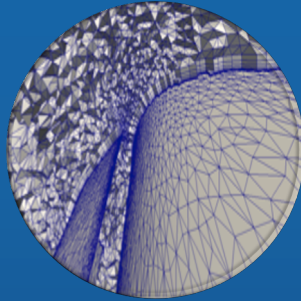
Unstructured grid capabilities focus on adaptivity, high-order, and the tools needed for extreme scaling



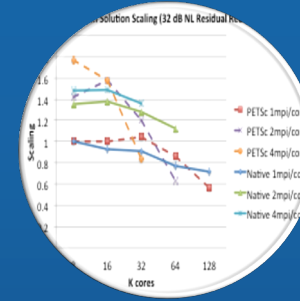
Parallel mesh infrastructures



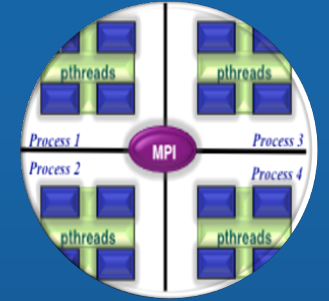
Dynamic load balancing



Mesh adaptation and quality control



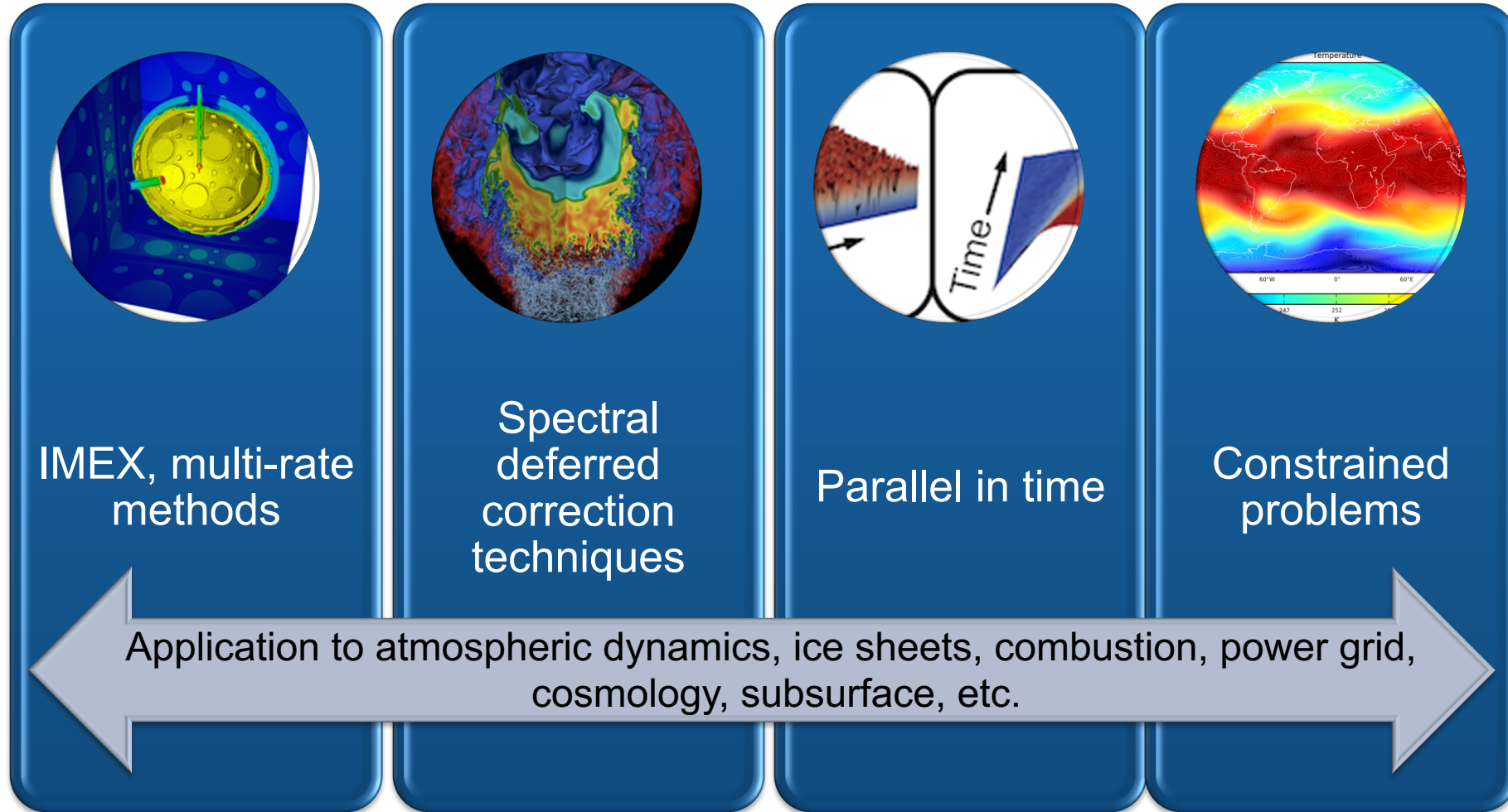
Parallel performance on unstructured meshes



Architecture aware implementations

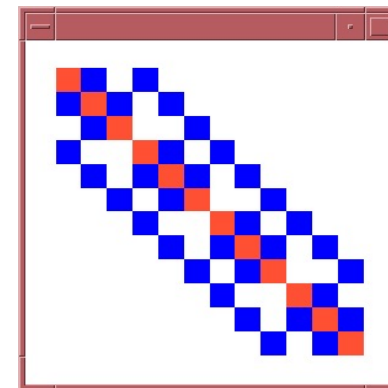
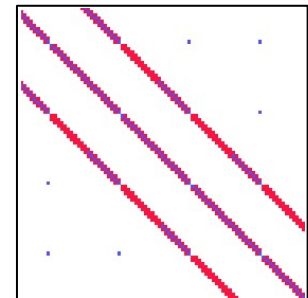
Application to fusion, climate, accelerator modeling, NNSA applications, nuclear energy, manufacturing processes, etc.

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

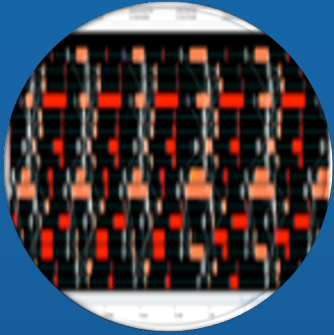


As problems grow in size, so do corresponding discrete systems

- 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.



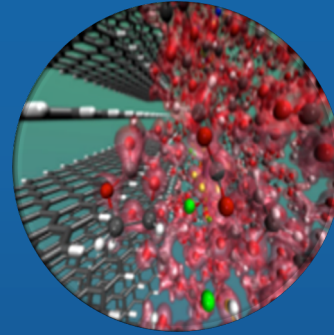
Research on algebraic systems provides key solution technologies to applications



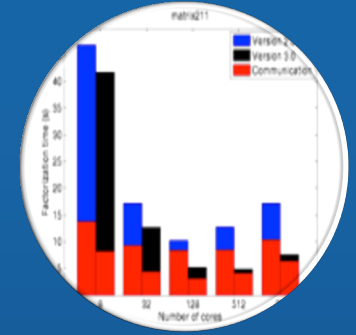
Linear system
solution using direct
and iterative solvers



Nonlinear system
solution using
acceleration
techniques and
globalized Newton
methods



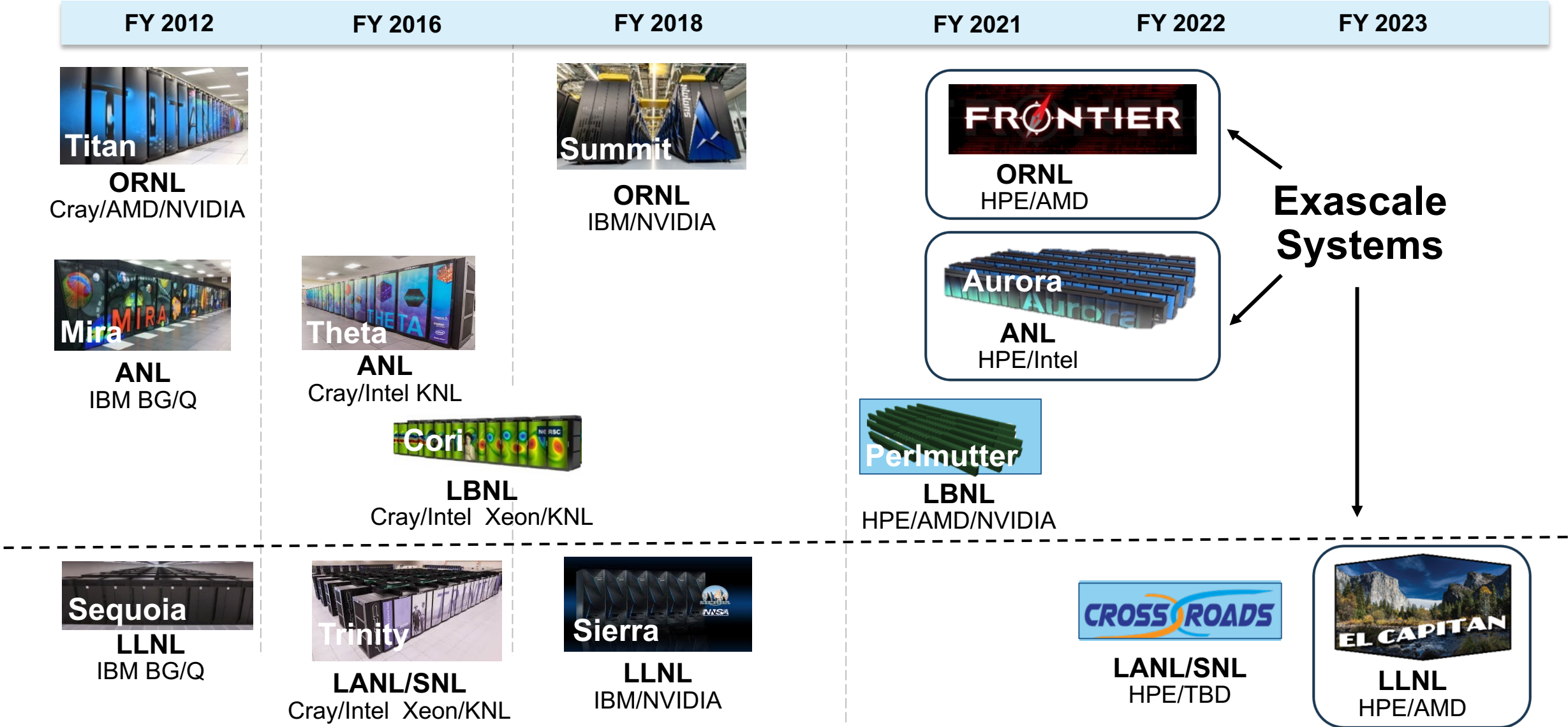
Eigensolvers using
iterative techniques
and optimization



Architecture aware
implementations

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

DOE HPC Roadmap to Exascale Systems



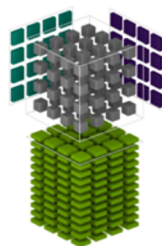
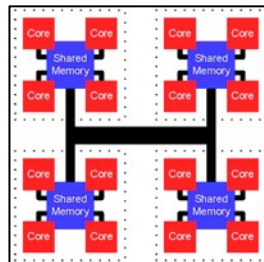
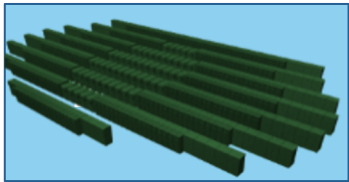
Disruptive changes in HPC architectures

- **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.



$$D = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} + \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

FP16 or FP32 FP16 FP16 FP16 or FP32

- **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.

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>
- ★ • **hypr** - <http://www.llnl.gov/CASC/hypr>
- **libMesh** - <https://libmesh.github.io>
- ★ • **MAGMA** - <http://icl.cs.utk.edu/magma>
- ★ • **MFEM** - <http://mfem.org/>
- ★ • **PETSc/TAO** – <http://petsc.org>
- ★ • **PUMI** - <http://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 ...

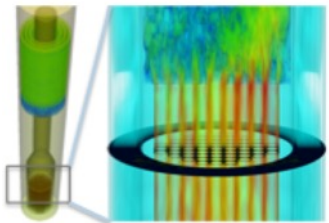
ECP Math Libraries



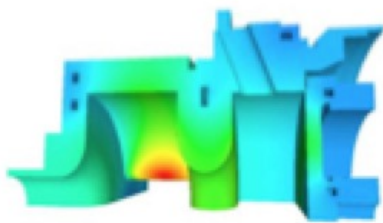
Multiphysics: A primary motivator for exascale

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

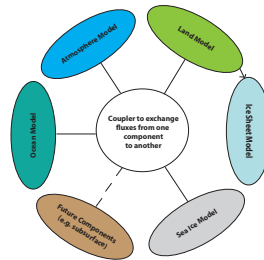
- Also: broad class of coarsely partitioned problems possess similarities



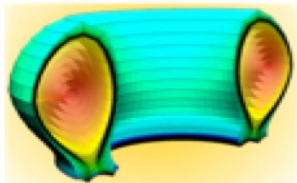
nuclear reactors
A. Siegel, ANL



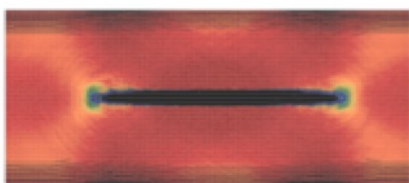
particle accelerators
K. Lee, SLAC



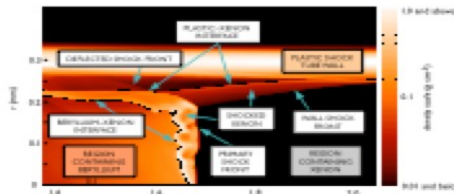
climate
K. Evans, ORNL



fusion
A. Hakim, PPPL



crack propagation
E. Kaxiras, Harvard



radiation hydrodynamics
E. Myra, Univ. of Michigan

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



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DOI: 10.1177/1094342012468181
hpc.sagepub.com
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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, Efthimios 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 Riviere²⁵, 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

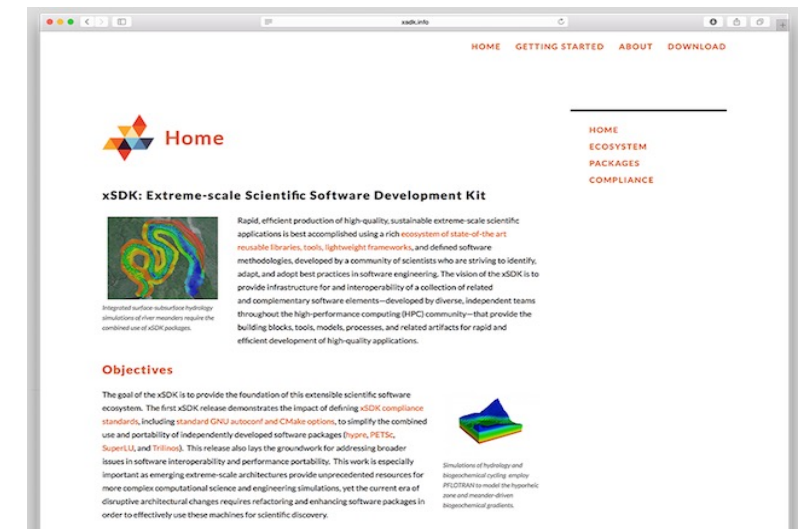


Building the foundation of a highly effective extreme-scale scientific software ecosystem

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

Impact:

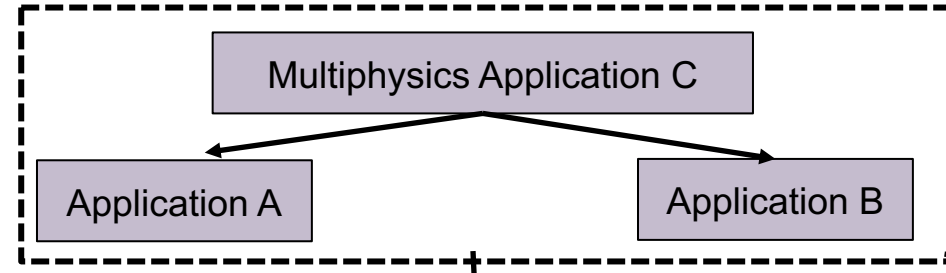
- Improved code quality, usability, access, sustainability
- Inform potential users that an xSDK member package can be easily used with other xSDK packages
- Foundation for work on performance portability, deeper levels of package interoperability



website: xSDK.info

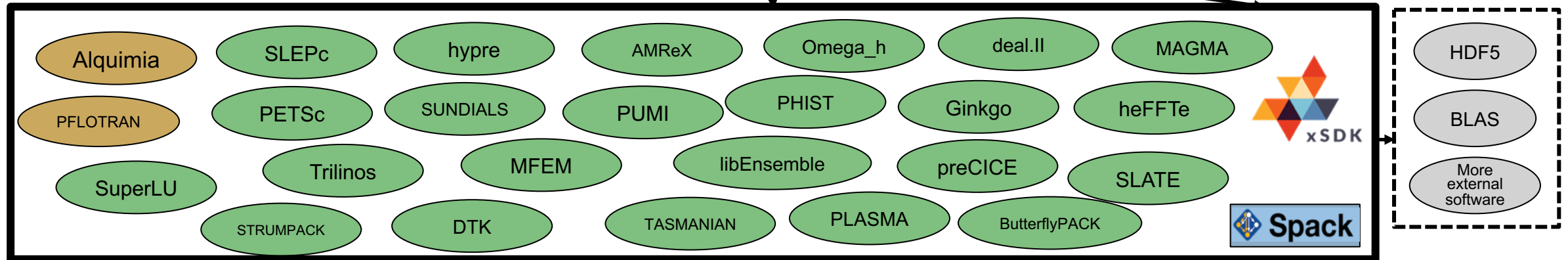
<https://xsdk.info>

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



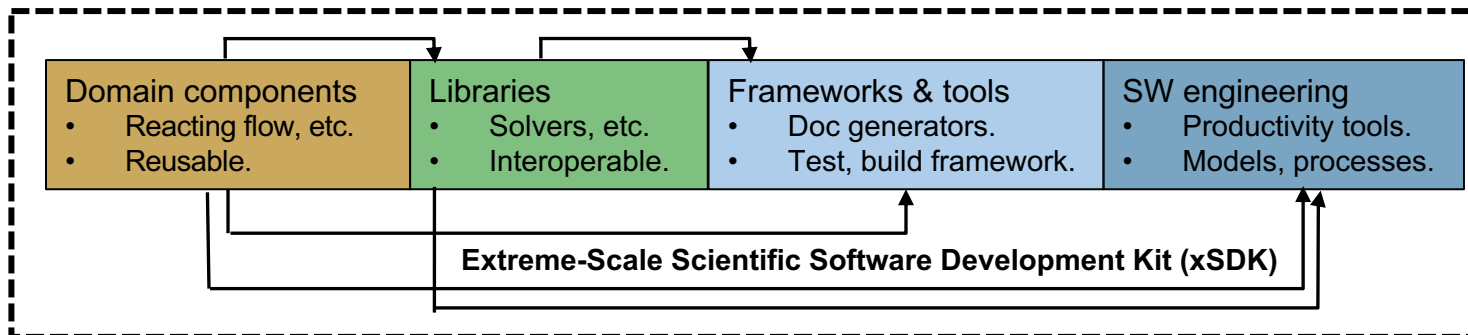
xSDK functionality, Nov 2020

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



November 2019

- 23 math libraries
- 2 domain components
- 16 mandatory (+ 8 recommended) xSDK community policies
- Spack xSDK installer



Impact: Improved code quality, usability, access, sustainability

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

xSDK collaborators



xSDK Release 0.6.0, Nov 2020

- **xSDK release lead:** Satish Balay, SNL
- **xSDK planning**
 - Ulrike Meier Yang (LLNL)
- **Leads for xSDK testing**
 - Satish Balay, ANL: ALCF testing
 - Piotr Luszczek, UTK: OLCF testing
 - Aaron Fischer, 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:

- **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, PLASMA, heFFTe, SLATE:** Piotr Luszczek, Stan Tomov, Mark Gates (UTK)
- **MFEM:** Aaron Fischer, Tzanio Kolev (LLNL)
- **Omega_h:** Dan Ibanez (SNL)
- **PETSc/TAO:** Satish Balay, Alp Dener, Todd Munson (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 (SNL)



xSDK community policies

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

<https://xsdk.info/policies>



Version 0.6.0,
October 2020

Mandatory xSDK policies: must be satisfied

- M1.** Support portable installation through Spack (includes xSDK Spack variant guidelines)
- 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.** Have a debug build option.

Recommended xSDK policies: currently 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.
- R8.** Provide sufficient documentation to support use and further development.

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?**



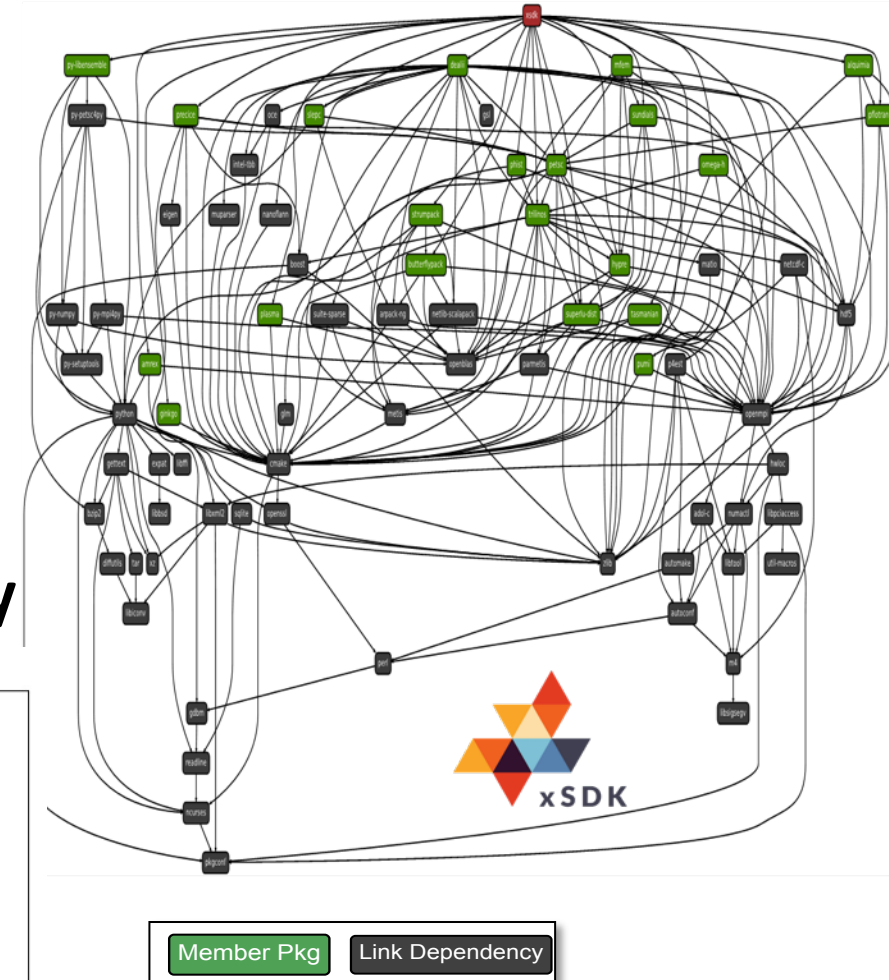
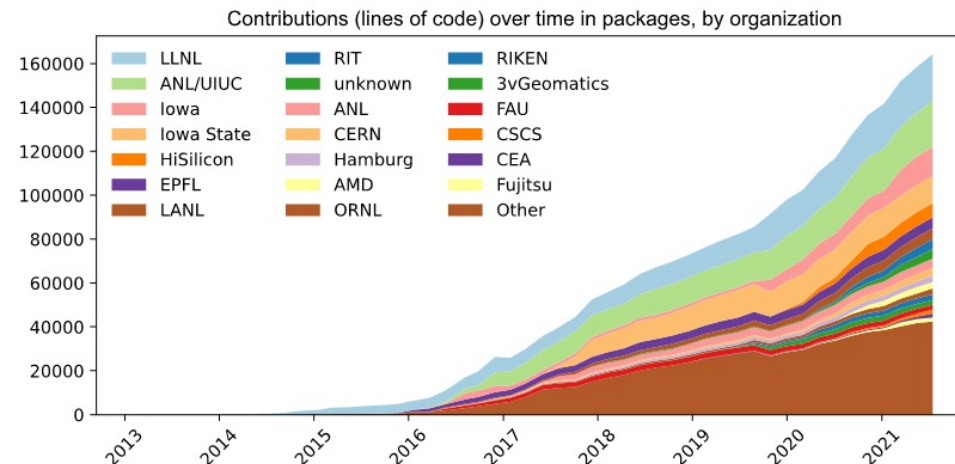
The xSDK is using Spack to deploy its software

- 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



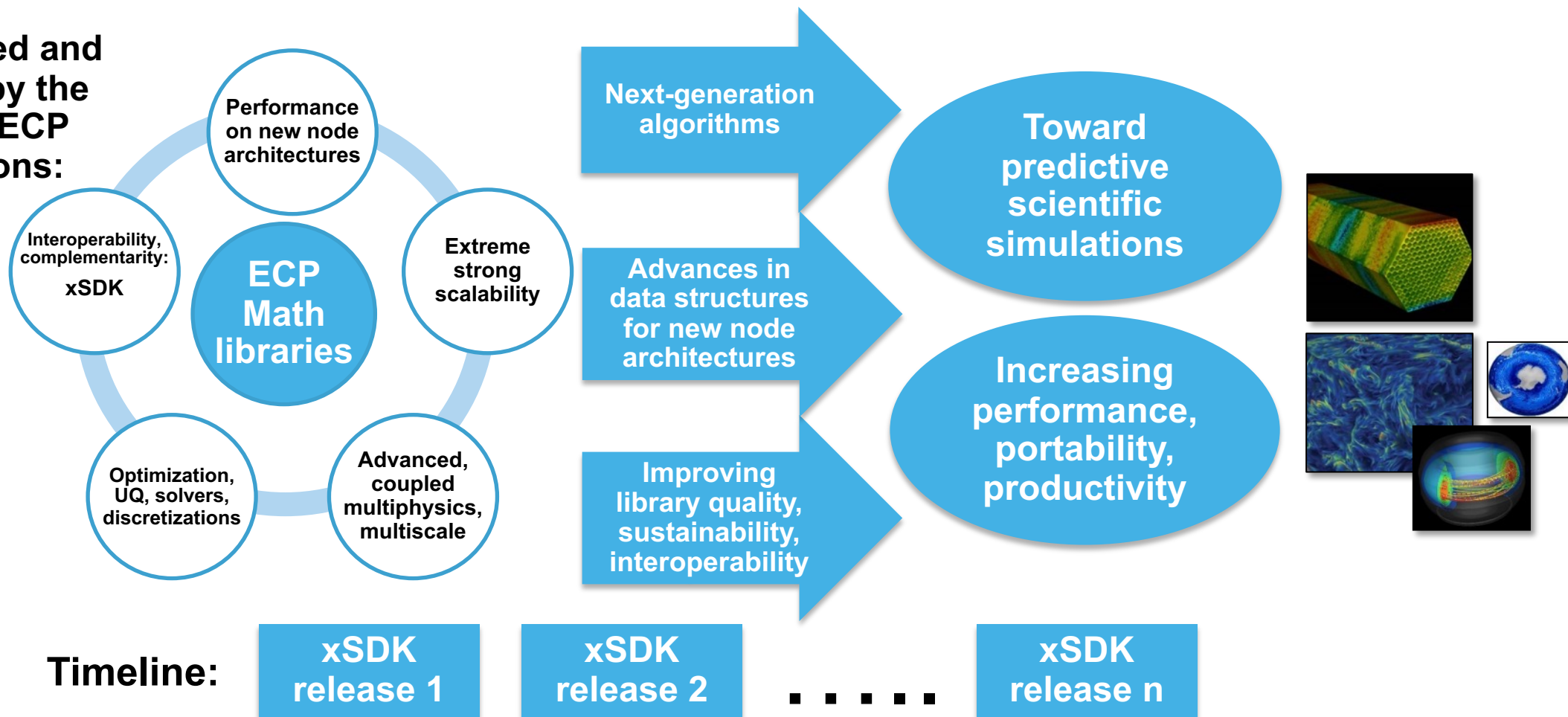
Spack has grown into a thriving open-source community

- Over 840 contributors
- Over 5,700 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:



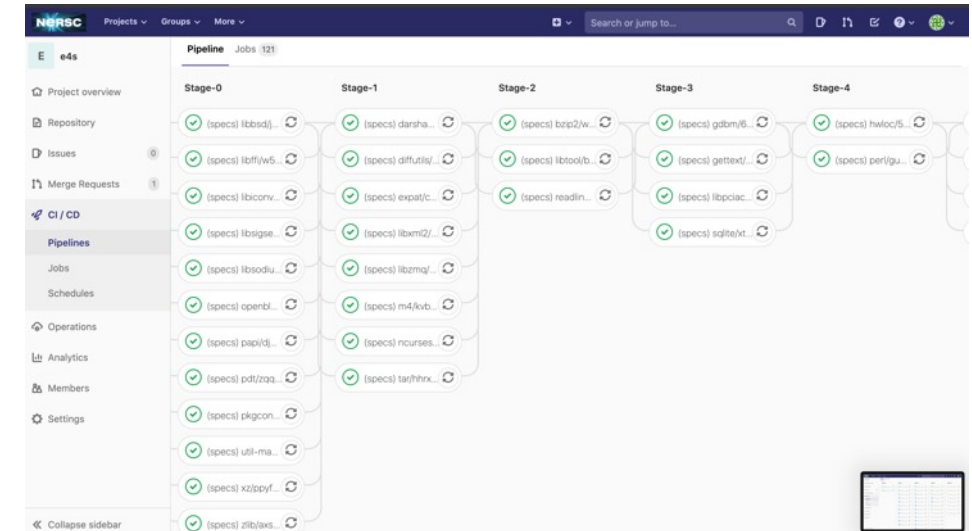
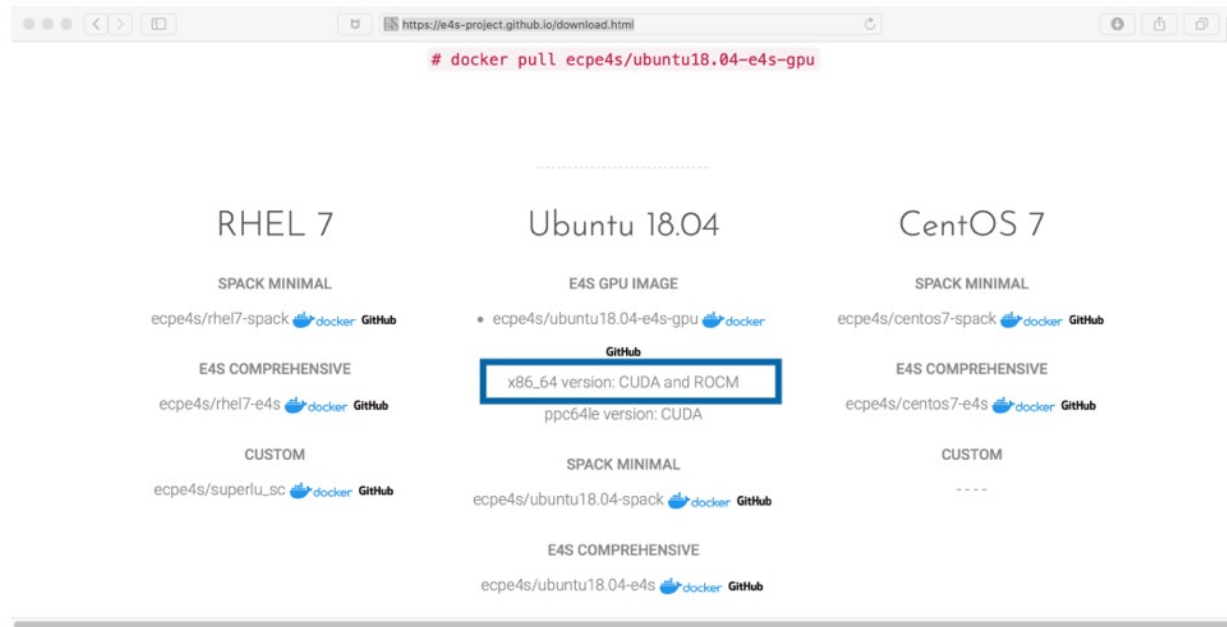
Extreme-scale Scientific Software Stack (E4S)

<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 76+ 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 37,000 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 2021-02 GPU Container Image



E4S build pipeline
• Cori, NERSC

21.05 Release: 76 Official Products + dependencies

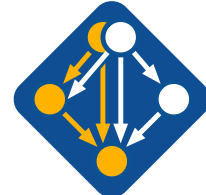
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E4S 2021.05 release

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



<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.

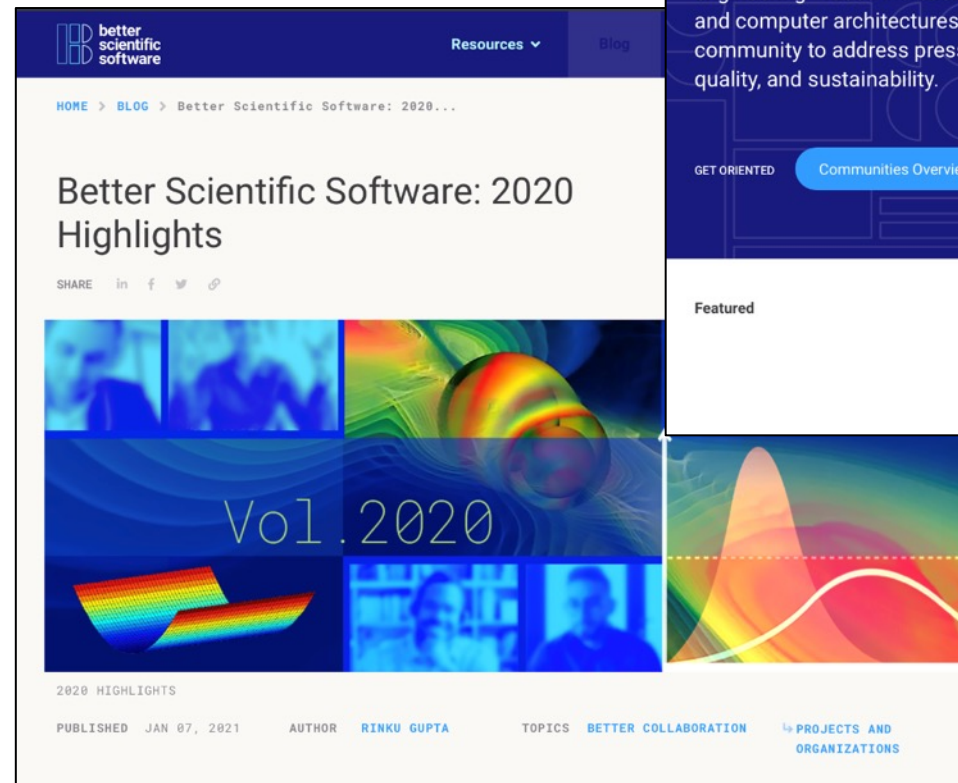
What E4S is



- Extensible, open architecture software ecosystem accepting contributions from US and international teams.
- Framework for collaborative open-source product integration.
- A full collection of 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.
- New entity in the HPC ecosystem enabling first-of-a-kind relationships with Facilities, vendors, other DOE program offices, other agencies, industry & international partners.
- Hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations.
- Conduit for future leading edge HPC software targeting scalable next-generation computing platforms.

Further reading

- [Building community through software policies](#), P. Luszczek & U. Yang
- [SuperLU: How advances in software practices are increasing sustainability and collaboration](#), S. Li
- [Porting the Ginkgo package to AMD's HIP ecosystem](#), H. Anzt
- [Scientific software packages and their communities](#), R. Gassmoeller
- [Leading a scientific software project: It's all personal](#), W. Bangerth
- [The art of writing scientific software in an academic environment](#), H. Anzt
- [Working Remotely: The Exascale Computing Project \(ECP\) panel series](#), E. Raybourn et al.
- [A Gentle Introduction to GPU Programming](#), M. Rosso and A. Myers
- [Performance Portability and the Exascale Computing Project](#), A. Dubey
- [Better Scientific Software: 2020 highlights](#), R. Gupta
- And many more ...



See also Track 7:
Software Productivity &
Sustainability (Aug 12)

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 2021 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.

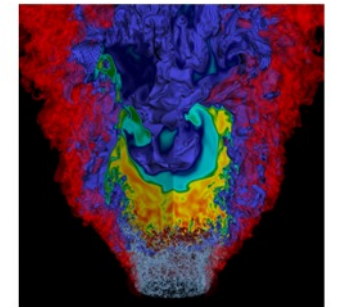
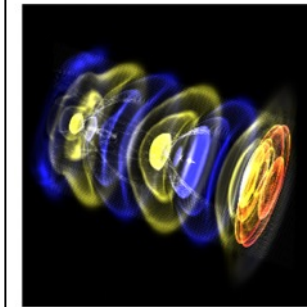
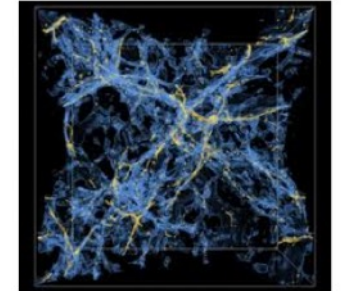
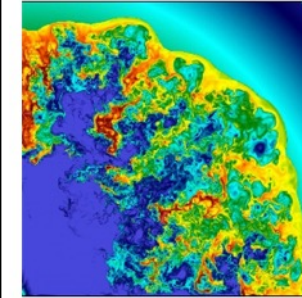
■ Capabilities

- 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 diverse 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



FAST MATH



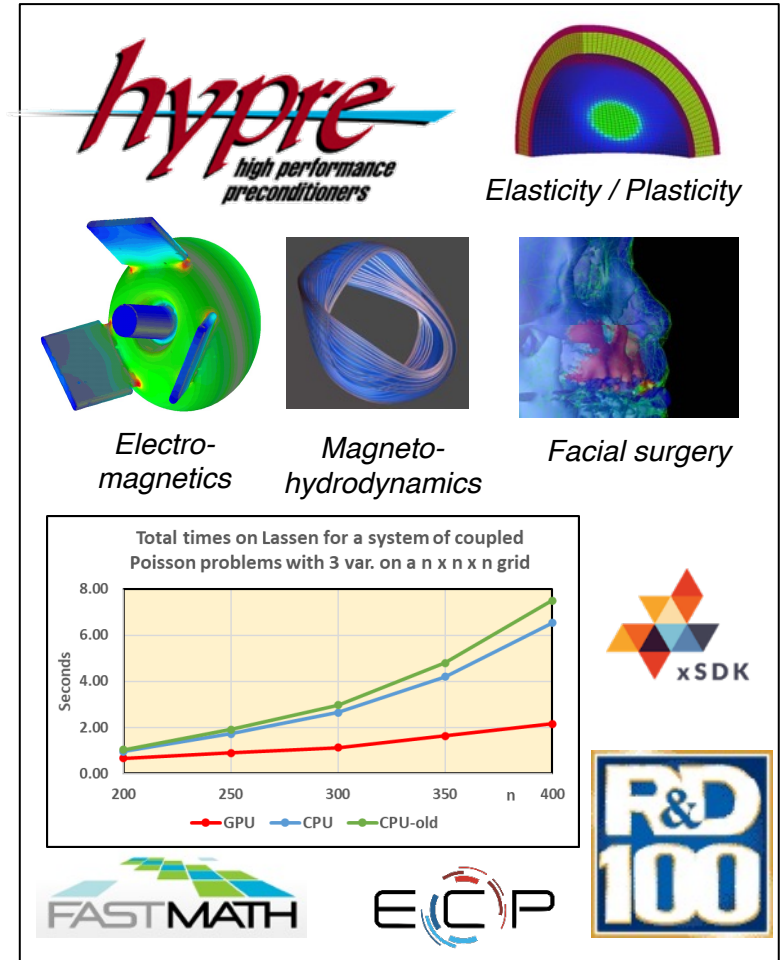
ECIP

<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 efficient (scalable) linear solvers through effective data storage schemes
- **Scalable preconditioners and solvers**
 - Structured and unstructured algebraic multigrid solvers
 - Maxwell solvers, H-div solvers
 - Multigrid solvers for nonsymmetric systems: pAIR, MGR
 - Matrix-free Krylov solvers
- **Exascale early systems GPU-readiness**
 - Available: Nvidia GPU (CUDA), AMD GPU (HIP)
 - In progress: Intel GPU (SYCL)
- **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/hypre-space/hypre>



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

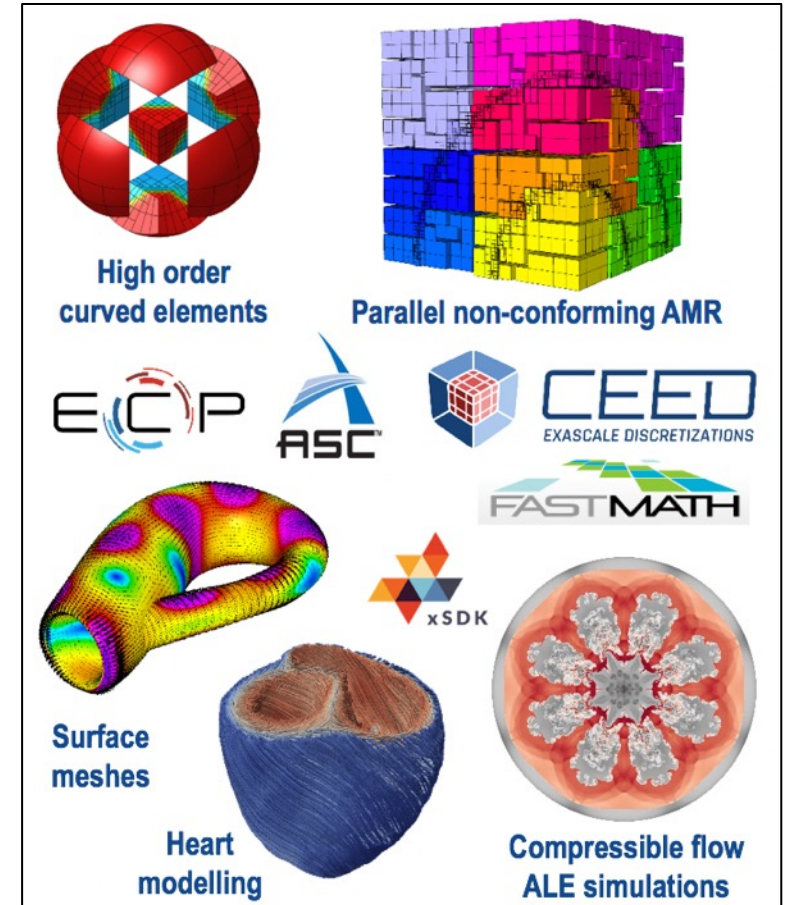
MFEM

Lawrence Livermore National Laboratory



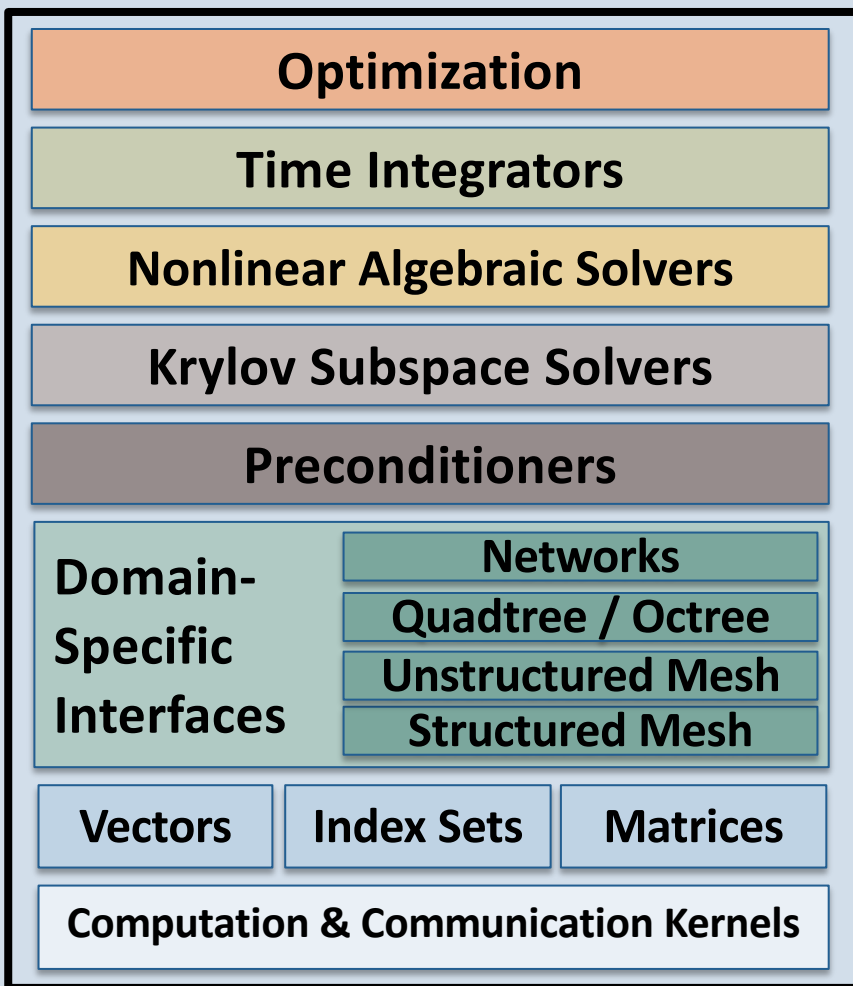
Free, lightweight, scalable C++ library for finite element methods. Supports arbitrary high order discretizations and meshes for wide variety of applications.

- **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 H^1 , $H(\text{curl})$, $H(\text{div})$ - and L^2 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>

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

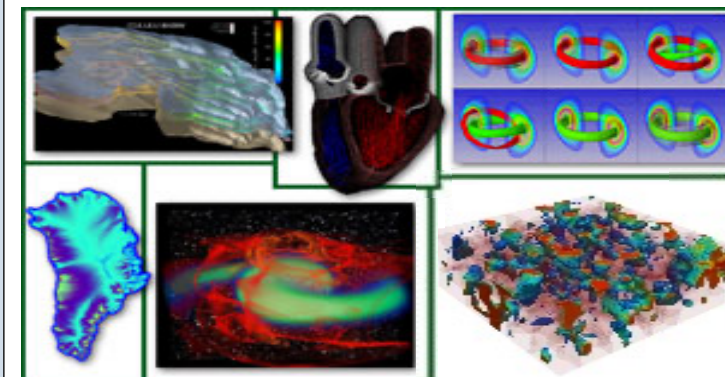


▪ **Easy customization and composability of solvers at runtime**

- 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; NVIDIA, AMD, and Intel GPUs
- Thousands of users worldwide



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



<https://petsc.org>

Parallel Unstructured Mesh Infrastructure

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

■ Core functionality

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

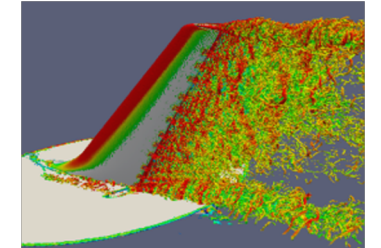
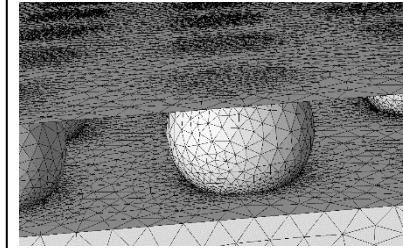
■ Designed for integration into existing codes

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

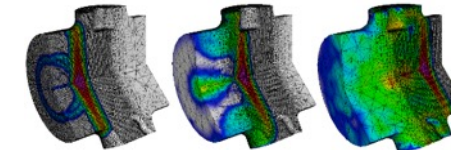
■ In-memory integrations developed

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

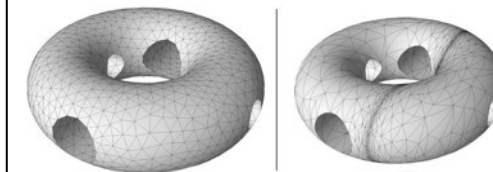
PUMi



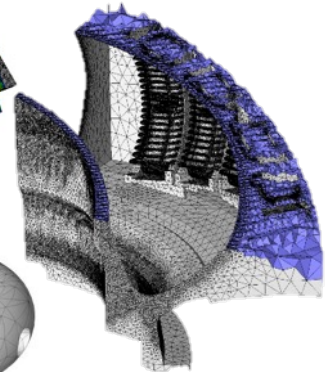
Applications with billions of elements: flip-chip (L), flow control (R)



Mesh adaptation for evolving features



Anisotropic adaptation for curved meshes



RF antenna and plasma surface in vessel.

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

PUMIPic Parallel Unstructured Mesh Infrastructure for Particle-in-Cell

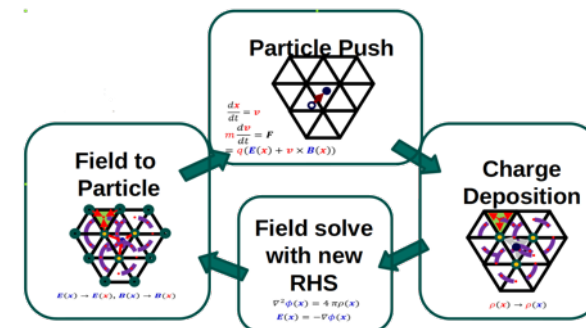
Parallel management of unstructured meshes with particles.
Framework for GPU accelerated particle-in-cell applications using unstructured meshes.

Core functionality

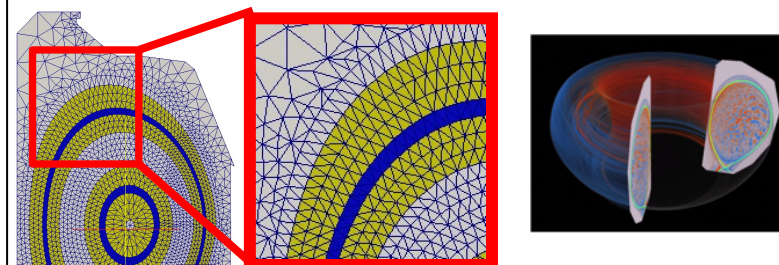
- Unstructured mesh-based approach
 - Particles accessed through mesh
 - Particle search through mesh adjacencies
 - Effective coupling to PDE solvers
 - Partitioning using bounding flux surfaces, graph, or geometric methods
 - PICpart: owned elements (defined by partition) + copied elements from topologically 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
 - Multiple choices for particle storage using abstraction layer: Sell-C-Sigma [Kreutzer 2014], COPA Cabana, and CSR.
- Parallel kernel launch function abstracts underlying particle and mesh storage

Applications Supported

- GITRm: impurity transport
- XGCm: 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 XGCm tokamak mesh and domain decomposition



Stages of a PIC application supported by PUMIPic



(Left) Two PICparts defined as sets of flux faces in XGCm mesh. (Center) The blue face is the 'core' and the yellow faces are its 'buffers'. (Right) Two poloidal planes in a toroidal domain.

Source Code: github.com/SCOREC/pumi-pic
Paper: scorec.rpi.edu/REPORTS/2020-2.pdf

PUMIPic Applications

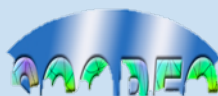
Unstructured mesh particle-in-cell fusion applications using PUMIPic. Supporting the analysis of tokamak plasma physics and impurity transport using extensions to the PUMIPic framework.

■ 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 verification and performance.

■ 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



HBPS
High-fidelity
Boundary
Plasma Simulation

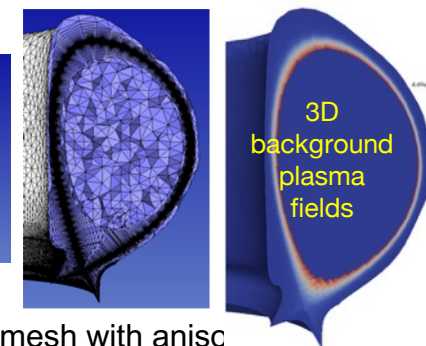
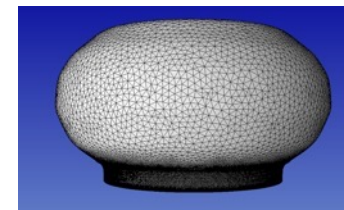
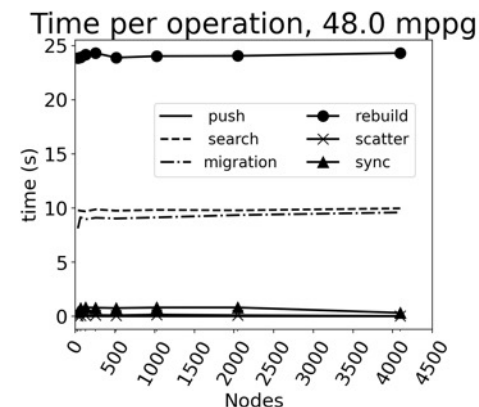


Rensselaer



XGCm weak scaling on Summit

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



3D unstructured mesh with anisotropic refinement. Less than 1% difference vs. GITR in gross erosion and deposition.

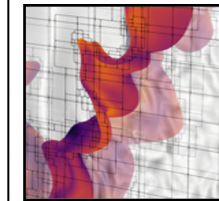
GITRm ITER test case

Contact: Mark S. Shephard
shephard@rpi.edu

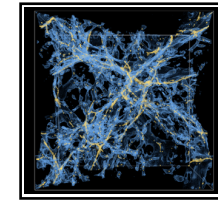
Adaptive time integrators for ODEs and DAEs and efficient nonlinear solvers
Used in a variety of applications. Freely available. Encapsulated solvers & parallelism.

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

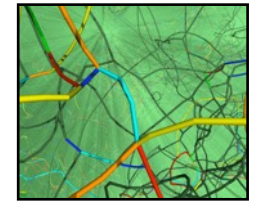
SUNDIALS is used worldwide in applications throughout research and industry



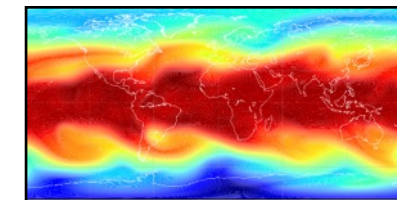
Combustion
(Pele)



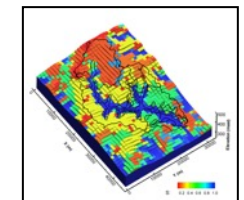
Cosmology
(Nyx)



Dislocation dynamics
(ParaDiS)



Atmospheric Dynamics
(Tempest)



Subsurface flow
(ParFlow)

 **Lawrence Livermore
National Laboratory**

 **ECP**

 **FAST MATH**

 **xSDK**

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

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

Capabilities

- Serial (thread-safe), shared-memory (SuperLU_MT, OpenMP or Pthreads), distributed-memory (SuperLU_DIST, hybrid MPI+ OpenM + CUDA/HIP).
 - Written in C, with Fortran interface
- Sparse LU decomposition (can be nonsymmetric sparsity pattern), triangular solution with multiple right-hand sides
- Incomplete LU (ILUTP) preconditioner in serial SuperLU
- Sparsity-preserving ordering: minimum degree or graph partitioning applied to $A^T A$ or $A^T + A$
- User-controllable pivoting: partial pivoting, threshold pivoting, static pivoting
- Condition number estimation, iterative refinement, componentwise error bounds

Exascale early systems GPU-readiness

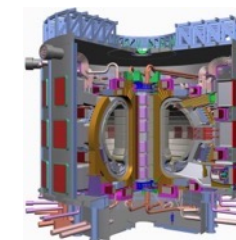
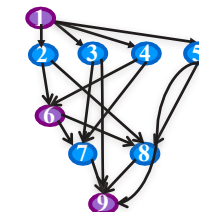
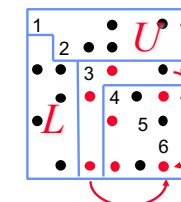
- Available: Nvidia GPU (CUDA), AMD GPU (HIP)
- In progress: Intel GPU (DPC++ planned)

Parallel Scalability

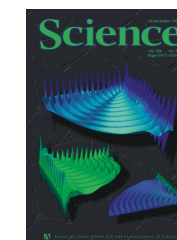
- Factorization strong scales to 32,768 cores with 4096 GPUs (IPDPS'18, PARCO'19)
- Triangular solve strong scales to 4000 cores (SIAM CSC'18, SIAM PP'20)

Open source software

- Used in a vast range of applications, can be used through PETSc and Trilinos, available on github



ITER tokamak



quantum mechanics

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



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

STRUMPACK

Structured Matrix Package



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



■ Dense Matrix Solvers using Hierarchical Approximations

- Hierarchical partitioning, low-rank approximations
- Hierarchically Semi-Separable (HSS), Hierarchically Off-Diagonal Low-Rank (HODLR), Hierarchically Off-Diagonal Butterfly (HODBF), Block Low-Rank (BLR), Butterfly
- C++ Interface to ButterflyPACK (Fortran)
- Applications: BEM, Cauchy, Toeplitz, kernel & covariance matrices, ...
- Asymptotic complexity much lower than LAPACK/ScaLAPACK routines

■ Sparse Direct Solver

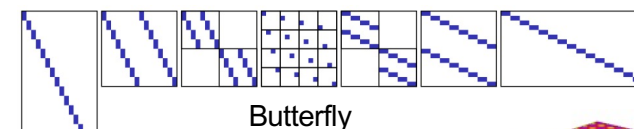
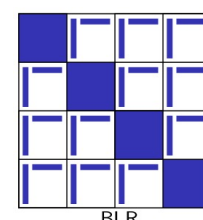
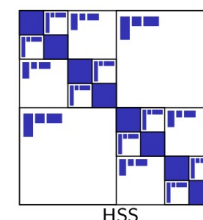
- Algebraic sparse direct solver
- GPU: CUDA, HIP/ROCm, DPC++ (in progress)
- Orderings: (Par)METIS, (PT)Scotch, RCM

■ Preconditioners

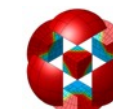
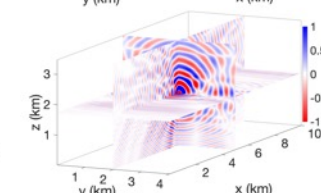
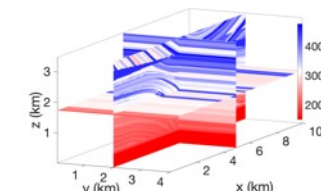
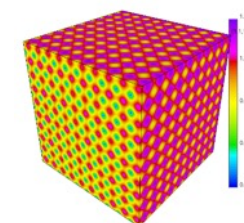
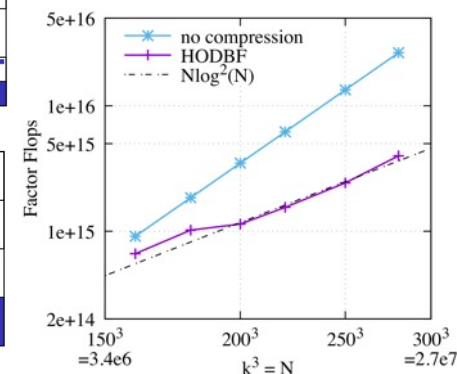
- Approximate sparse factorization, using hierarchical matrix approximations
- Scalable and robust, aimed at PDE discretizations, indefinite systems, ...
- Iterative solvers: GMRES, BiCGStab, iterative refinement

■ Software

- BSD license
- Interfaces from PETSc, MFEM, Trilinos, available in Spack



Near linear scaling for high-frequency wave equations



github.com/pghysels/STRUMPACK



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

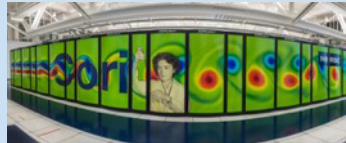
- **Optimal kernels to optimal solutions**

- Scalable linear, nonlinear, eigen, transient, optimization, UQ solvers
- Discretization, geometry, meshing
- Load balancing

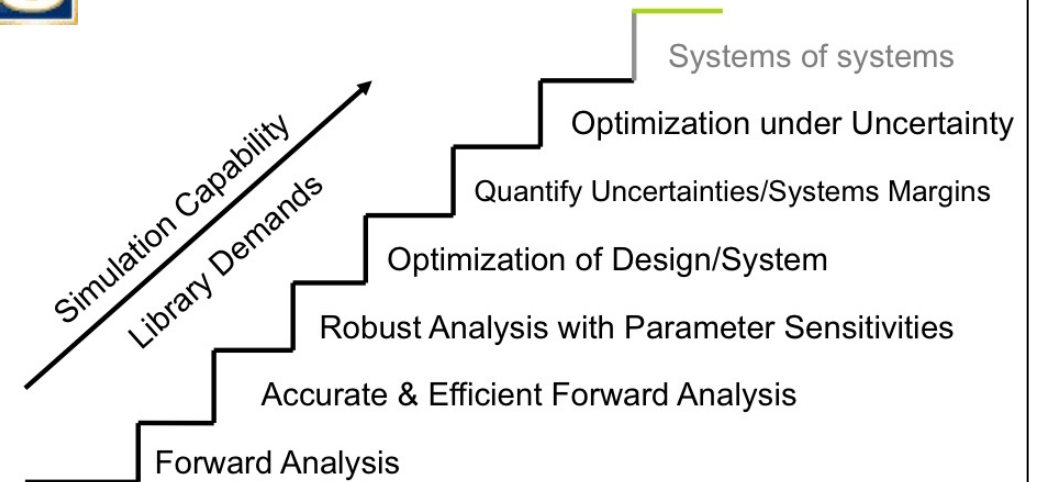
- ***Performance Portability across multiple platforms (GPU, multicore) provided by Kokkos***

- **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. Templated C++ allows for generic scalar, ordinal, and compute node types.

- **Ability to solve single or sequence of linear systems**

- Simultaneously solved systems w/ multiple-RHS: $AX = B$
- Sequentially solved systems w/ multiple-RHS: $AX_i = B_i, i=1,...,t$
- Sequences of multiple-RHS systems: $A_i X_i = B_i, i=1,...,t$

- **Standard methods**

- Conjugate Gradients (CG), GMRES
- TFQMR, BiCGStab, MINRES, fixed-point

- **Advanced methods**

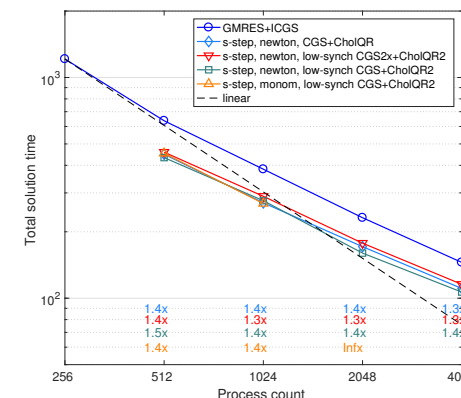
- Block GMRES, block CG/BICG
- Hybrid GMRES, CGRODR (block recycling GMRES)
- TSQR (tall skinny QR), LSQR
- Pipelined and s-step methods
- Stable polynomial preconditioning

- **Performance portability via Kokkos (CPUs, NVIDIA/Intel/AMD GPUs, Phi)**

- **Ongoing research**

- Communication avoiding methods

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



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



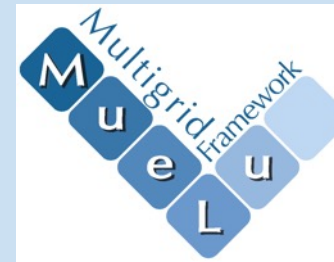
<https://trilinos.github.io/belos.html>

Trilinos/MueLu

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

- **Robust, scalable, portable AMG preconditioning critical for many large-scale simulations**

- Multifluid plasma simulations
- Shock physics
- Magneto-hydrodynamics (MHD)
- Low Mach computational fluid dynamics (CFD)



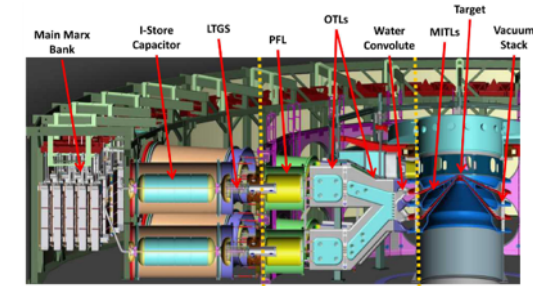
- **Capabilities**

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

- **Research Areas**

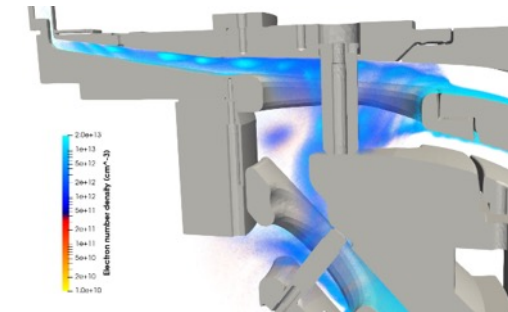
- AMG for multiphysics
- Multigrid for coupled structured/unstructured meshes
- Algorithm selection via machine learning

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

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



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



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

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)

ArborX/ DataTransferKit



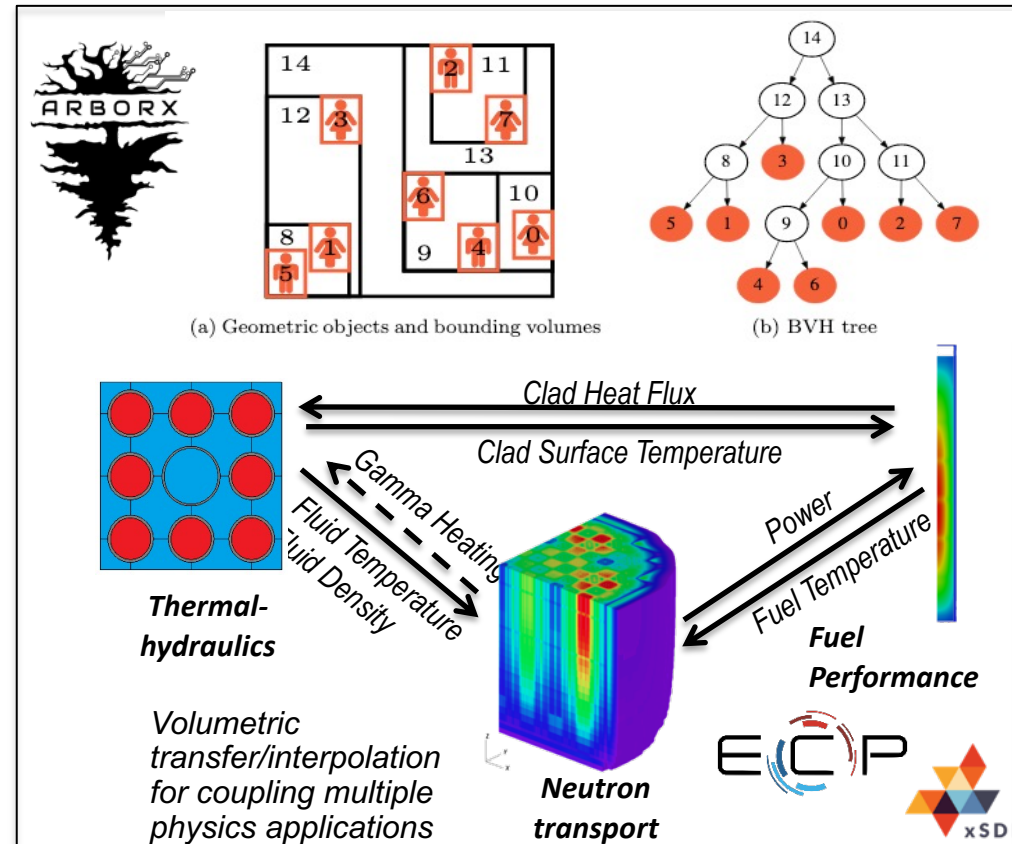
Open source libraries for geometric search and parallel solution transfer. Support for grid-based and mesh-free applications.

■ ArborX

- Geometric search and clustering algorithms
 - Provides both neighborhood search (rNN) and nearest neighbors (kNN)
 - Provides density-based clustering algorithms (DBSCAN, HDBSCAN)
- Performance portable
 - Serial performance is comparable to widely used libraries (Boost R-tree, Nanoflann)
 - Supports all DOE leadership class machines
- Used for Kokkos performance benchmarking
 - The first libraries to support all Kokkos backends (OpenMP, CUDA, HIP, SYCL, OpenMPTarget)

■ DataTransferKit

- Efficient and accurate solution transfers between applications of different mesh layouts on parallel accelerated architectures
- Used for a variety of applications including conjugate heat transfer, fluid structure interaction, computational mechanics, and reactor analysis



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

ButterflyPACK



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

■ Capabilities

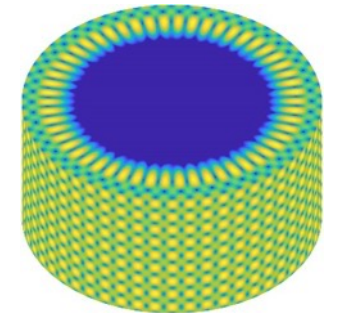
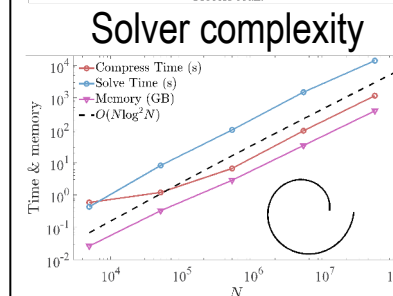
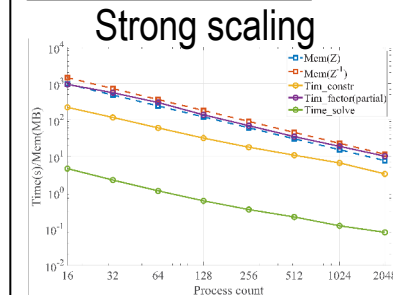
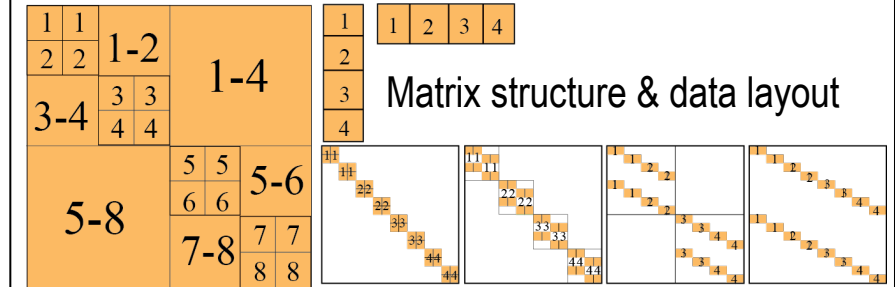
- Fast algebraic operations for rank-structured dense and sparse matrices, including matrix compression, multiplication, factorization and solution
- Support distributed-memory H-matrix, HODLR formats with low-rank and butterflies
- Particularly targeted at high-frequency electromagnetic, acoustic and 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/liuyangzhuan/ButterflyPACK/tree/master/EXAMPLE>



Accelerator cavity



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

Chombo



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

■ Adaptive Mesh Refinement (AMR)

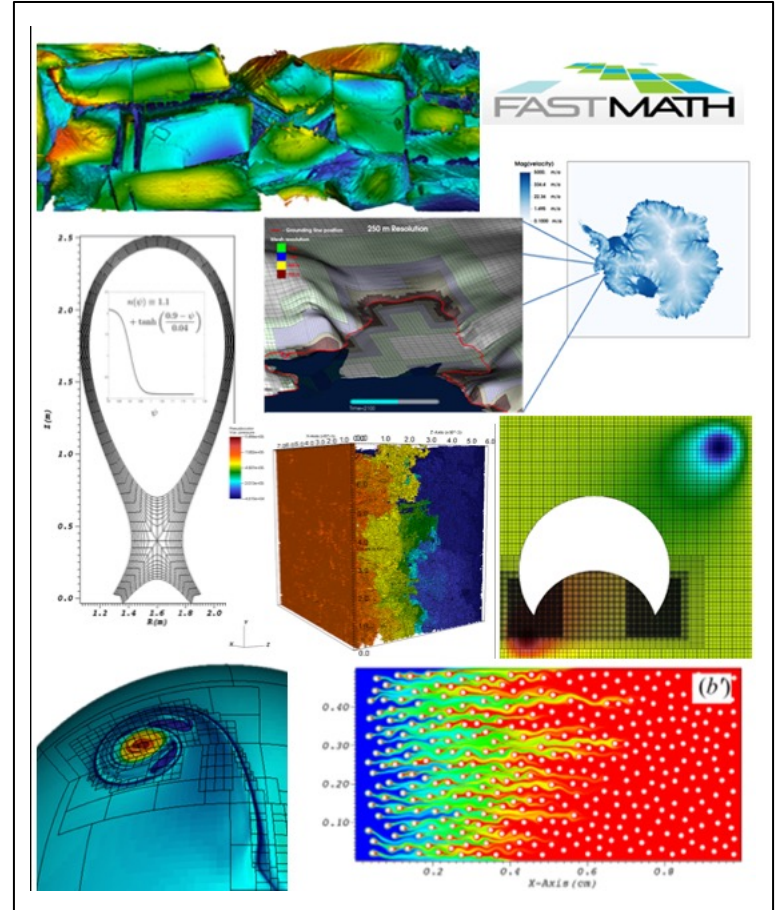
- Block structured AMR dynamically focuses computational effort where needed to improve solution accuracy
- Designed as a developers' toolbox for implementing scalable AMR applications
- Implemented in C++/Fortran
- Solvers for hyperbolic, parabolic, and elliptic systems of PDEs

■ 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

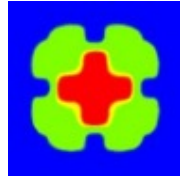
■ Higher-order finite-volume

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



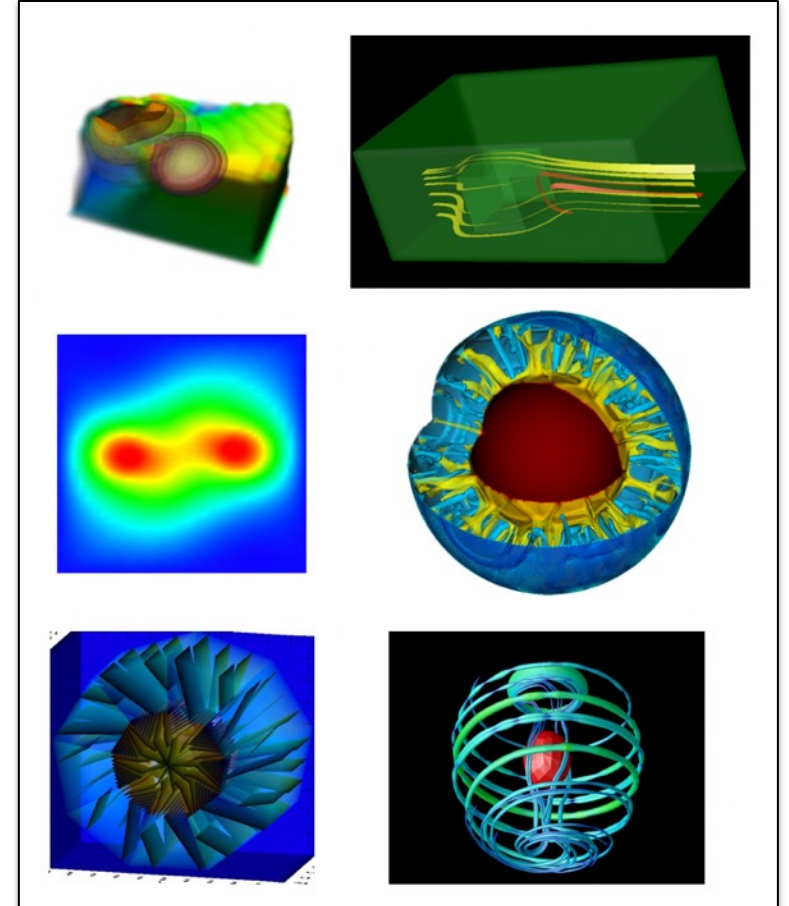
<http://Chombo.lbl.gov>

deal.II



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>

Ginkgo



GPU-centric high performance sparse linear algebra. Sustainable and extensible C++ ecosystem with full support for AMD, NVIDIA, Intel GPUs.

High performance sparse linear algebra

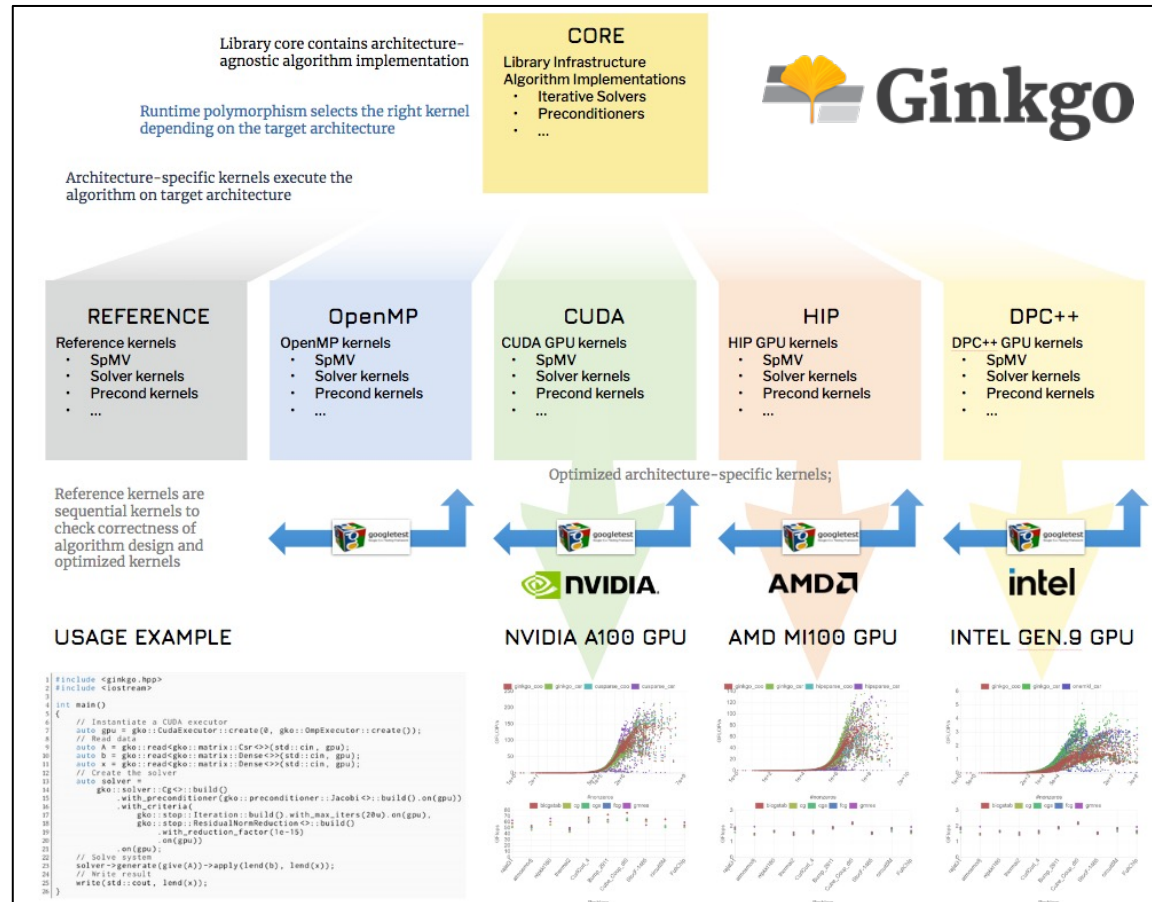
- Linear solvers: BiCG, BiCGSTAB, CG, CGS, FCG, GMRES, IDR;
- Advanced preconditioning techniques: ParILU, ParILUT, SAI;
- Mixed precision algorithms: adaptive precision Jacobi, FSPAI;
- Decoupling of arithmetic precision and memory precision;
- Batched iterative solvers;*
- Linear algebra building blocks: SpMV, SpGEAM,...;
- Extensible, sustainable, production-ready;

Exascale early systems GPU-readiness

- Available: Nvidia GPU (CUDA), AMD GPU (HIP), Intel GPU (DPC++), CPU Multithreading (OpenMP);
- C++, CMake build;

Open source, community-driven

- Freely available (BSD License), GitHub, and Spack;
- Part of the **xSDK** and **E4S** software stack;
- Can be used from **deal.II** and **MFEM**;



<https://ginkgo-project.github.io/>



heFFTe



Highly Efficient FFT for Exascale (heFFTe). Scalable, high-performance multidimensional FFTs; Flexible; User-friendly interfaces (C++/C/Fortran/python); Examples & benchmarks; Testing; Modified BSD license.

Capabilities:

- Multidimensional FFTs
- C2C, R2C, C2R
- Support flexible user data layouts
- Leverage and build on existing **FFT capabilities**

Pre-exascale environment:

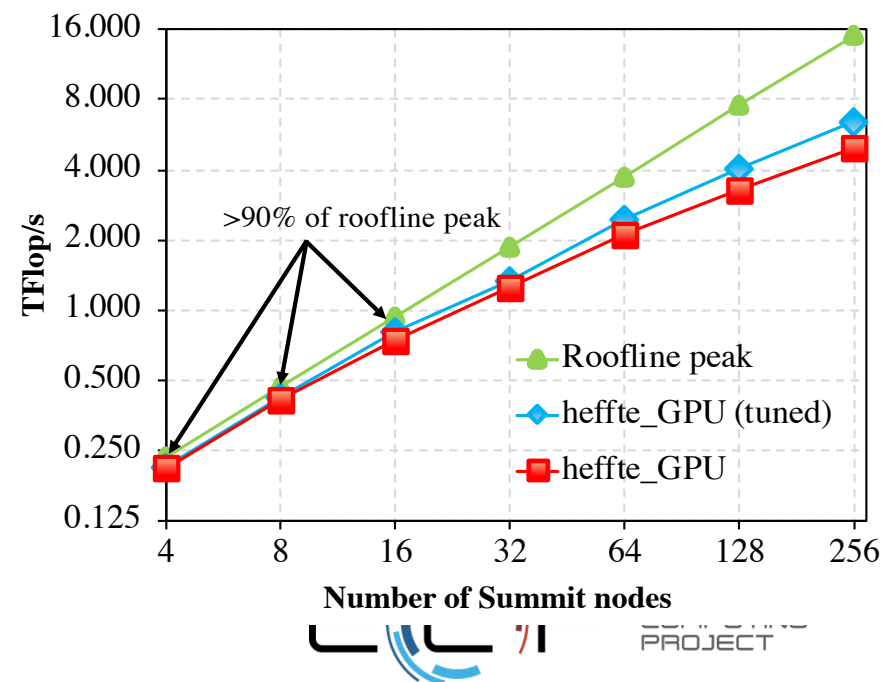
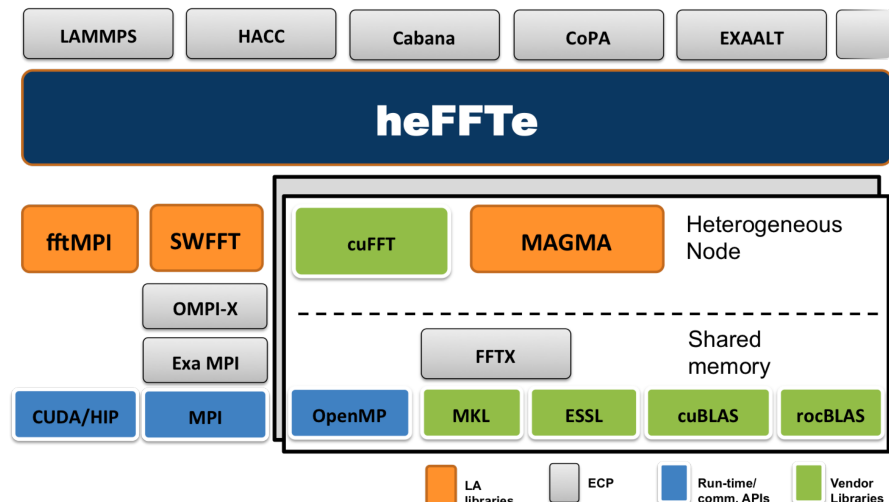
- **Summit @ OLCF (Nvidia GPUs), Poplar (AMD GPUs), and others**
- **In progress: Intel GPU**

Current status:

- heFFTe 2.0 with support for CPUs, Nvidia GPUs, AMD GPUs
- Very good strong and weak scaling, reaching up to 90% of roofline peak

Open Source Software

- **spack** installation and integration in xSDK
- heFFTe Integration and acceleration of CoPA projects using LAMMPS and HACC
- Homepage: <http://icl.utk.edu/fft/>
- Repository: <https://bitbucket.org/icl/heffte/>



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:

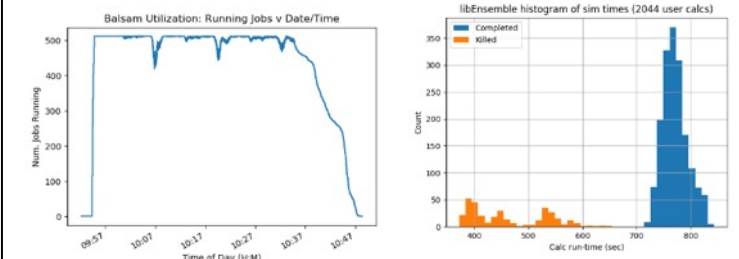
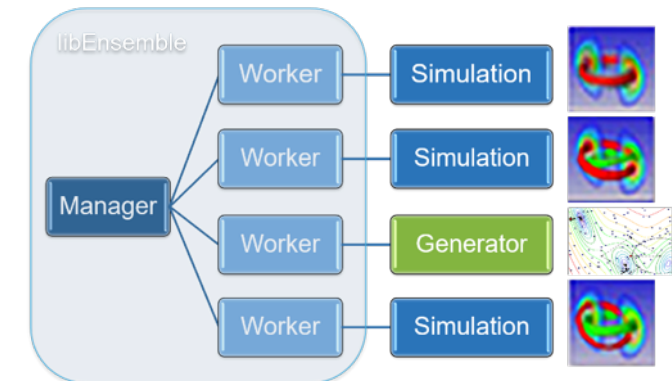
- Extreme scaling
- Resilience and fault tolerance
- Monitoring and killing tasks and recovering resources
- Portability and flexibility

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>

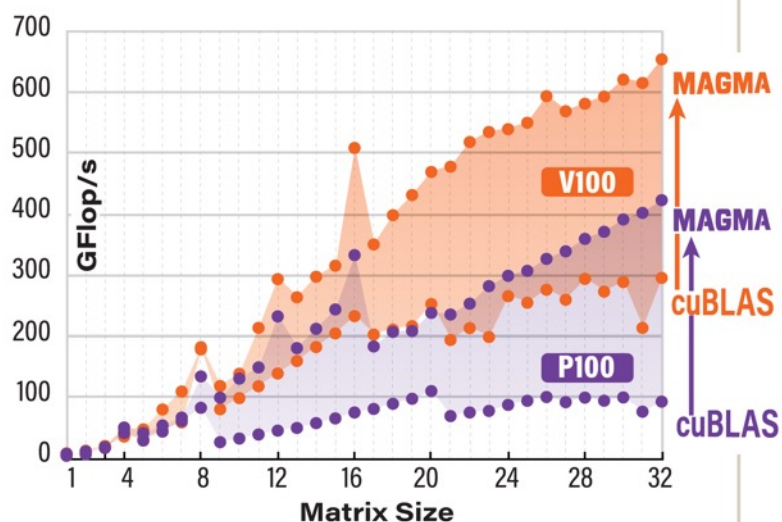


MAGMA

- Shared memory systems
- BLAS/LAPACK on GPUs
- Hybrid CPU-GPU Algorithms
 - Linear system solvers (+ mixed precision)
 - Eigenvalue problem solvers
- Batched LA
 - All BLAS-3 (fixed/variable), LU, QR, Cholesky
- Sparse LA
 - Solvers: BiCG, BiCGSTAB, GMRES
 - Preconditioners: ILU, Jacobi,
 - SPMV, SPM (CSR, ELL, ... etc.)

PERFORMANCE OF BATCHED LU

in double-precision arithmetic on 1 million matrices



Matrix Algebra on GPU and Multicore Architectures

PERFORMANCE & ENERGY EFFICIENCY

MAGMA LU factorization in double-precision arithmetic

CPU

Intel Xeon E5-2650 v3 (Haswell)
2 x 10 cores @ 2.30 GHz

P100

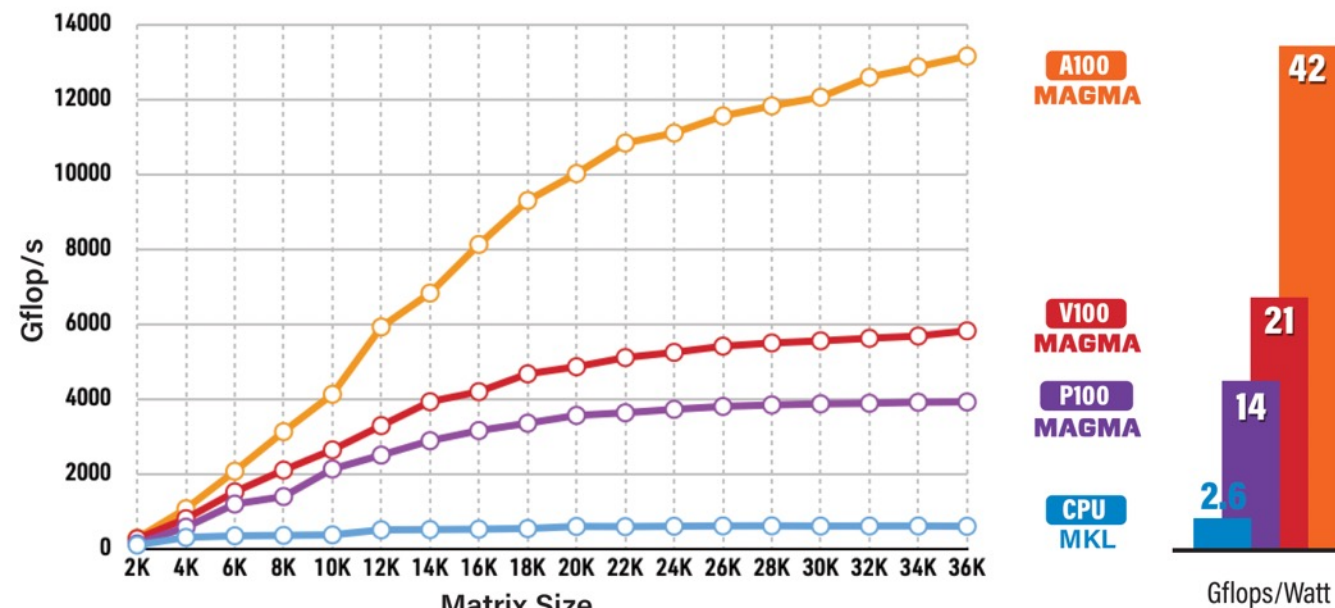
NVIDIA Pascal GPU
56 SMs x 64 @ 1.19 GHz

V100

NVIDIA Volta GPU
80 SMs x 64 @ 1.37 GHz

A100

NVIDIA Ampere GPU
108 SMs x 64 @ 1.41 GHz



- Support CUDA and ROCM/HIP

- <https://icl.utk.edu/magma>

IN COLLABORATION WITH

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Berkeley
UNIVERSITY OF CALIFORNIA

University of Colorado
Denver

U.S. Department of
Defense

U.S. DEPARTMENT OF
ENERGY

AMD

intel

Inria

KAUST

ECIP

National
Science
Foundation

MathWorks

nvidia

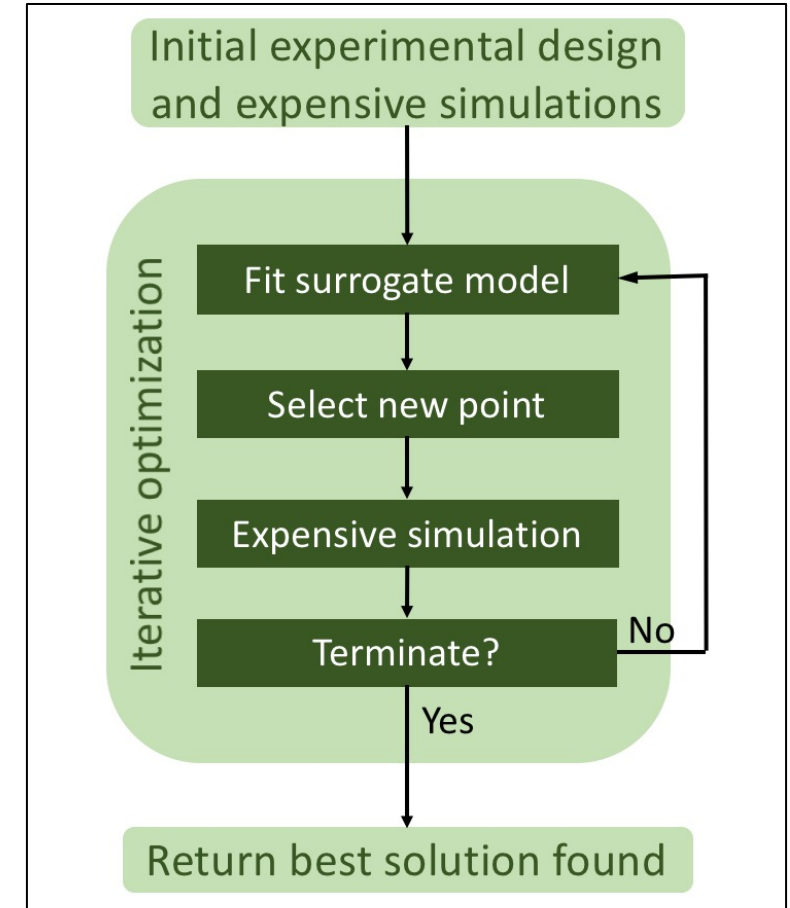
Efficient optimization of computationally-expensive black-box problems. For integer, mixed-integer, and continuous variables. Your choice of surrogate model, sampling method, and initial design strategy. Easy to use. Freely available.

■ 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 $\mathbf{Ax} = \lambda \mathbf{Bx}$ (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

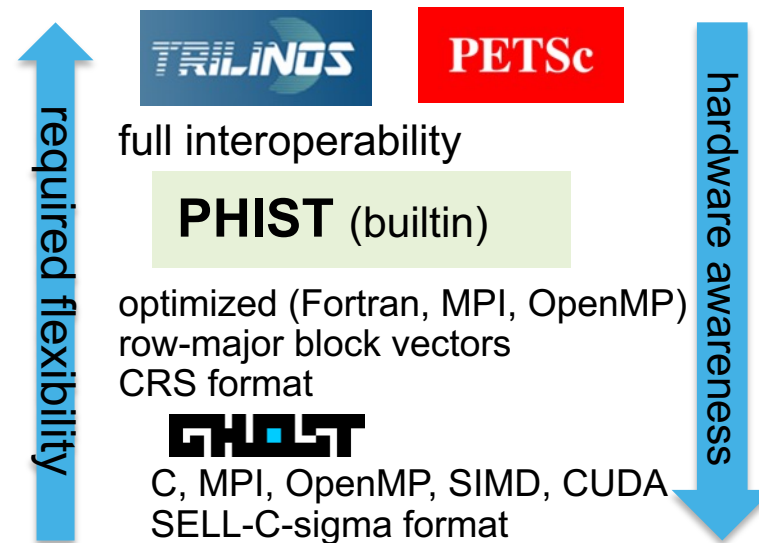
■ Algorithmic Building Blocks

- 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



Funded by the DFG
project ESSEX



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

PLASMA: Parallel Linear Algebra for Multicore Architectures

Functional scope

- Dense: linear systems, least-squares, EIG/SVD
- Tile matrix layout and tile algorithms
- OpenMP: v4 tasking, v4.5 priorities, v5 offload variants

```
int dev = omp_get_default_device(); double *a = mkl_malloc(a_ld * n * 8, 64);  
#pragma omp target data map(to:a,b) map(tofrom:c)  
{  
#pragma omp target variant dispatch use_device_ptr(a,b,c) device(dev) nowait  
mkl_dgemm(tA, tB, m, n, k, alpha, a, a_ld, b, b_ld, beta, c, c_ld);  
#pragma omp taskwait  
}
```

Accessing
device-specific
asynchronous
dispatch for low-level
runtime integration

```
#pragma omp target data map(a[0:n*n],b[0:n*n]) map(alloc:c[0:n*n])  
#pragma omp target data use_device_ptr(a,b,c)  
{  
    cudaStream_t omp_stream = (cudaStream_t) omp_get_cuda_stream(dev);  
    cublasSetStream(handle, stream);  
    cublasDgemm(handle, CUBLAS_OP_N, CUBLAS_OP_N, m, n, k, &alpha, a, a_ld, b, b_ld, &beta, c, c_ld);  
}
```

Compiler framework targets: Clang 11, AOMP 11, XL 16, OneAPI 1, Cray 9, NVHPC

```
double*a_dev=omp_target_alloc(device, a_ld * n);
```

Device-resident pointers for
persistent on-device storage

Accessing native libraries for vendor-level on-
device performance

SLATE

Software for Linear Algebra Targeting Exascale

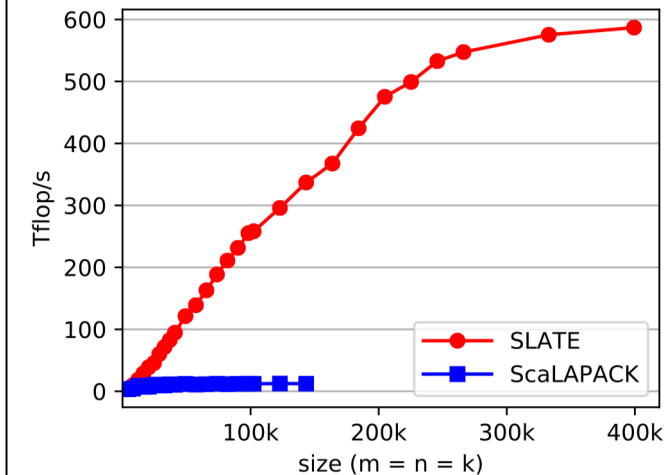


Distributed, GPU-accelerated, dense linear algebra library.
Modern replacement for ScaLAPACK. BSD license.

- **Made for distributed HPC with accelerators**
 - BLAS: matrix multiply ($C = AB$), etc.
 - Linear systems ($Ax = b$): LU, Cholesky, symmetric indefinite
 - Least squares ($Ax \approx b$): QR, LQ
 - Eigenvalue ($Ax = \lambda x$)
 - SVD ($A = U\Sigma V^H$)
- **GPU-readiness: Uses BLAS++ as abstraction layer**
 - Initial implementation: Nvidia GPUs (cuBLAS)
 - Recent: AMD GPU (hip/rocBLAS).
 - In progress Intel GPUs (OpenMP, oneAPI).
- **Software design**
 - C++ library built on MPI, OpenMP, batch-BLAS, vendor-BLAS.
 - Build: CMake, Makefile, Spack. APIs: C, Fortran, ScaLAPACK.
- **BLAS++ and LAPACK++**
 - C++ wrappers for BLAS and LAPACK routines. Independent projects.



Summit 16 nodes: 672 POWER9 cores+96 NVIDIA V100
CPU + GPU **peak 765 Tflop/s** in double precision



Matrix multiply (dgemm)
47x speedup
77% of peak



<https://icl.utk.edu/slate/>



■ 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

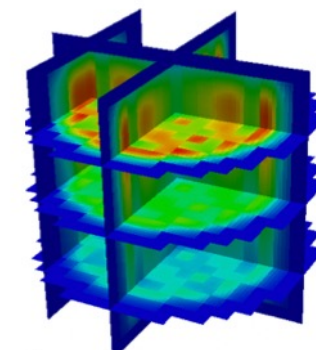
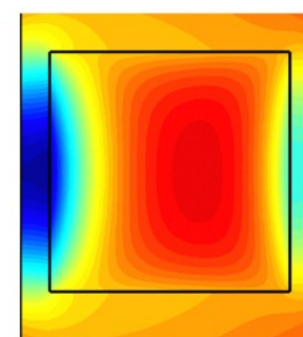
- Parallel Krylov solver to evaluate $y=f(A)v$
- Support for matrix exponential, square root, etc. and combinations thereof

■ Extension of PETSc

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



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



<http://slepc.upv.es>

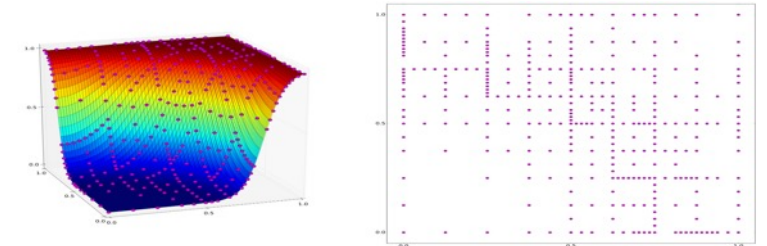
■ Capabilities

- Sparse Grid Surrogate modeling using structured and unstructured data
 - Statistical analysis
 - Fast surrogates for multiphysics simulations
- Hierarchical data representation for data-reduction and data-mining
- Markov Chain Monte Carlo methods for Bayesian inference
 - Model calibration and validation
 - Sensitivity analysis and multidimensional anisotropy

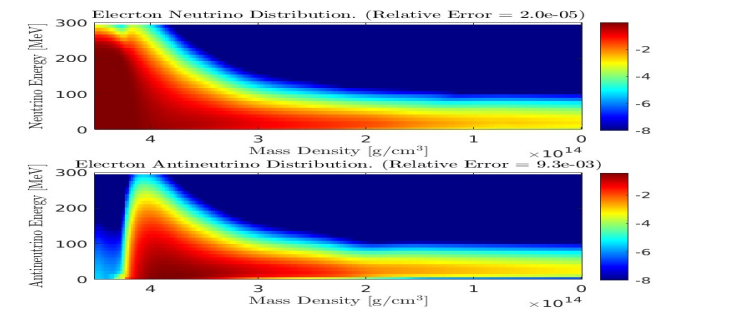
■ GPU Accelerated Capabilities

- Fast surrogates using Nvidia (CUDA), AMD (HIP), Intel (DPC++)
- Accelerated linear algebra using UTK MAGMA
- Parallel surrogate construction using libEnsemble
- Mixed single-double precision methods for low memory footprint

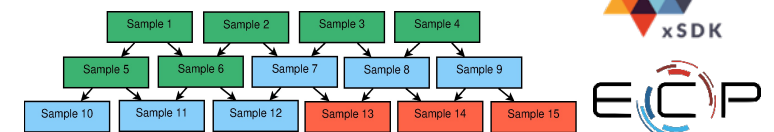
Adaptive Sparse Grid Sampling



Multiphysics simulation of Neutrino Radiation



Dynamic Adaptive Sampling



<https://github.com/ORNLTASMANIAN>

Zoltan/Zoltan2

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

■ Partitioning & load-balancing support many applications

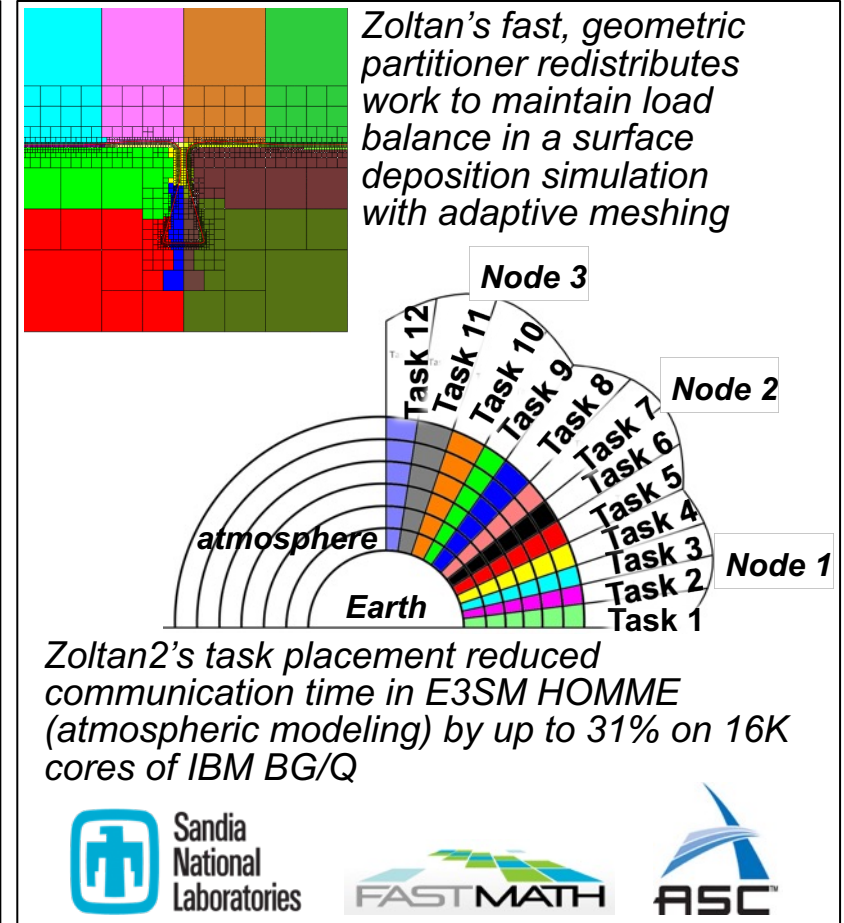
- Fast geometric methods maintain spatial locality of data (e.g., for adaptive finite element methods, particle methods, crash/contact simulations)
- Graph and hypergraph methods explicitly account for communication costs (e.g., for electrical circuits, finite element meshes, social networks)
- Single 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

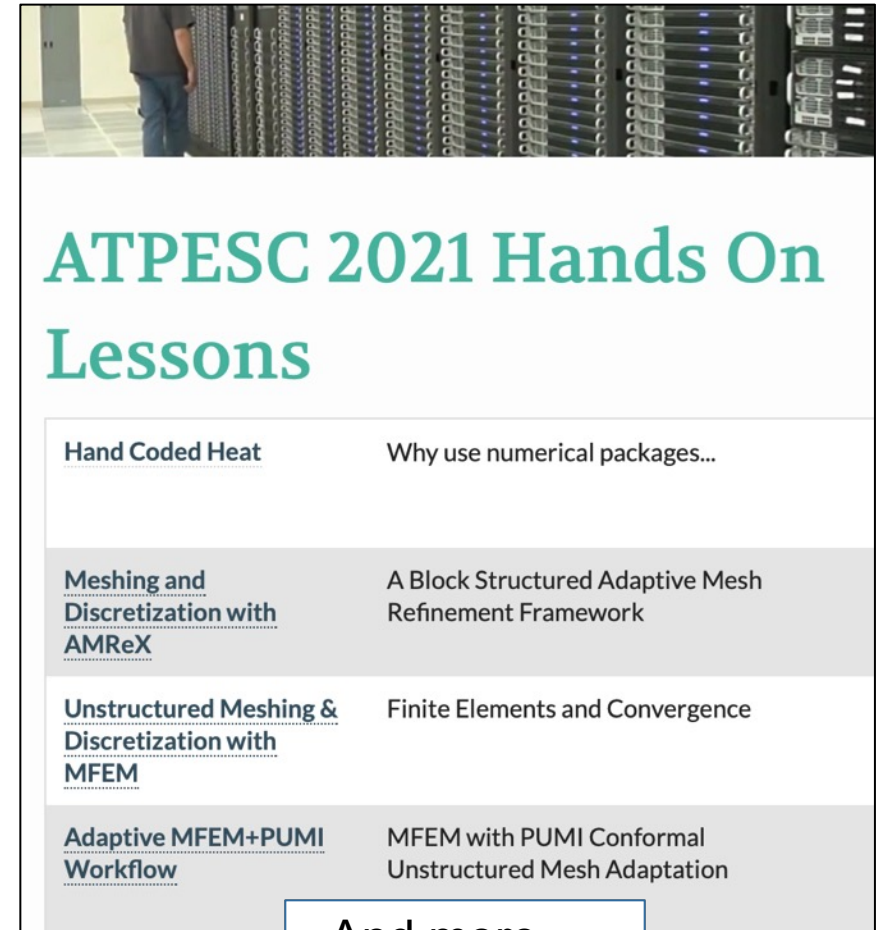
■ Use as a stand-alone library or as a Trilinos component



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

HandsOn Lessons

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



The poster features a header image of a server room with a person standing in the aisle. Below the header, the title "ATPESC 2021 Hands On Lessons" is displayed in large teal font. A table lists five topics, each with a title and a brief description. The topics are: "Hand Coded Heat" (Why use numerical packages...), "Meshing and Discretization with AMReX" (A Block Structured Adaptive Mesh Refinement Framework), "Unstructured Meshing & Discretization with MFEM" (Finite Elements and Convergence), and "Adaptive MFEM+PUMI Workflow" (MFEM with PUMI Conformal Unstructured Mesh Adaptation). A fifth entry, "And more ...", is shown in a separate box below the table.

Hand Coded Heat	Why use numerical packages...
Meshing and Discretization with AMReX	A Block Structured Adaptive Mesh Refinement Framework
Unstructured Meshing & Discretization with MFEM	Finite Elements and Convergence
Adaptive MFEM+PUMI Workflow	MFEM with PUMI Conformal Unstructured Mesh Adaptation

And more ...

Github pages site:

<https://xsdk-project.github.io/MathPackagesTraining2021/lessons/>

Hello World (for numerical packages)

Alp Dener

Mathematics and Computer Science

Argonne National Laboratory

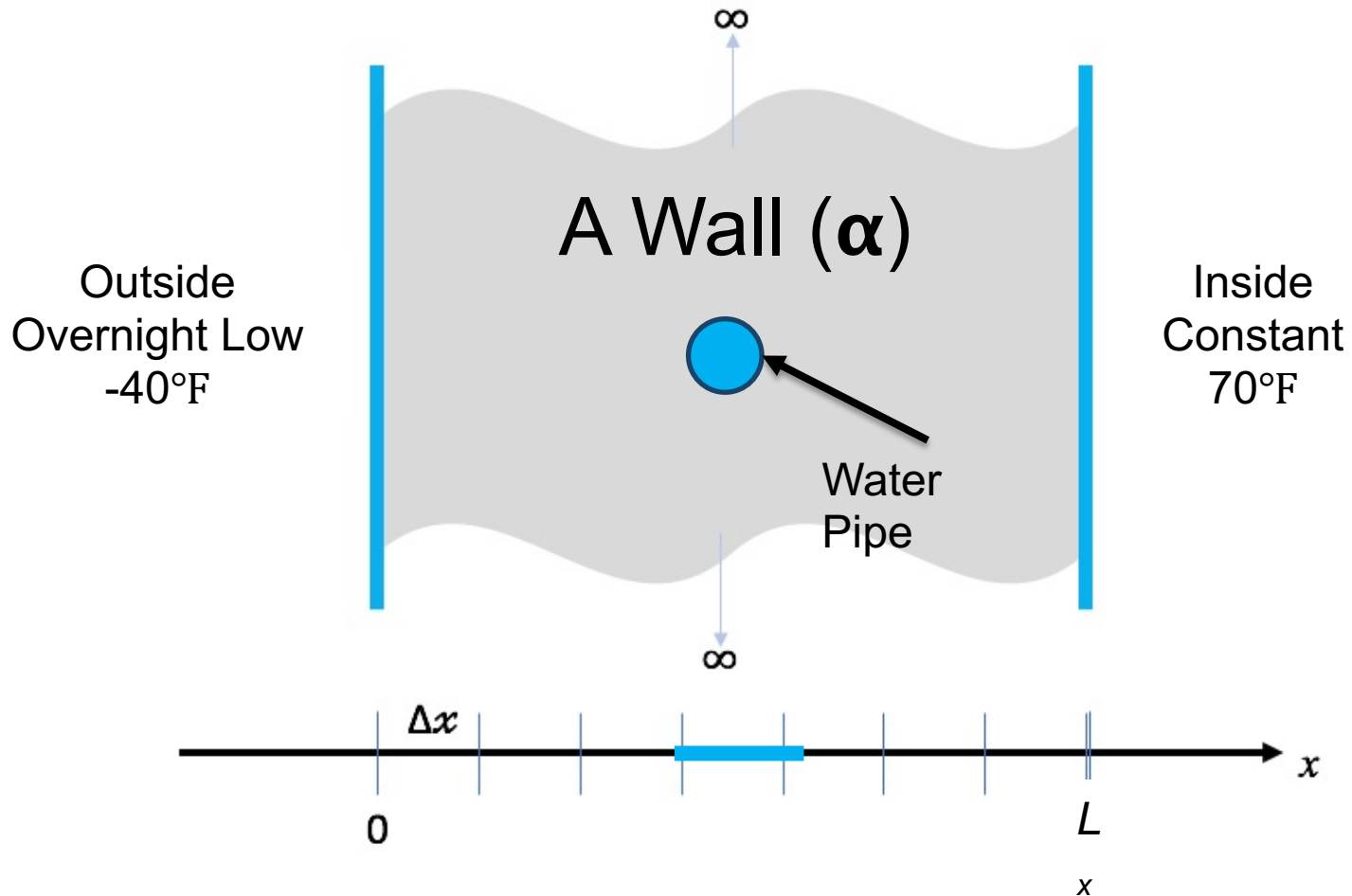
with special thanks to Mark Miller, LLNL



ATPESC Numerical Software Track



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: $u(x,0) = U(x)$

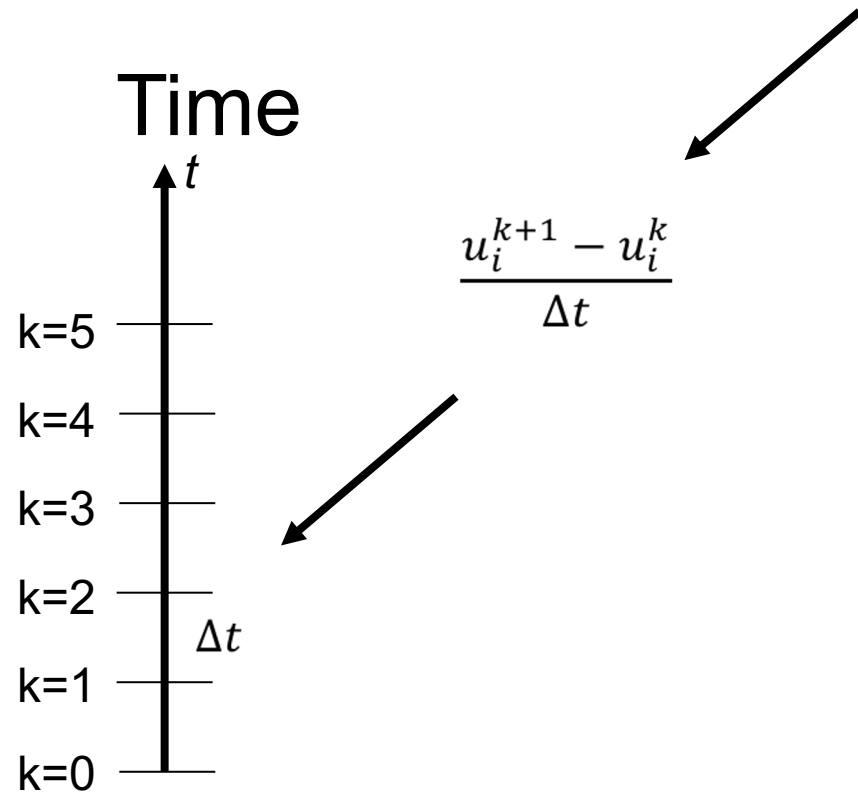
We seek a numerical software solution for $u(x,t)$ (all space & time)

Discretize: Continuous ☐ Discrete

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

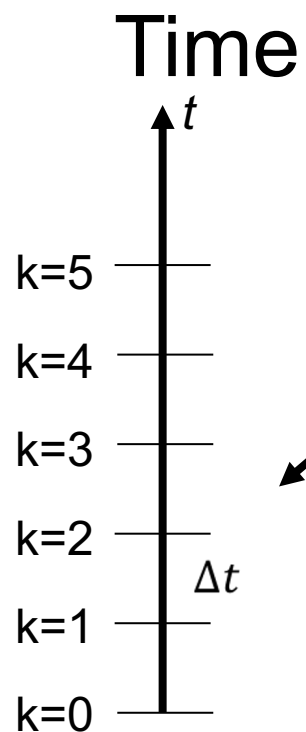
Discretize: Continuous \square Discrete

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



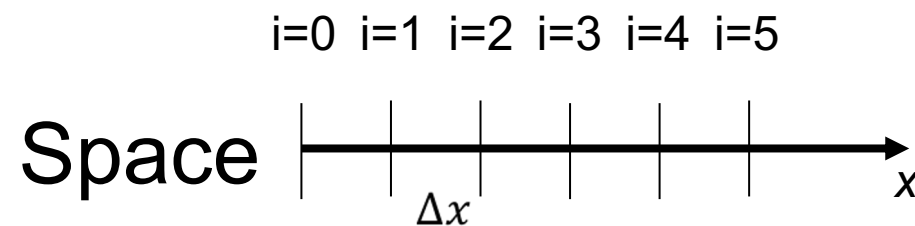
Discretize: Continuous \square Discrete

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



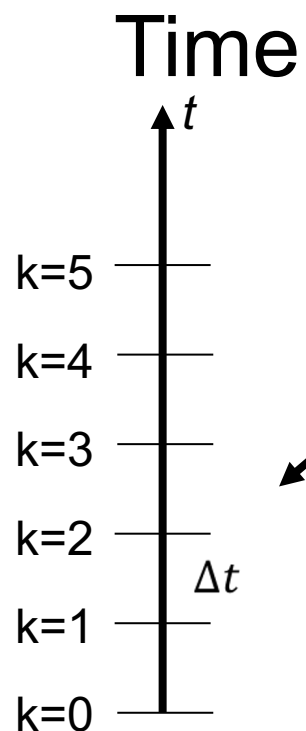
$$\frac{u_i^{k+1} - u_i^k}{\Delta t}$$

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

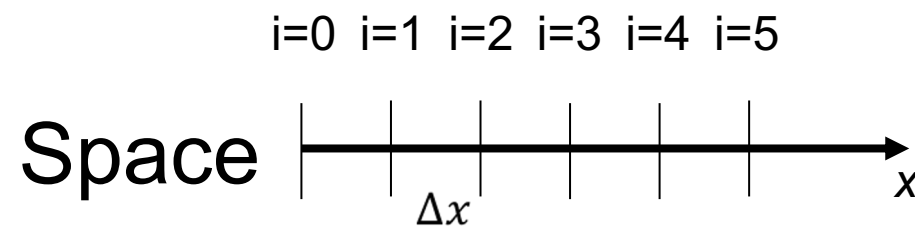


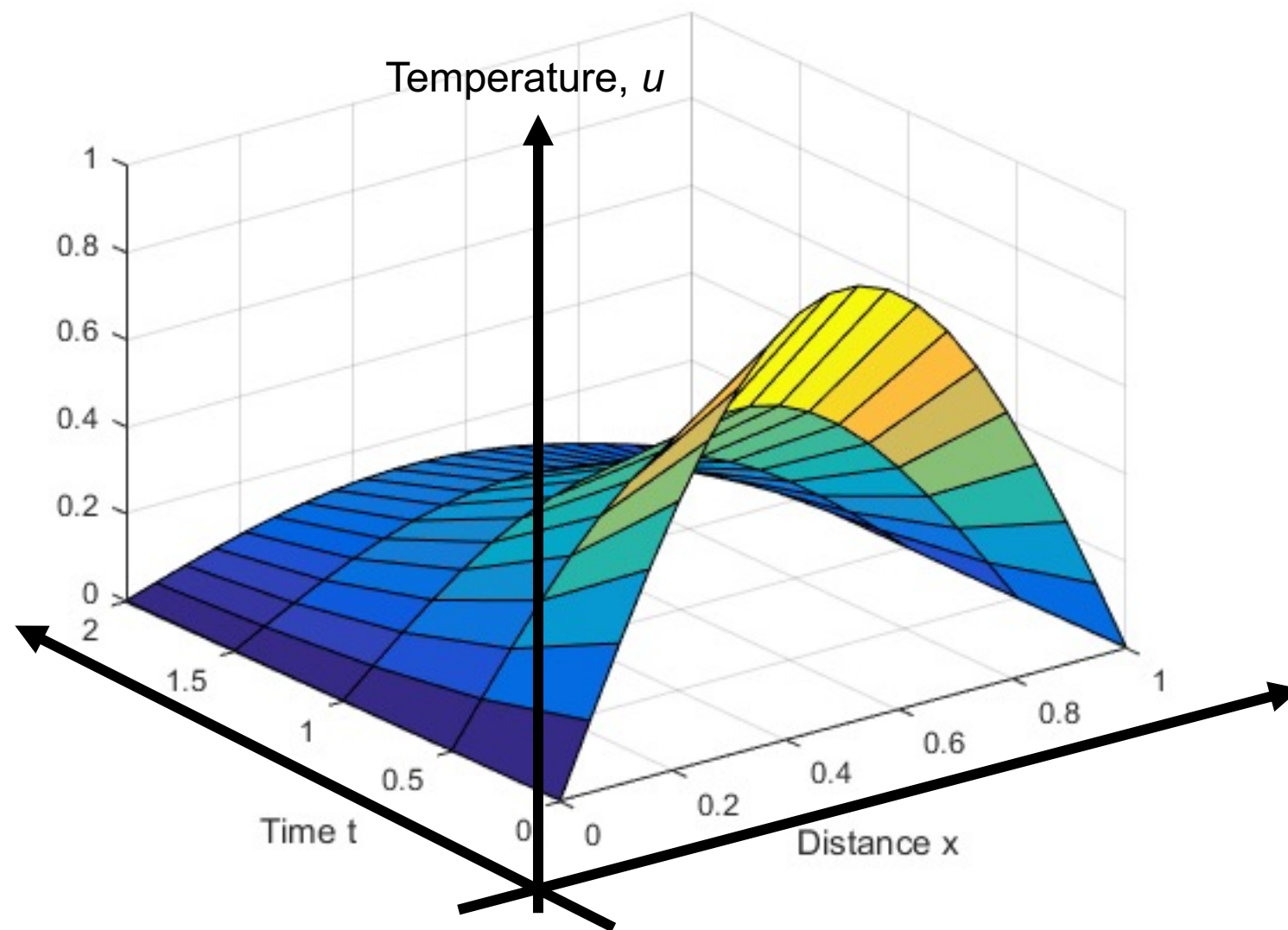
Discretize: Continuous \square Discrete

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



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





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

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

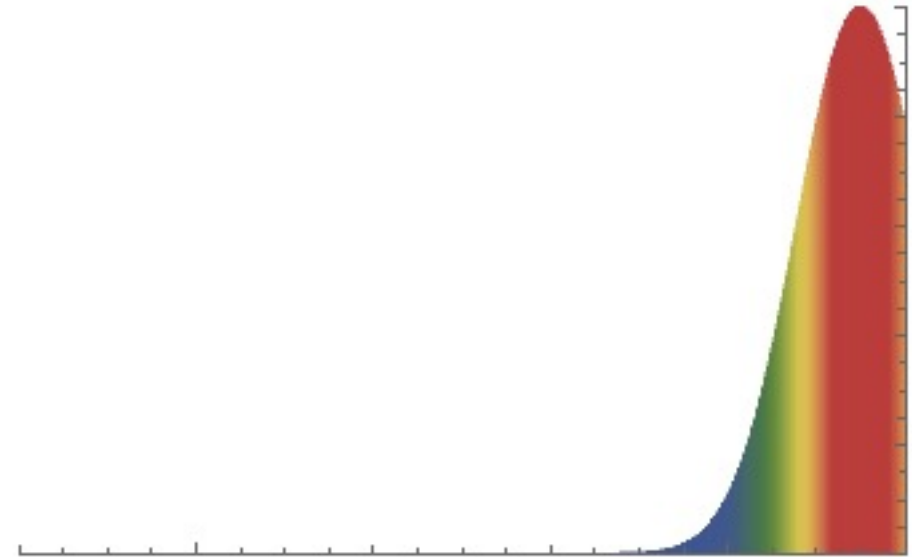
```
bool                                     // true if valid, false if not
update_solution_ftcs(
    int n,                             // number of values
    Double *uk1,                       // new values: u(i) i=0...n-1 @ t=k+1
    Double const *uk0,                 // last values: u(i) i=0...n-1 @ t=k
    Double alpha,                      // thermal diffusivity
    Double dx, Double dt,              // spacing in space, x, and time, t.
    Double bc0, Double bc1)           // boundary conditions @ x=0 & x=L
{

}
```


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, 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 developing large-scale scientific computing applications

- We can code this all from scratch because...
 - Solid wall, single material, constant diffusion coefficient
 - 1-dimension in space, uniform grid
 - Spatial derivatives via second central finite difference
 - Simple explicit time integration scheme
- Large-scale scientific computing applications need...
 - Advanced discretization tools to capture complex geometries and domains
 - Scalable linear and nonlinear solvers for challenging systems of equations
 - Sophisticated time integration schemes for stability

Simplifications hide challenges of developing large-scale scientific computing applications

- Physical and mathematical modeling
- High-performance algorithm development
- Scalable & portable implementation
- Extensibility and interoperability with external libraries
- Documentation, ease of installation, ease of use
- Sustainable open source, supported with regular updates, bug tracking/fixing

Very few possess the domain-specific, mathematics, computer science and software development expertise necessary to do it all on their own

We share expertise through numerical packages...

- **Discretization:** Structured (AMReX), Unstructured (MFEM/PUMI)
- **Systems of Equations:** Krylov solvers, preconditioners & algebraic multigrid (HYPRE & MueLu), Direct solvers (SuperLU/Strumpack), Nonlinear solvers (PETSc)
- **Time Integration** (SUNDIALS)
- **Optimization** (TAO)

Agenda (Time Zone: CDT)

<https://extremecomputingtraining.anl.gov/agenda-2021/#Track-5>

10:30 Parallel Session 1

- **ROOM FRONTIER:** Structured Discretization (with AMReX) Ann Almgren, LBL
Don Willcox, LBL
- **ROOM AURORA:** Unstructured Discretization (with MFEM/PUMI) Aaron Fisher, LLNL
Cameron Smith, RPI
- **ROOM PERLMUTTER:** Iterative Solvers & Algebraic Multigrid (with HYPRE) Sarah Osborn, LLNL
Ulrike Yang, LLNL
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack) Sherry Li, LBL
Pieter Ghysels, LBL

11:30 Break

11:45 Parallel Session 2

- **ROOM FRONTIER:** Structured Discretization (with AMReX) Ann Almgren, LBL
Don Willcox, LBL
- **ROOM AURORA:** Unstructured Discretization (with MFEM/PUMI) Aaron Fisher, LLNL
Cameron Smith, RPI
- **ROOM PERLMUTTER:** Iterative Solvers & Preconditioners (with MueLu) Christian Glusa, SNL
Graham Harper, SNL
Peter Ohm, SNL
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack) Sherry Li, LBL
Pieter Ghysels, LBL

12:45 p.m. Lunch

1:45 MAIN ROOM:

Panel Discussion: Contributing to the Numerical Package Community

Ann Almgren, LBL
Aaron Fisher, LLNL
Christian Glusa, SNL
Richard Tran Mills, ANL
Dan Reynolds, SMU
Cameron Smith, RPI
Alp Dener, ANL

2:35 Parallel Session 3

- **ROOM FRONTIER:** Nonlinear Solvers (with PETSc) Richard Tran Mills, ANL
- **ROOM AURORA:** Optimization (with TAO) Alp Dener, ANL
- **ROOM PERLMUTTER:** Time Integration (with SUNDIALS) Dan Reynolds, SMU
- **ROOM EL CAPITAN:** Iterative Solvers & Algebraic Multigrid (with HYPRE) Sarah Osborn, LLNL
Ulrike Yang, LLNL

3:25 Break

3:40 Parallel Session 4

- **ROOM FRONTIER:** Nonlinear Solvers (with PETSc) Richard Tran Mills, ANL
- **ROOM AURORA:** Optimization (with TAO) Alp Dener, ANL
- **ROOM PERLMUTTER:** Time Integration (with SUNDIALS) Dan Reynolds, SMU
- **ROOM EL CAPITAN:** Direct Solvers (with SuperLU/Strumpack) Sherry Li, LBL
Pieter Ghysels, LBL

4:35 Working with Numerical Packages in Practice Ann Almgren, LBL

5:00 Adjourn

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

Sample Schedules (Time Zone: CDT)

<https://xsdk-project.github.io/MathPackagesTraining2021/agenda/>

	Topics	S1 10:30am	S2 11:45am	S3 02:35pm	S4 03:40pm
Discretization	Structured (AMReX)	Frontier	Frontier		
	Unstructured (MFEM/PUMI)	Aurora	Aurora		
Linear Solvers	Iterative Solvers & Algebraic Multigrid (HYPRE)	Perlmutter		El-Capitan	
	Iterative Solvers & Preconditioners (MueLu)		Perlmutter		
	Direct Solvers (SuperLU/Strumpack)	El-Capitan	El-Capitan		El-Capitan
Nonlinear Solvers	Nonlinear Solvers (PETSc)			Frontier	Frontier
Outer Loop Tools	Optimization (TAO)			Aurora	Aurora
	Time Integration (SUNDIALS)			Perlmutter	Perlmutter

Sample 1: Balanced

- 10:30am – Structured Discretization (with AMReX)
- 11:34am – Iterative Solvers & Preconditioners (with MueLu)
- 02:35pm – Nonlinear Solvers (with PETSc)
- 03:40pm – Time Integration (with SUNDIALS)

Sample 3: Solvers

- 10:30am – Direct Solvers (with SuperLU/Strumpack)
- 11:34am – Iterative Solvers & Preconditioners (with MueLu)
- 02:35pm – Iterative Solvers & Algebraic Multigrid (with HYPRE)
- 03:40pm – Nonlinear Solvers (with PETSc)

Sample 2: Discretization

- 10:30am – Unstructured Discretization (with MFEM/PUMI)
- 11:34am – Structured Discretization (with AMReX)
- 02:35pm – Iterative Solvers & Algebraic Multigrid (with HYPRE)
- 03:40pm – Optimization (with TAO)

Sample 4: Outer Loop Tools

- 10:30am – Unstructured Discretization (with MFEM/PUMI)
- 11:34am – Direct Solvers (with SuperLU/Strumpack)
- 02:35pm – Optimization (with TAO)
- 03:40pm – Time Integration (with SUNDIALS)



CASC

Center for Applied
Scientific Computing



**Lawrence Livermore
National Laboratory**

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