Introduction to Numerical Software

Presented to
ATPESC 2021 Participants

Ulrike Meier Yang
Lawrence Livermore National Laboratory

Alp Dener
Argonne National Laboratory

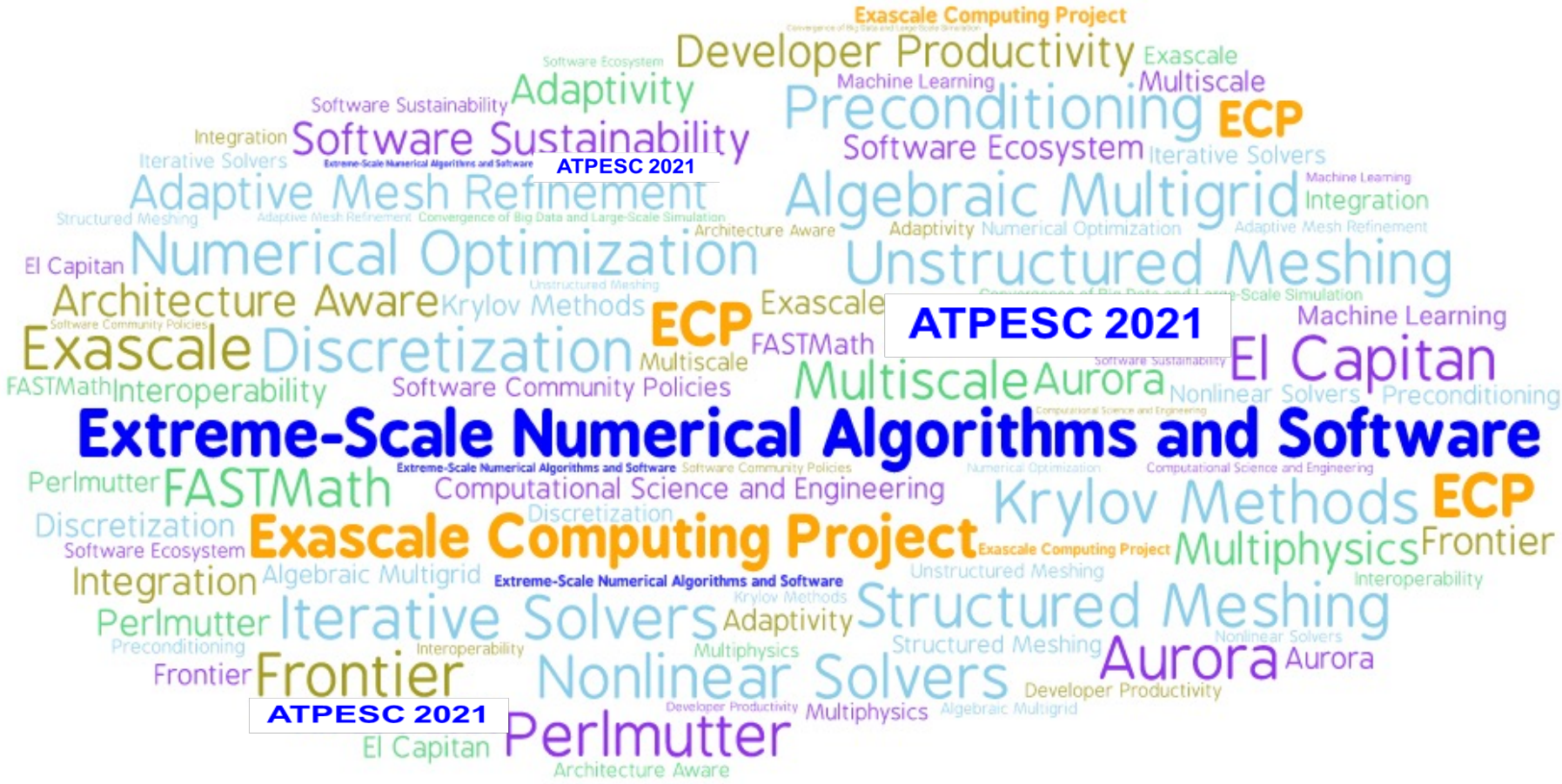
Date 08/10/2021

U.S. DEPARTMENT OF ENERGY | Office of Science

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)	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 Peter 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)

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

Mix-n-Match topics to your interests

See Synopses from Agenda

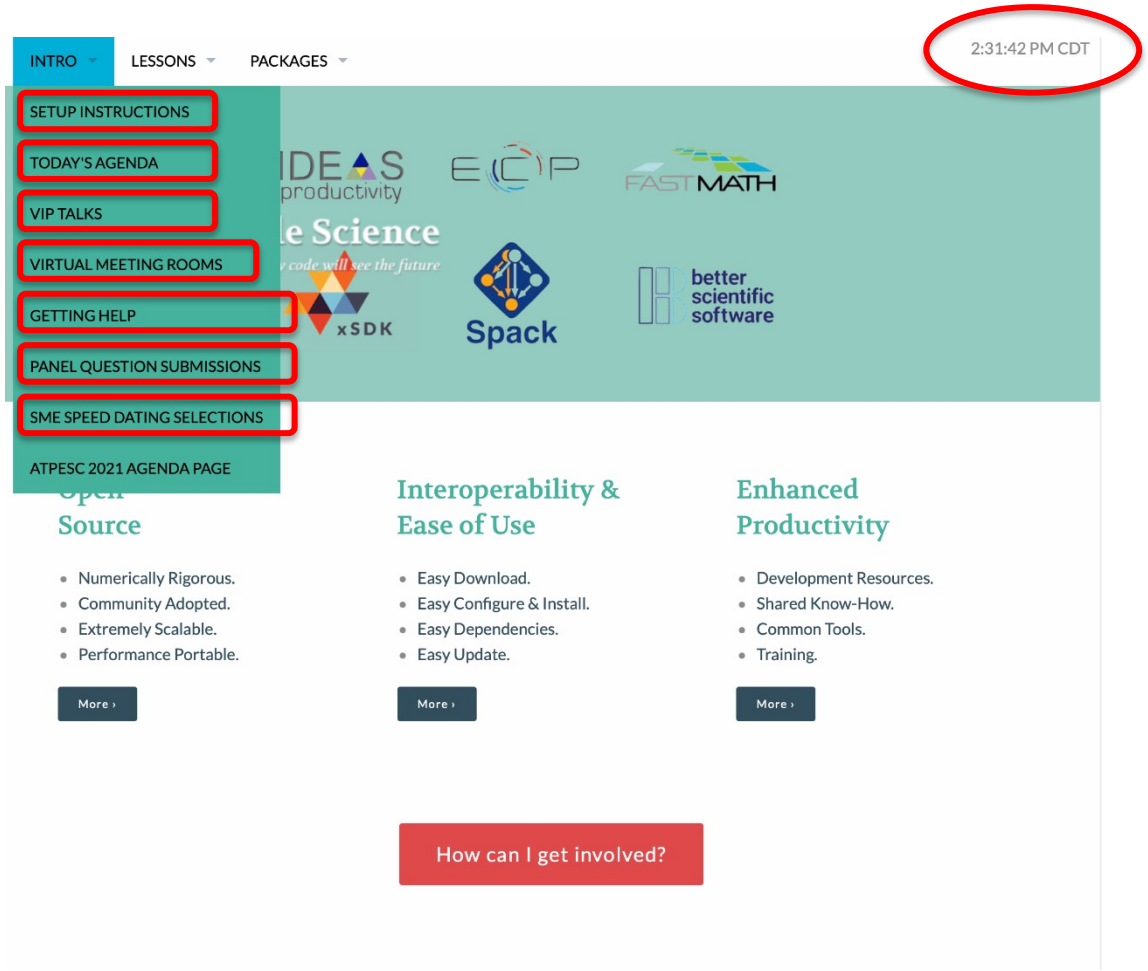
#1
- **Structured Discretization** (AMReX)
- **Unstructured Discretization** (MFEM/PUMI)
- **Iterative Solvers & Preconditioners** (hypre)
- **Direct Solvers** (SuperLU/Strumpack)

#2
- **Structured Discretization** (AMReX)
- **Unstructured Discretization** (MFEM/PUMI)
- **Iterative Solvers & Preconditioners** (Trilinos/MueLU)
- **Direct Solvers** (SuperLU/Strumpack)

#3
- **Nonlinear Solvers** (PETSc)
- **Optimization** (TAO)
- **Time Interation** (SUNDIALS)
- **Iterative Solvers & Preconditioners** (hypre)

#4
- **Nonlinear Solvers** (PETSc)
- **Optimization** (TAO)
- **Time Interation** (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

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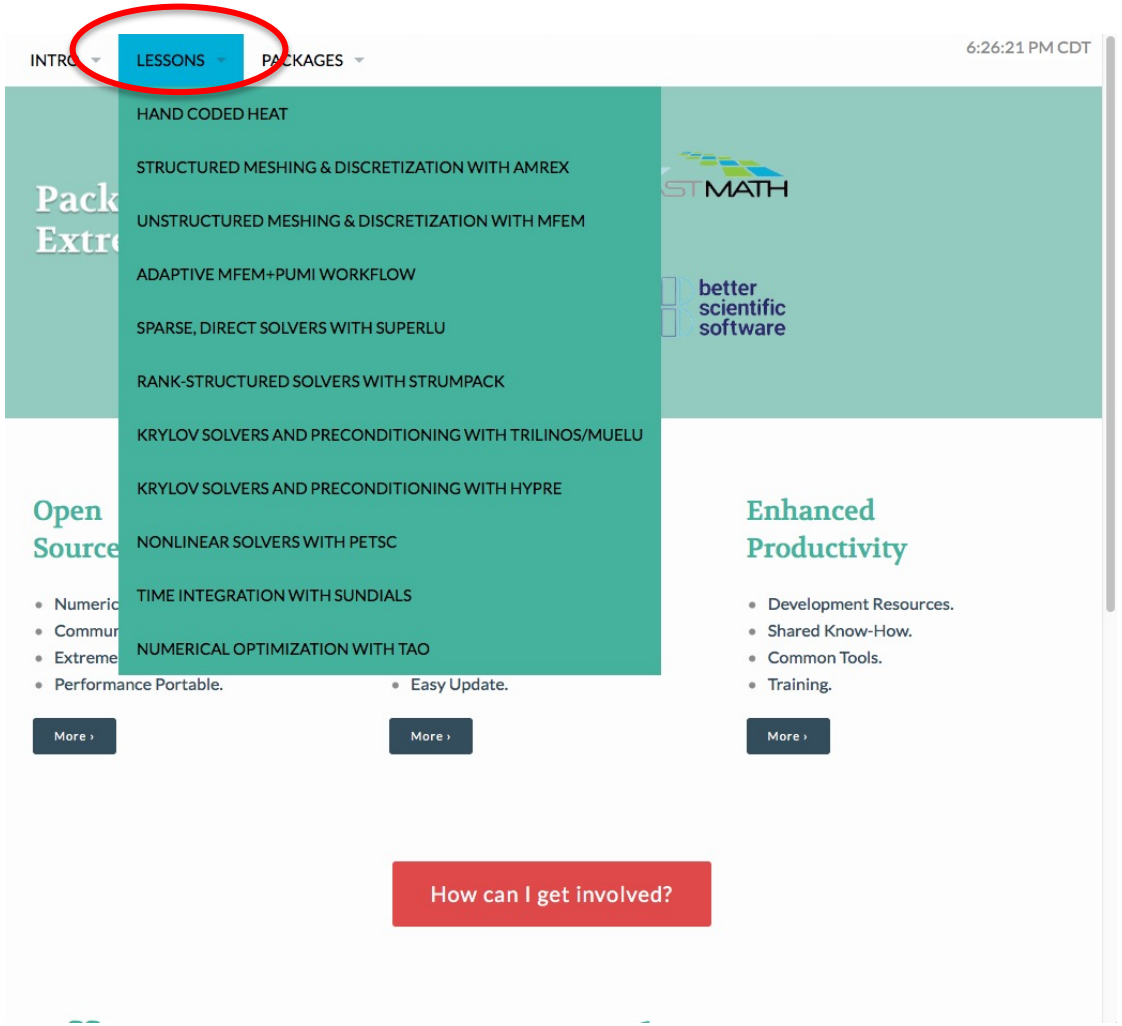
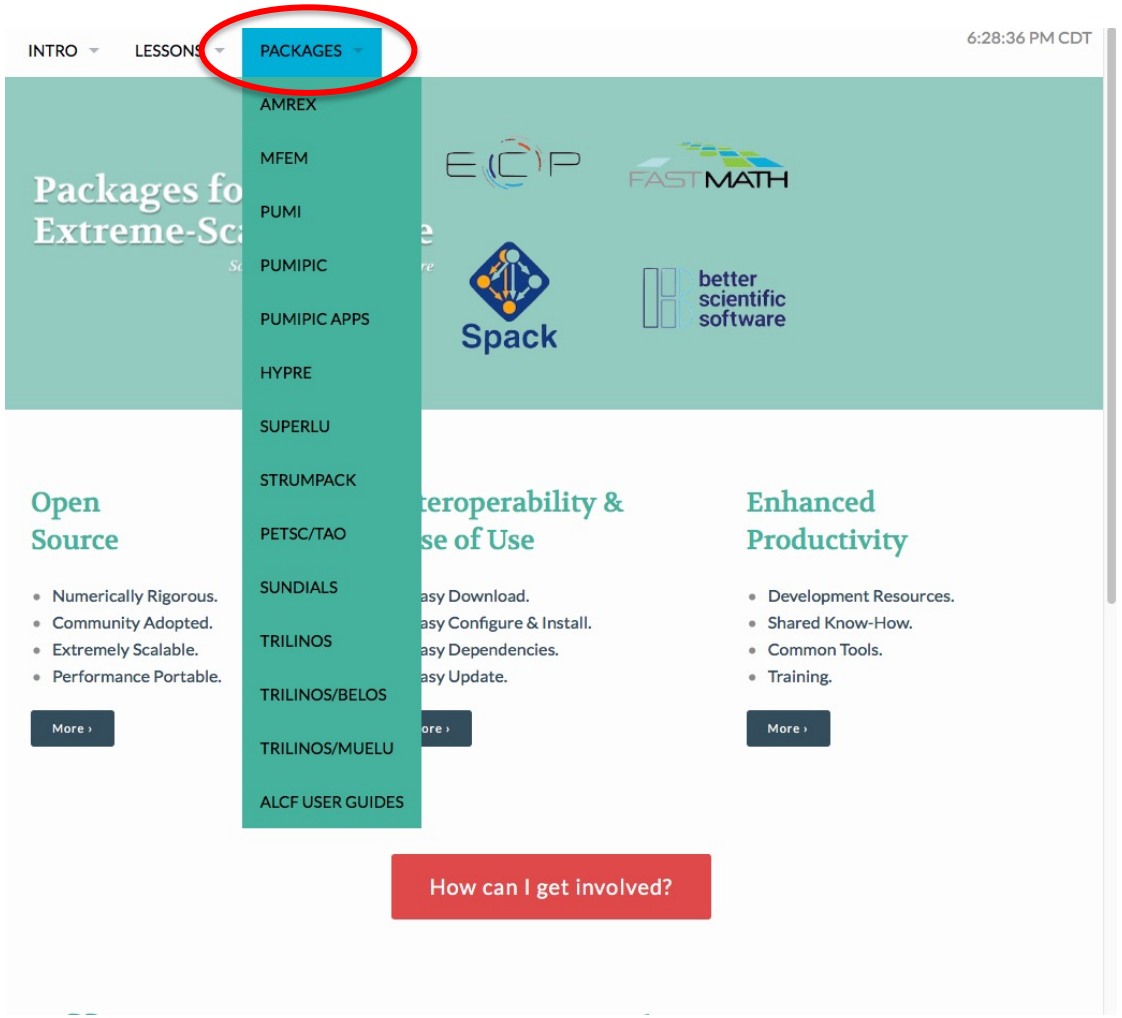
https://xsdk-project.github.io/MathPackagesTraining2021/



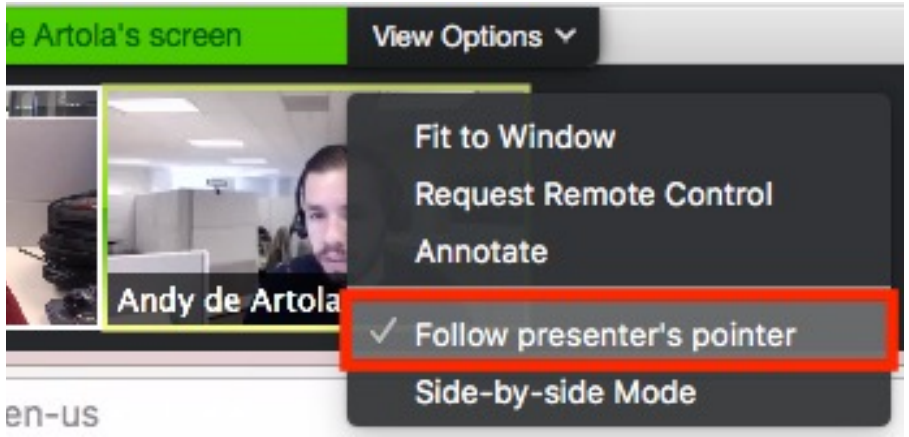
- Hands-on Lessons

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



- Hands-on Lessons
- Packages

Using Zoom

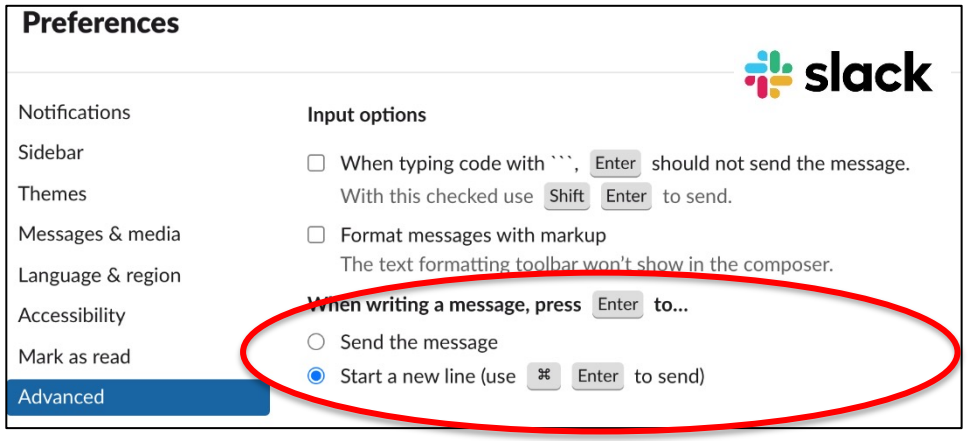


- Please stay muted unless asked to un-mute
- We're using Slack for chat, not Zoom's chat
- "Follow presenter's pointer" might be helpful
  - Available only if NOT in "Fit to Window" mode
- Download slide PDFs from ATPESC web site (agenda page) ahead of presentation as a backup
- Other useful tips
 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

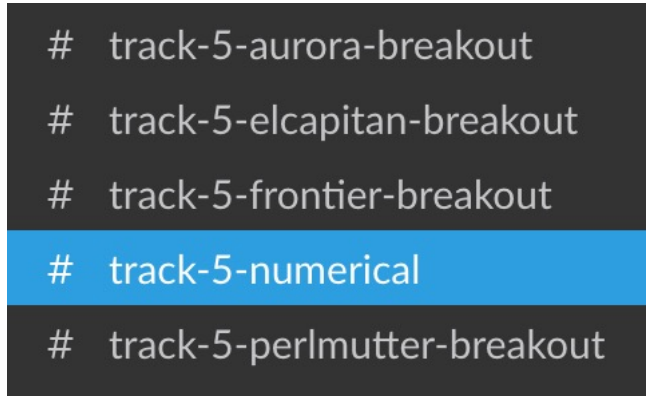
Using Slack

- 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 <u>on the current presentation topic only</u>
    - 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



slack ATPESC 2021 AUGUST 1–13



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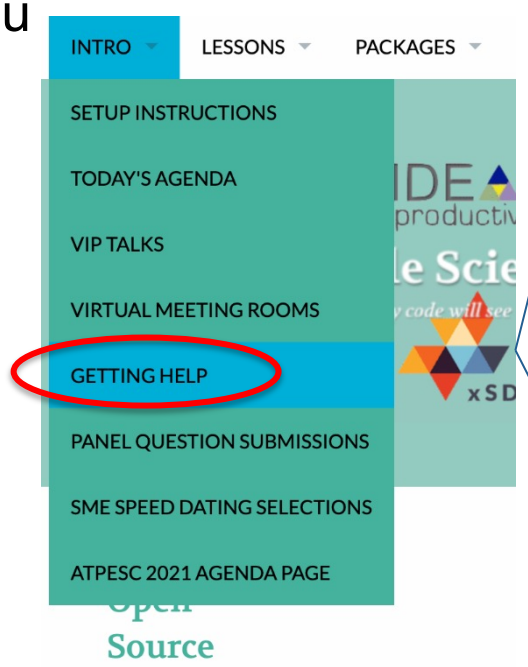
Getting help (“Getting help” menu item)

- **#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

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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

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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

ECP EXASCALE COMPUTING PROJECT

The ATPESC Team 2021

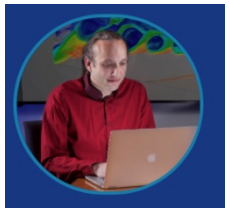
Extreme-scale numerical algorithms and software
Integrated lectures and hands-on examples, panel session, individual discussions … and more!

Alp Dener, ANL

Cameron Smith, RPI

David Gardner, LLNL

Ann Almgren, LBL


Aaron Fisher, LLNL

Christian Glusa, SNL

Richard Mills, ANL

Don Willcox, LBL

Ulrike Yang, LLNL

Satish Balay, ANL

Pieter Ghysels, LBL

Sherry Li, LBL

Dan Reynolds, SMU

Thank you to Peter Ohm and Graham Harper, SNL

Additional contributors to gallery of highlights:

Various HPC package developers

Sarah Osborn, LLNL

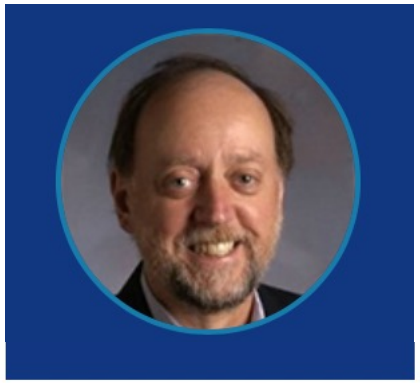
Mark Shephard, RPI

Lois Curfman McInnes, ANL

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 Benchmarker, 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]

ECP EXASCALE COMPUTING PROJECT

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

https://exascaleproject.org

https://fastmath-scidac.llnl.gov

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

Community efforts: Join us!

https://xsdk.info

https://bssw.io

https://e4s.io

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

https://ideas-productivity.org

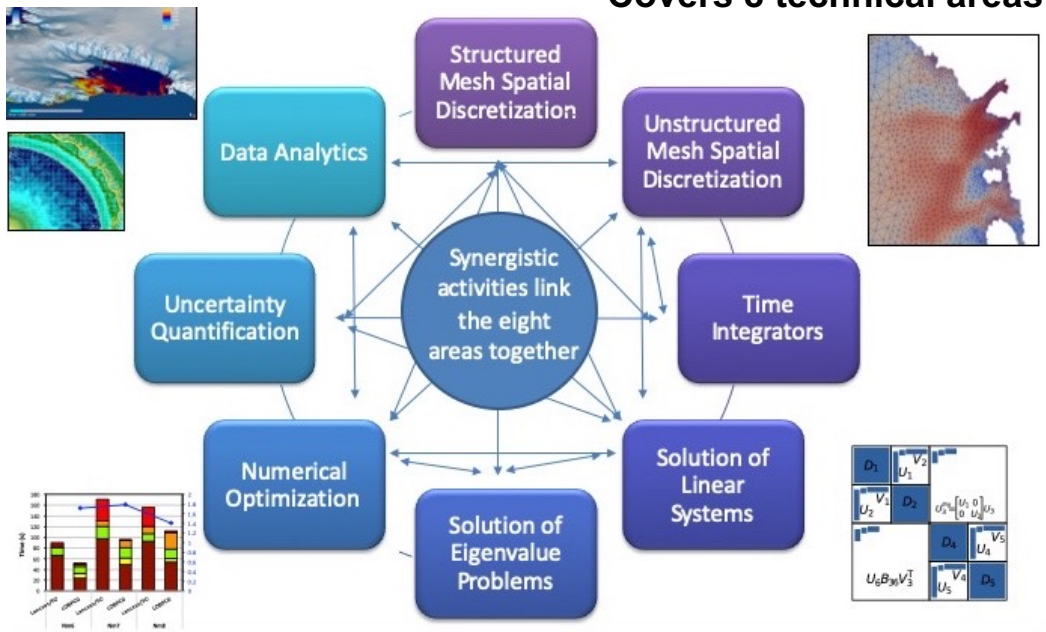
- IDEAS Software Productivity Project
- Better Scientific Software Community

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

FASTMath: Frameworks, Algorithms & Scalable Technologies for Mathematics

https://scidac-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

50+ researchers from 5 DOE labs and 5 universities

Berkeley Lab, Argonne National Laboratory, Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, Sandia National Laboratories

CU Boulder, USC, MIT, Rensselaer, SMU

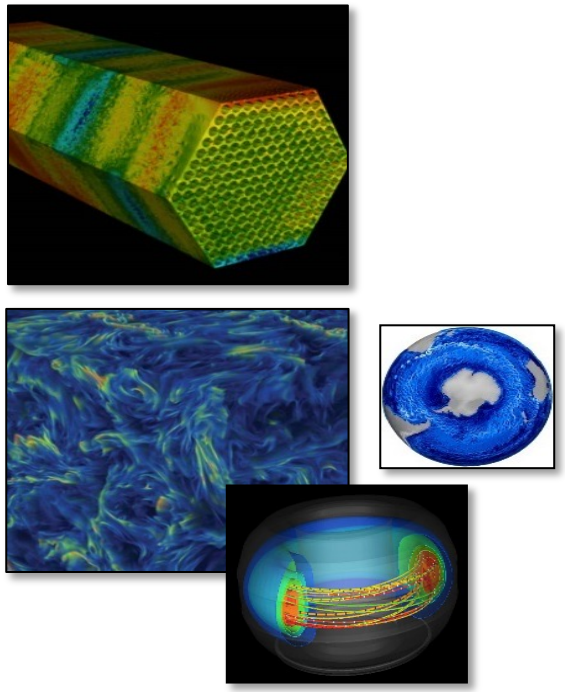
100's of person years of experience building math software

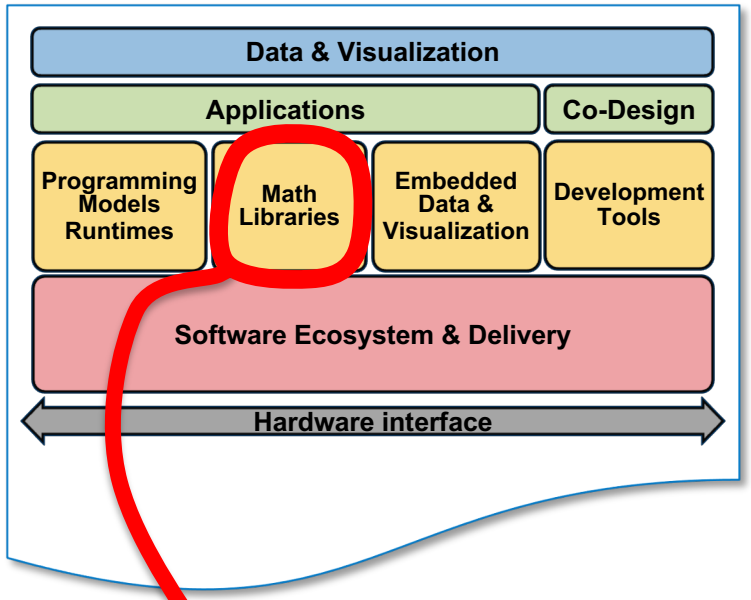
SuperLU, AMReX, sundials, ZOLTAN, mfem, PETSc, hypre high performance preconditioners, UQTk, symPACK, PUMI Parallel Unstructured Mesh Infrastructure, Trilinos, Albany, DAKOTA

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

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

Application Development	Software Technology	Hardware and Integration
Science and mission applications	Scalable software stack	Relationships: facilities with AD/ST, with vendors





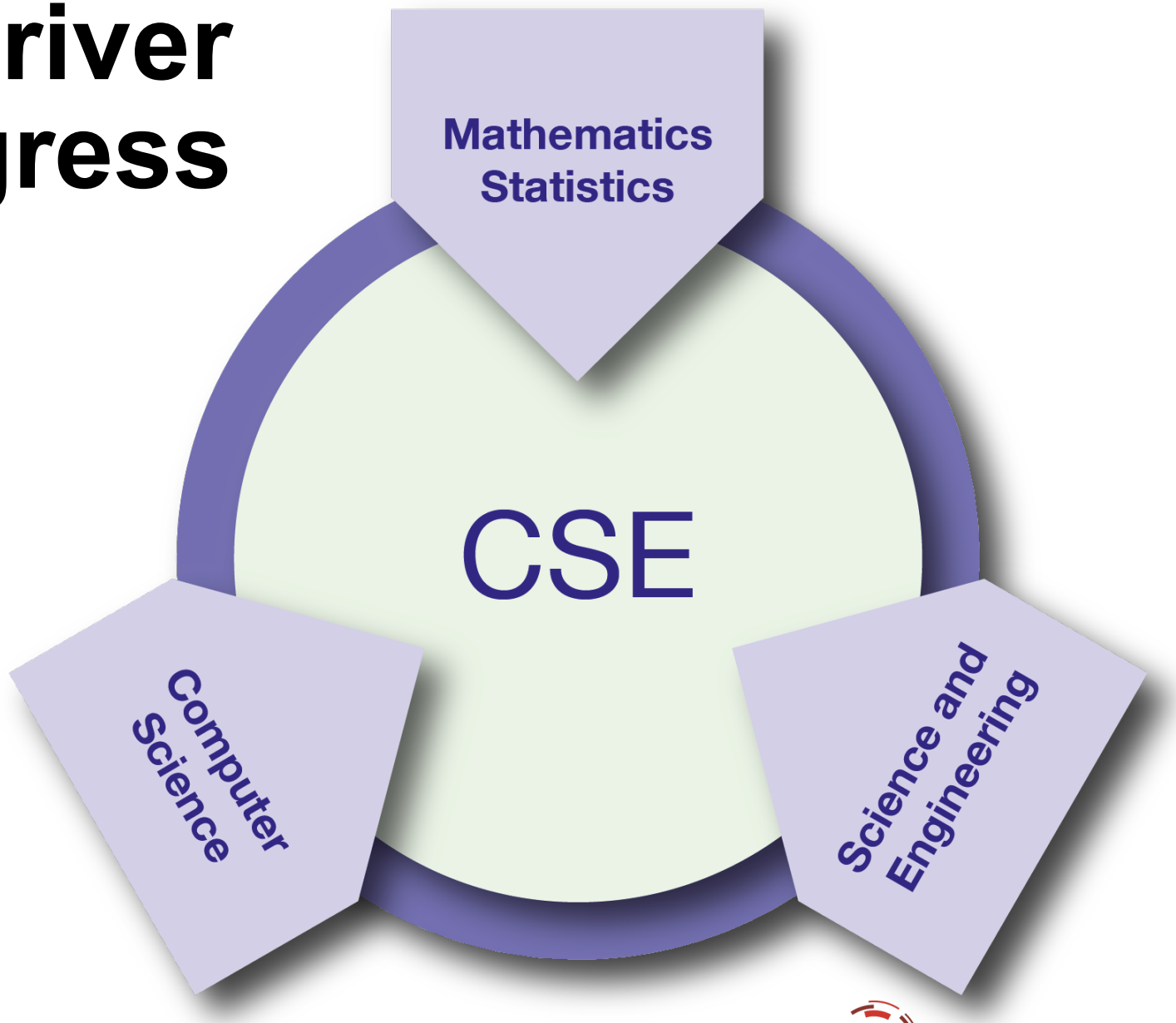
Emphasis for this presentation

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



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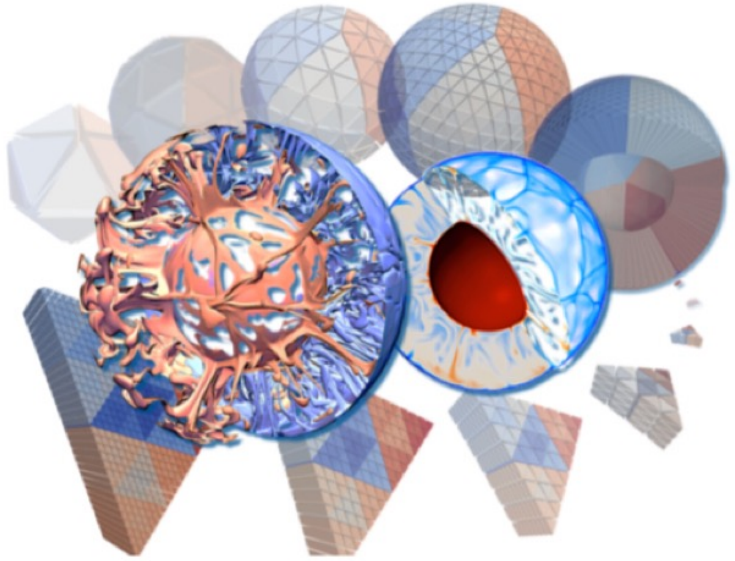
Rapidly expanding role of CSE: New directions toward predictive science

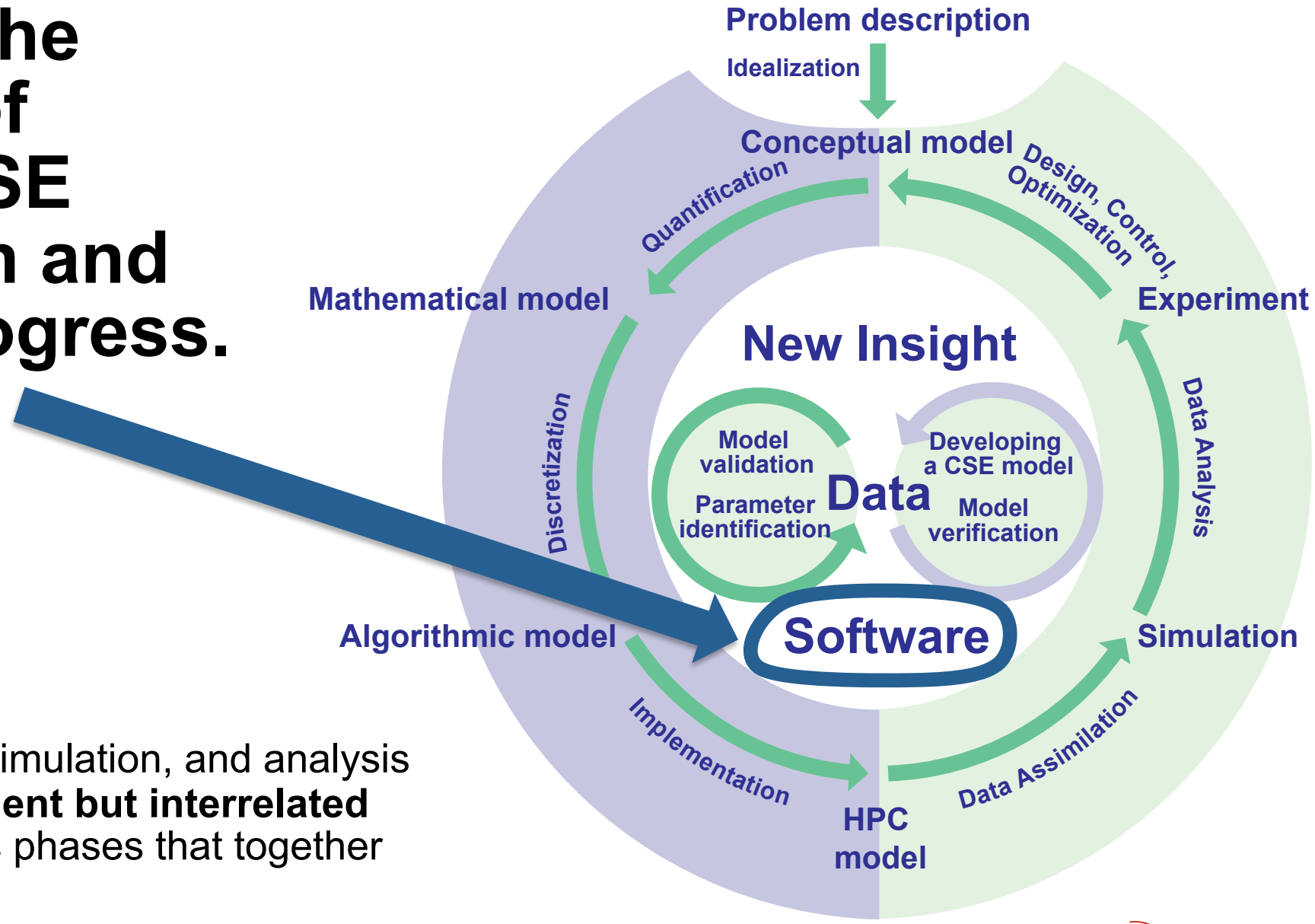
- Mathematical methods and algorithms
- CSE and HPC: Ubiquitous parallelism
- CSE and the data revolution
- CSE software
- CSE education & workforce development



Research and Education in Computational Science & Engineering

U. Rüde, K. Willcox, L.C. McInnes, H. De Sterck, G. Biros, H. Bungartz, J. Corones, 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

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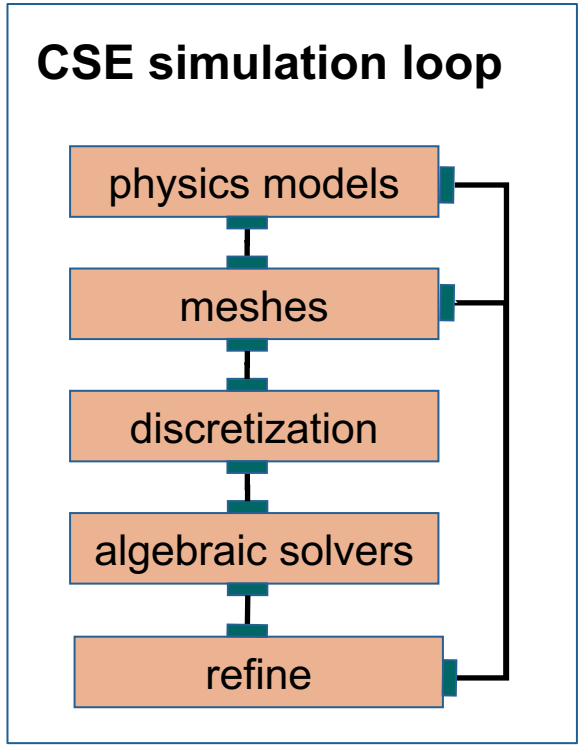
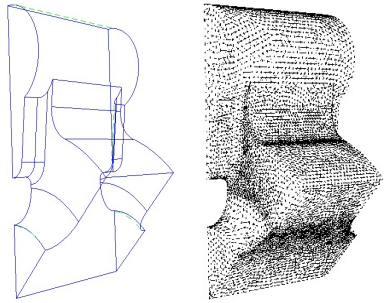
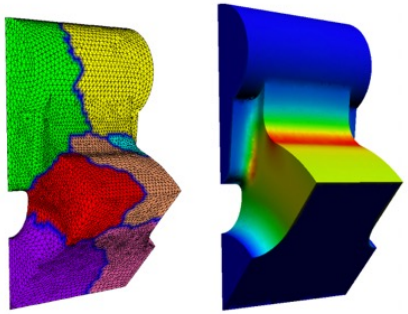
CSE simulation starts with a forward simulation that captures the physical phenomenon of interest

- 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







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

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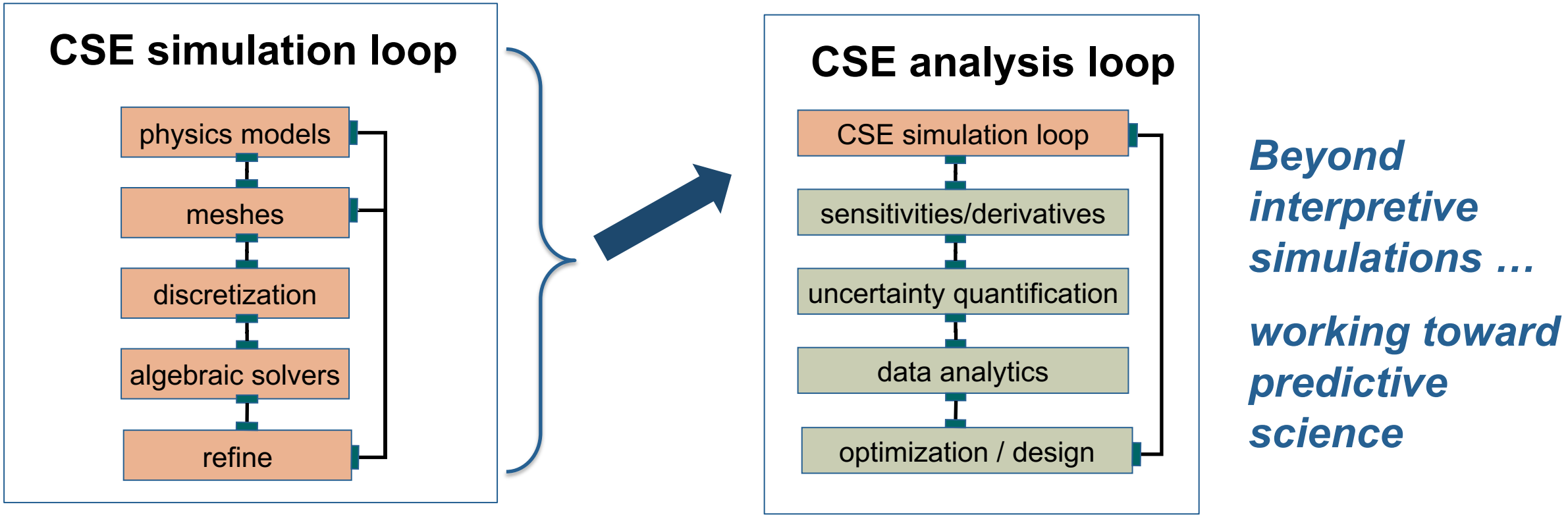
CSE analysis builds on the CSE simulation loop … and relies on even more numerical algorithms and software



Beyond interpretive simulations …

working toward predictive science

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

ECP EXASCALE COMPUTING PROJECT

First consider a very simple example

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

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

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

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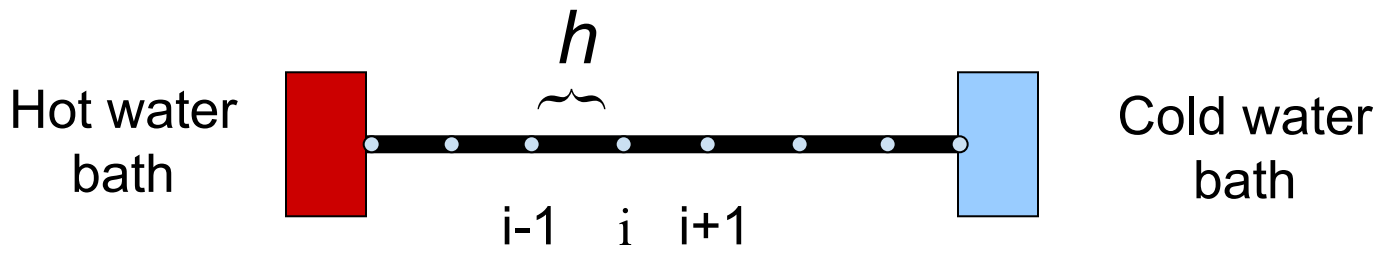
The first step is to discretize the equations

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

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

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



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Then you can solve for the unknowns T_i

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

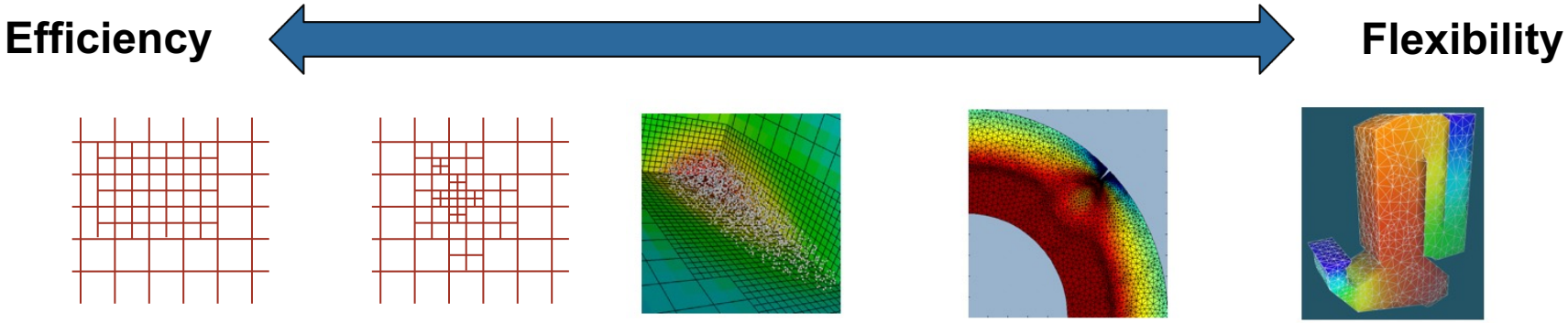
$$\begin{pmatrix} 2 & -1 & 0 & \ldots\ldots\ldots\ldots & 0 \\ -1 & 2 & -1 & 0 & \ldots\ldots\ldots & 0 \\ 0 & -1 & 2 & -1 & 0 & \ldots. & 0 \\ & & & \ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ . \\ T_{n-1} \end{pmatrix}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

- Visualize and analyze the results

ECP EXASCALE COMPUTING PROJECT

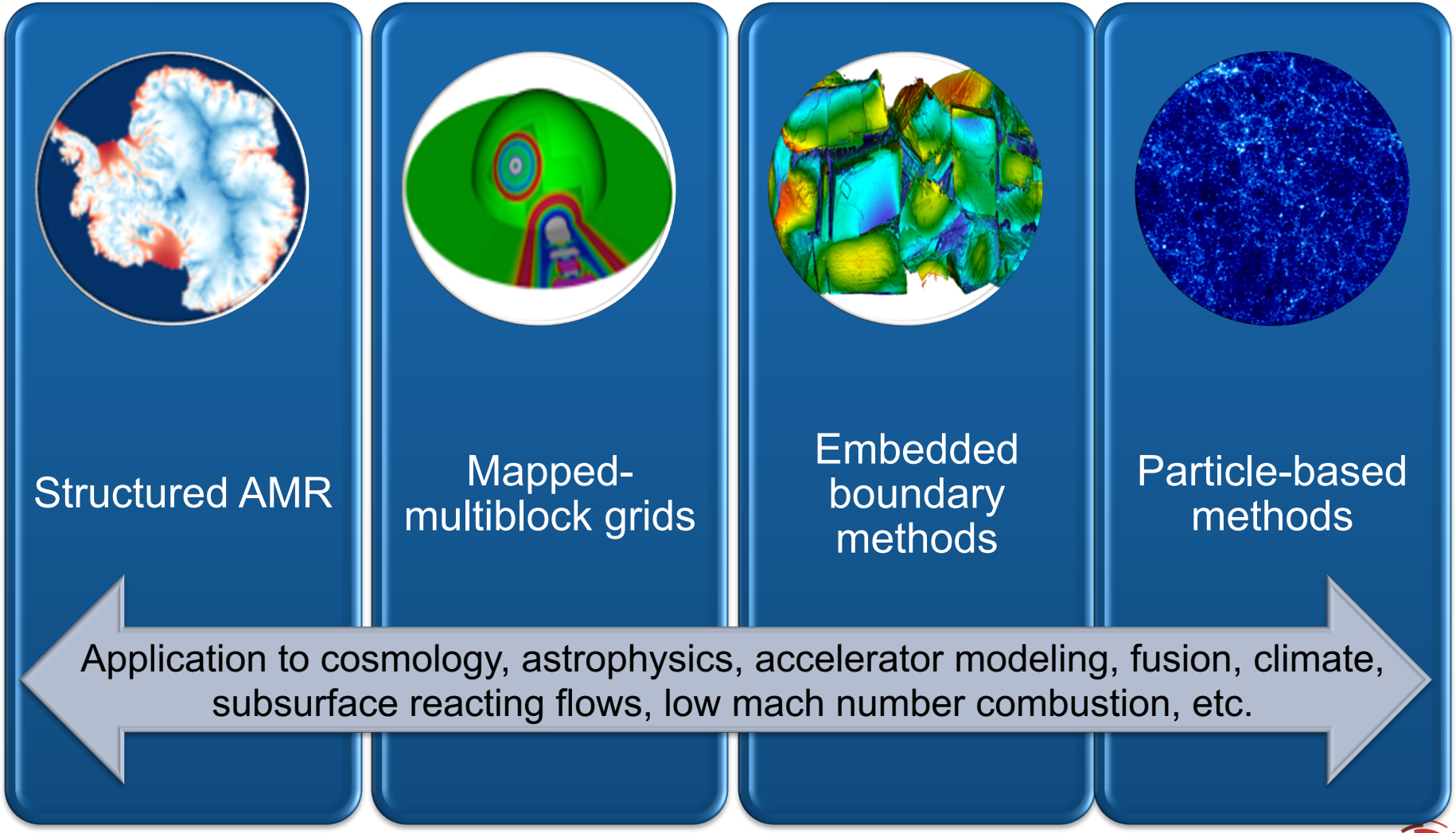
As problems get more complicated, so do the steps in the process

- Different discretization strategies exist for differing needs



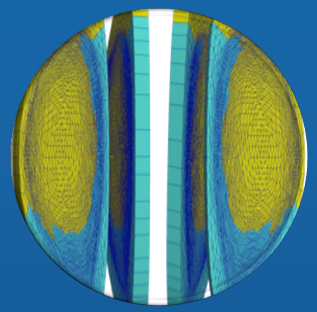
- Most problems are time dependent and nonlinear
  - Need higher algorithmic levels than linear solvers
- Increasingly combining multiple physical processes
  - Interactions require careful handling
- Goal-oriented problem solving requires optimization, uncertainty quantification

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



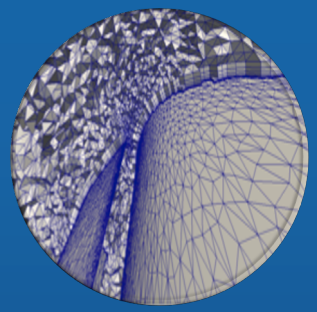
ECP EXASCALE COMPUTING PROJECT

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

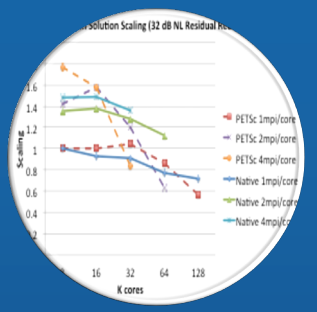


Parallel mesh infrastructures

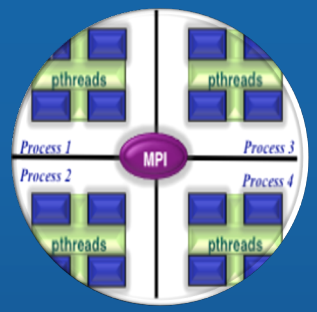
Dynamic load balancing



Mesh adaptation and quality control



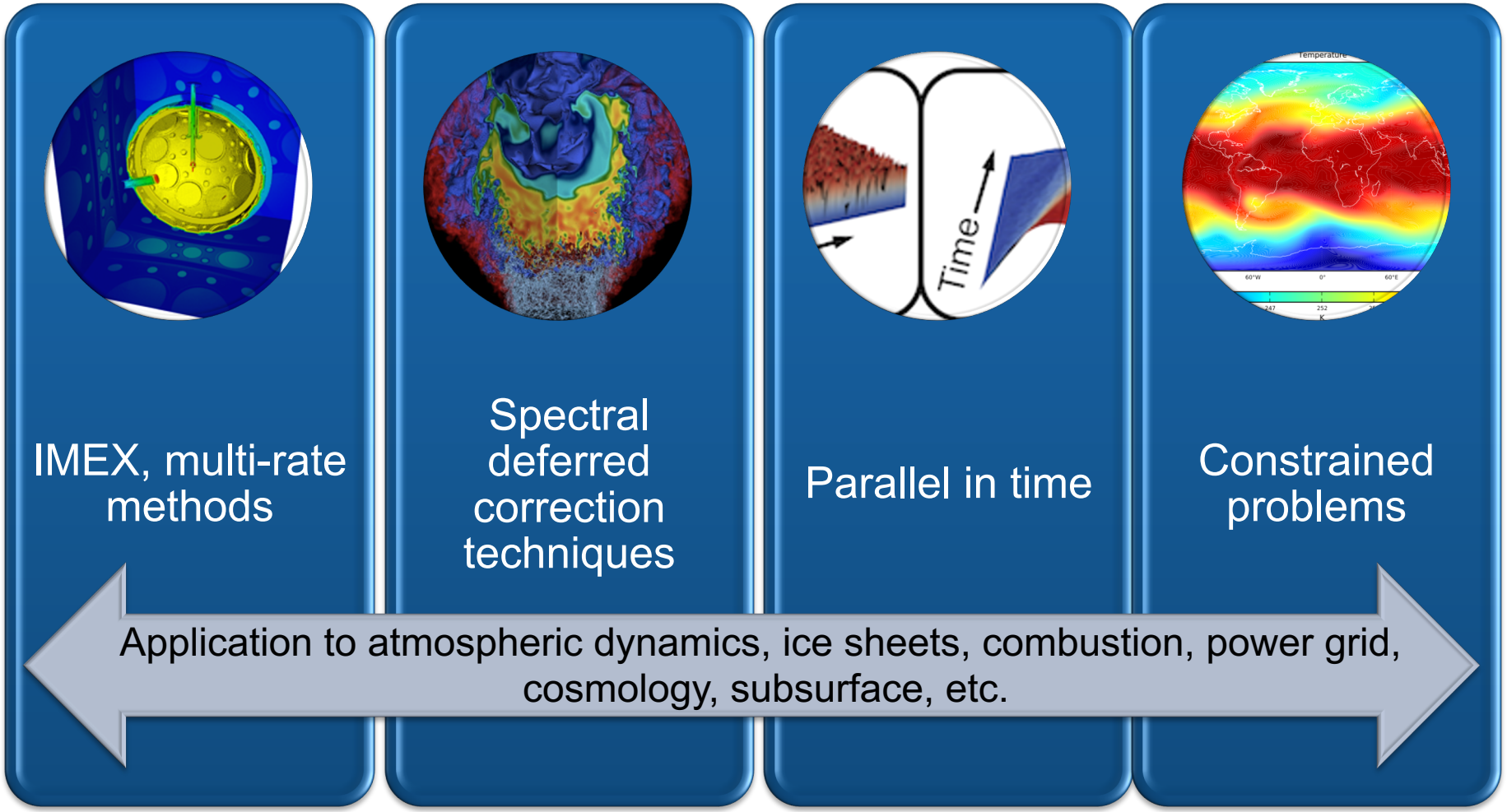
Parallel performance on unstructured meshes



Architecture aware implementations

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

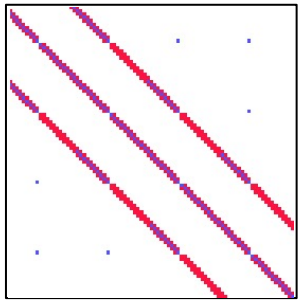
Time discretization methods provide efficient and robust techniques for stiff implicit, explicit and multi-rate systems

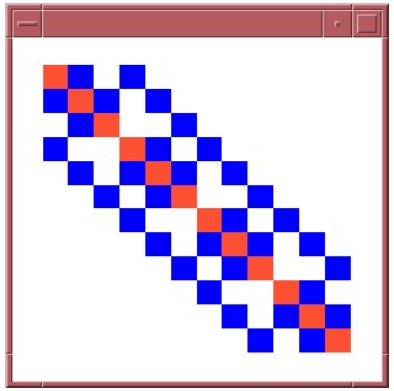


ECP EXASCALE COMPUTING PROJECT

As problems grow in size, so do corresponding discrete systems

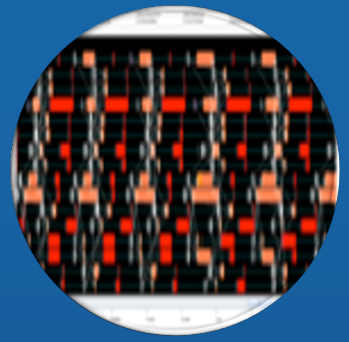
- Targeting applications with billions grid points and unknowns
- Most linear systems resulting from these techniques are LARGE and sparse
- Often most expensive solution step
- Solvers:
  - Direct methods (e.g., Gaussian Elimination)
  - Iterative methods (e.g., Krylov Methods)
    - Preconditioning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





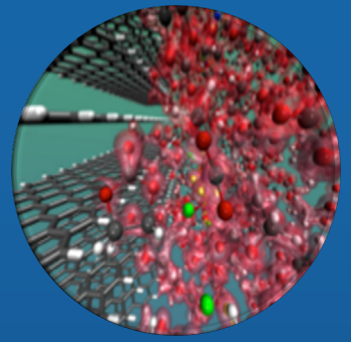
ECP EXASCALE COMPUTING PROJECT

Research on algebraic systems provides key solution technologies to applications

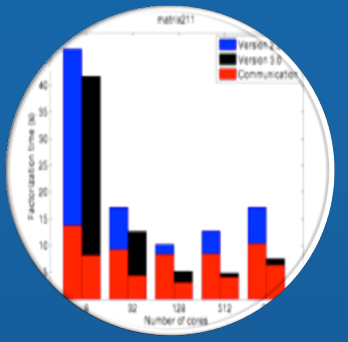


Linear system solution using direct and iterative solvers

Nonlinear system solution using acceleration techniques and globalized Newton methods



Eigensolvers using iterative techniques and optimization



Architecture aware implementations

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

DOE HPC Roadmap to Exascale Systems

FY 2012	FY 2016	FY 2018	FY 2021	FY 2022	FY 2023

ORNL
Cray/AMD/NVIDIA

ORNL
IBM/NVIDIA

ANL
IBM BG/Q

ANL
Cray/Intel KNL

LBNL
Cray/Intel Xeon/KNL

LBNL
HPE/AMD/NVIDIA

ORNL
HPE/AMD

ANL
HPE/Intel

Exascale Systems

LLNL
IBM BG/Q

LANL/SNL
Cray/Intel Xeon/KNL

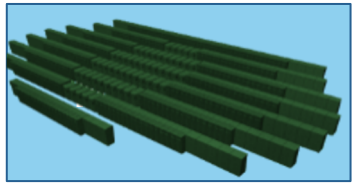
LLNL
IBM/NVIDIA

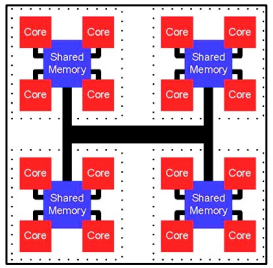
LANL/SNL
HPE/TBD

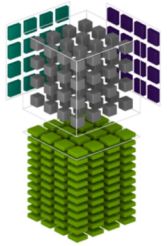
LLNL
HPE/AMD

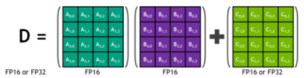
Disruptive changes in HPC architectures

- **Extreme levels of concurrency**
  - Increasingly deep memory hierarchies
  - Very high node and core counts
- **Additional complexities**
  - Hybrid architectures
  - GPUs, multithreading, manycore
  - Relatively poor memory latency and bandwidth
  - Challenges with fault resilience
  - Must conserve power – limit data movement
  - New (not yet stabilized) programming models
  - Etc.









- **Research advances: On-node and inter-node capabilities**
  - Reduce communication and synchronization
  - Increase concurrency
  - Address memory footprint
  - Enable large communication/computation overlap
  - Use GPUs and multithreading
  - Compare task and data parallelism
  - Low-level kernels for vector operations that support hybrid programming models
  - Mixed precision (leverage compute power available in low-precision tensor cores)
  - Etc.

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)
  - What are Interoperable Software Libraries? Introducing the xSDK

Broad range of HPC numerical software

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

- ★ **AMReX** – https://github.com/AMReX-codes/amrex
- ★ **Chombo** - https://commons.lbl.gov/display/chombo
- **Clawpack** - http://www.clawpack.org
- ★ **Deal.II** - https://www.dealii.org
- **FEniCS** - https://fenicsproject.org
- ★ **hypre** - http://www.llnl.gov/CASC/hypre
- **libMesh** - https://libmesh.github.io
- ★ **MAGMA** - http://icl.cs.utk.edu/magma
- ★ **MFEM** - http://mfem.org/
- ★ **PETSc/TAO** – http://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 EXASCALE COMPUTING PROJECT

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

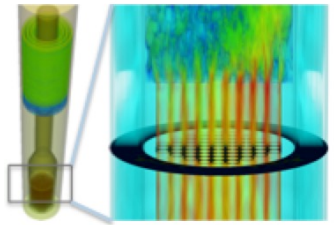
hypre high performance preconditioners
PETSc
TAO
TRILINOS
STRUMPACK
MFEM
SuperLU
sundials
MAGMA
ARBORX
PLASMA
DTK
ECP SLATE ICL
FFTX
heFFTe
libEnsemble
Ginkgo
TASMANIAN

ECP EXASCALE COMPUTING PROJECT

Multiphysics: A primary motivator for exascale

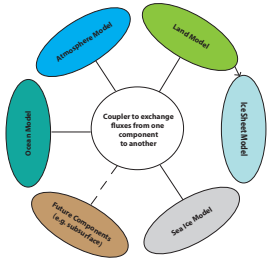
Multiphysics: greater than 1 component governed by its own principle(s) for evolution or equilibrium

- Also: broad class of coarsely partitioned problems possess similarities

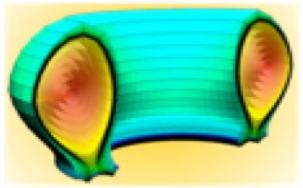


nuclear reactors
A. Siegel, ANL

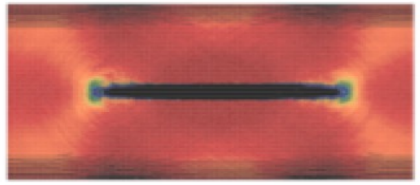
particle accelerators
K. Lee, SLAC



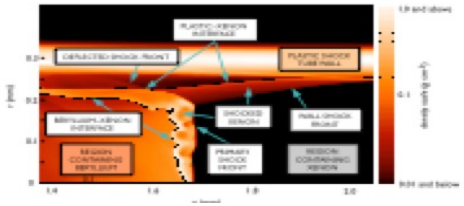
climate
K. Evans, ORNL



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

THE INTERNATIONAL JOURNAL of HIGH PERFORMANCE COMPUTING APPLICATIONS

Multiphysics simulations: Challenges and opportunities

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

doi:10.1177/1094342012468181

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

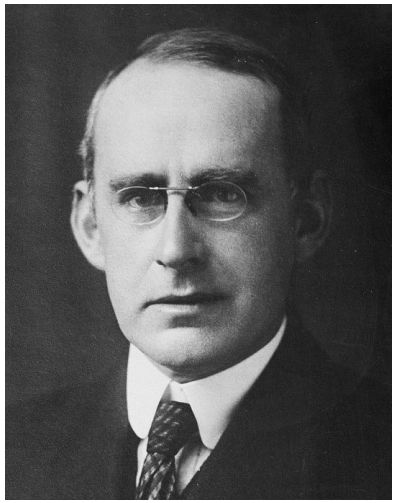
ECP EXASCALE COMPUTING PROJECT

Need software ecosystem perspective

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

Ecosystems are challenging!

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



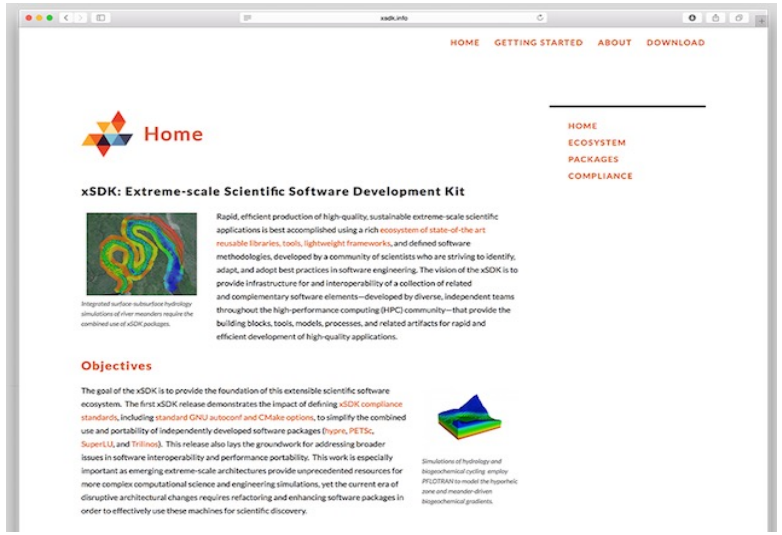
− Sir Arthur Stanley Eddington (1892−1944), British astrophysicist

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

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

Impact:

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



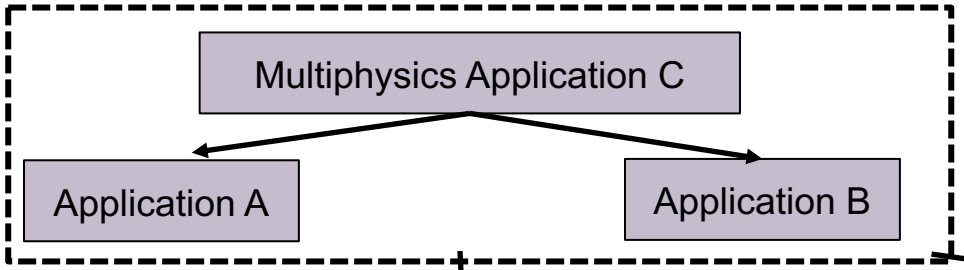
website: xSDK.info

xSDK Version 0.6.0: November 2020

https://xsdk.info

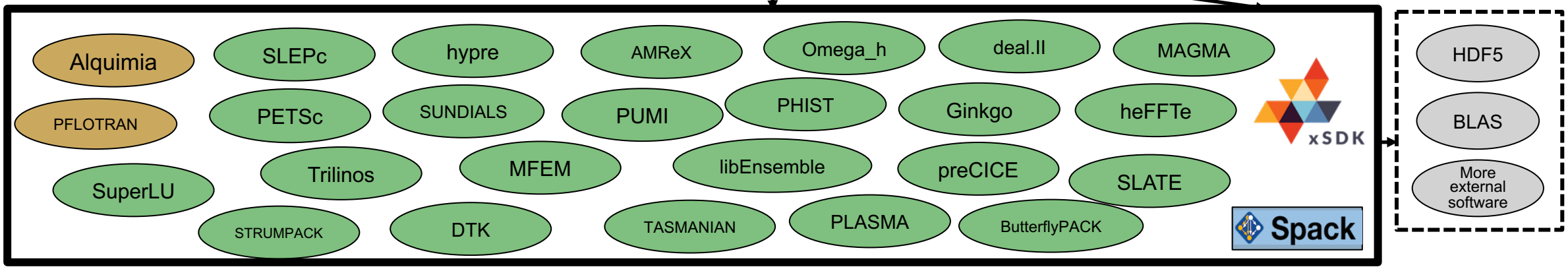
https://xsdk.info

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



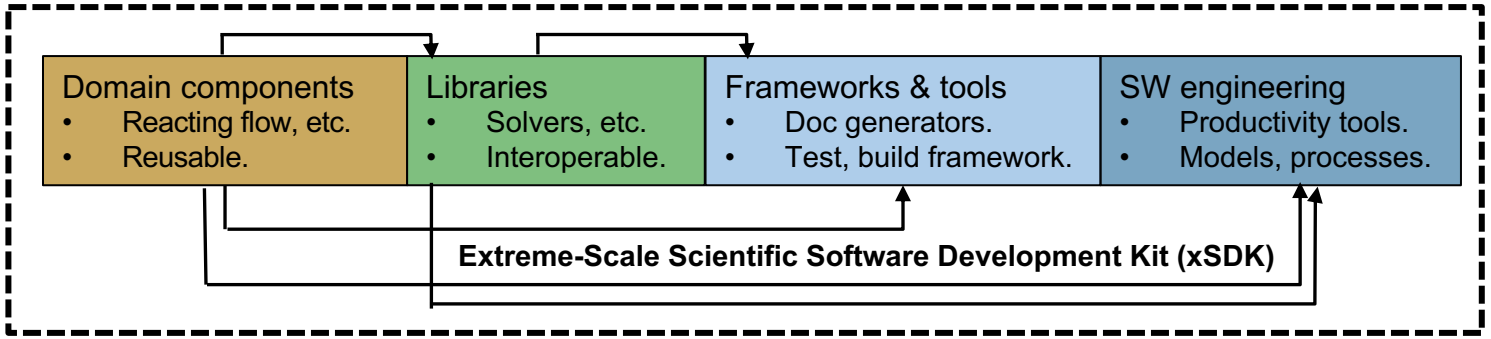
xSDK functionality, Nov 2020

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

EXASCALE COMPUTING PROJECT

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 guildelines)

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.

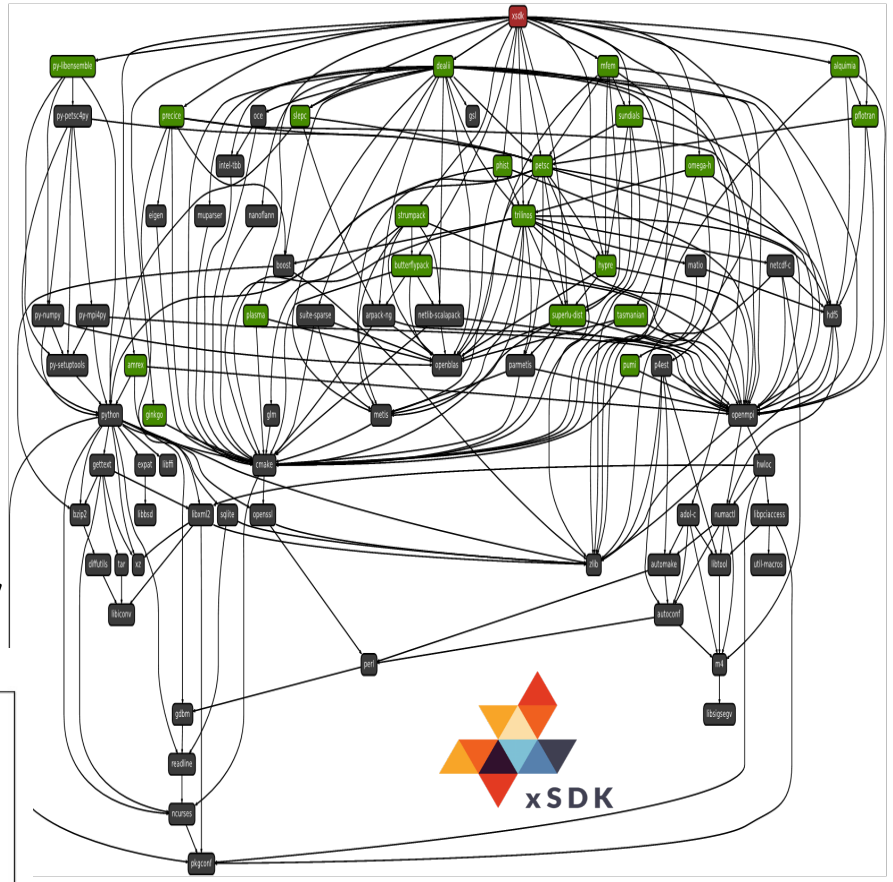
We welcome feedback. What policies make sense for your software?

EXASCALE COMPUTING PROJECT

The xSDK is using Spack to deploy its software

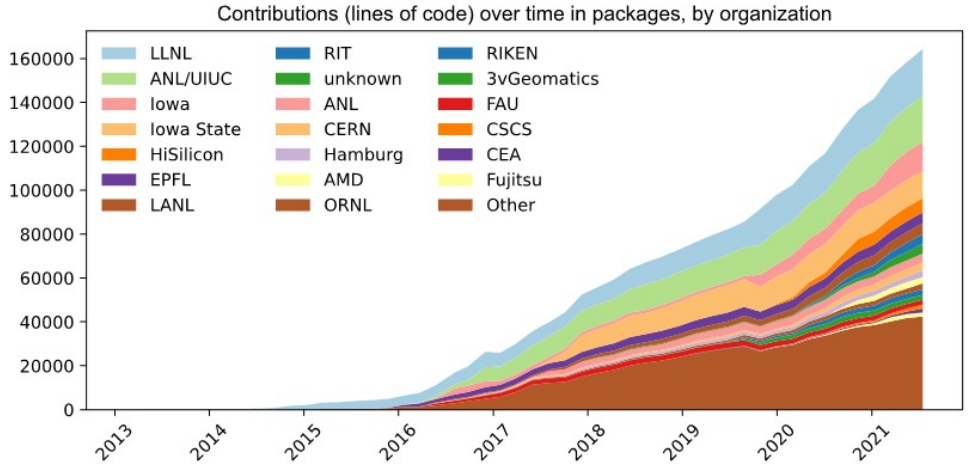
- The xSDK packages depend on a number of open-source libraries
- Spack is a flexible package manager for HPC
- Spack allows the xSDK to be deployed with a single command
  - User can optionally choose compilers, build options, etc.
  - Will soon support combinatorial test dashboards for xSDK packages

Spack



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

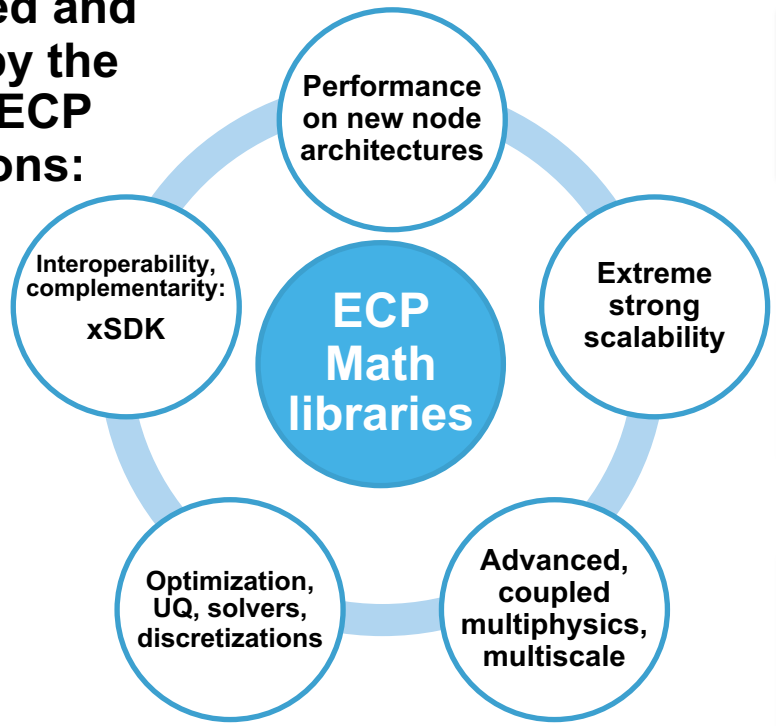


https://spack.io github.com/spack

EXASCALE COMPUTING PROJECT

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

As motivated and validated by the needs of ECP applications:



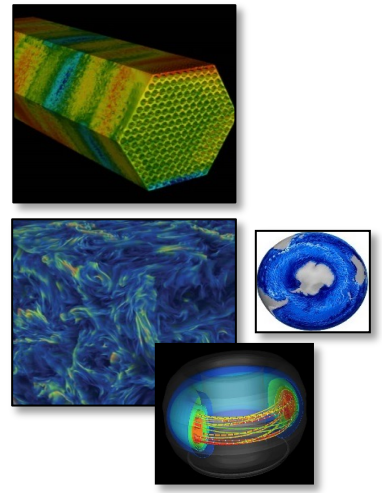
Next-generation algorithms

Advances in data structures for new node architectures

Improving library quality, sustainability, interoperability

Toward predictive scientific simulations

Increasing performance, portability, productivity



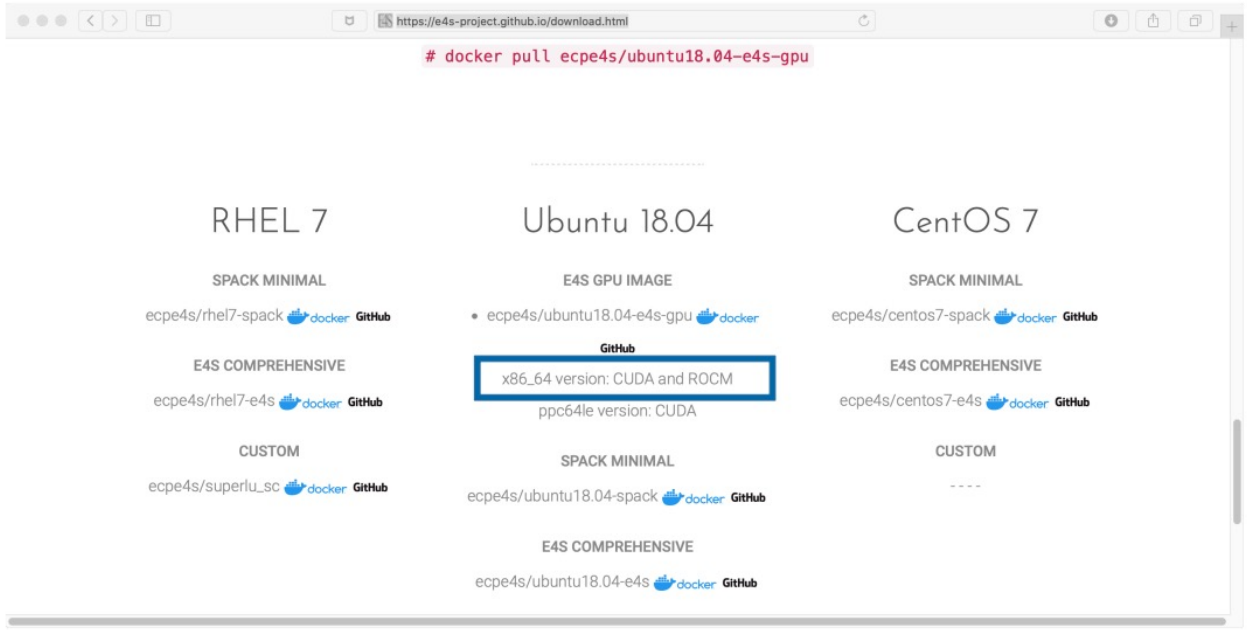
Timeline:

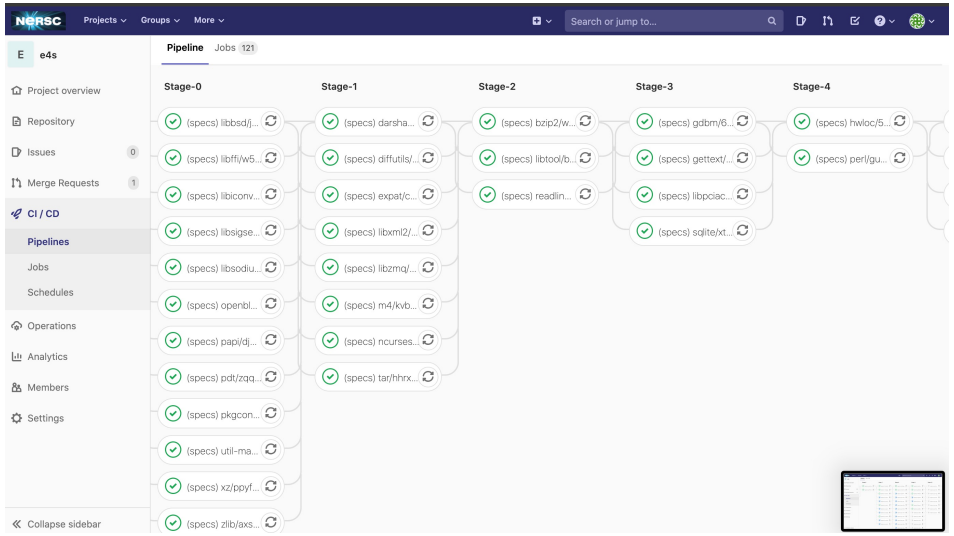
xSDK release 1 — xSDK release 2 — . . . . . — xSDK release n

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

EXASCALE COMPUTING PROJECT

E4S Summary

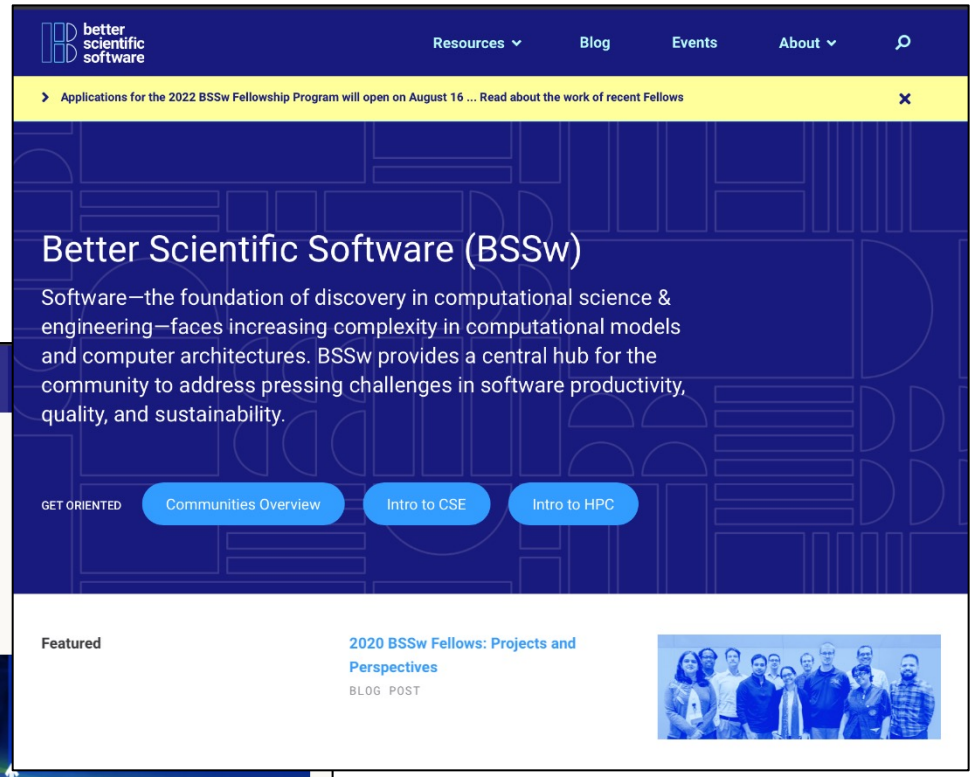
What E4S is not	What E4S is
• A closed system taking contributions only from DOE software development teams.	• Extensible, open architecture software ecosystem accepting contributions from US and international teams. • Framework for collaborative open-source product integration.
• A monolithic, take-it-or-leave-it software behemoth.	• A full collection if compatible software capabilities **and** • A manifest of a la carte selectable software capabilities.
• A commercial product.	• 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.
• A simple packaging of existing software.	• 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.

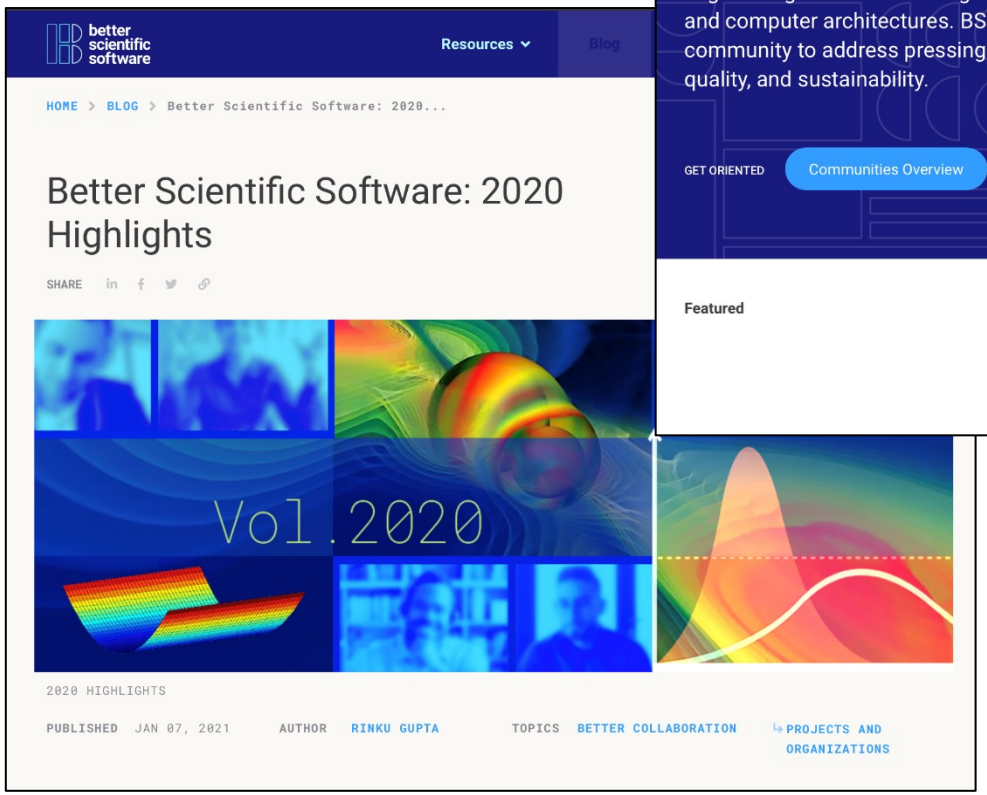
Further reading

better scientific software

https://bssw.io

- 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)

EXASCALE COMPUTING PROJECT

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)

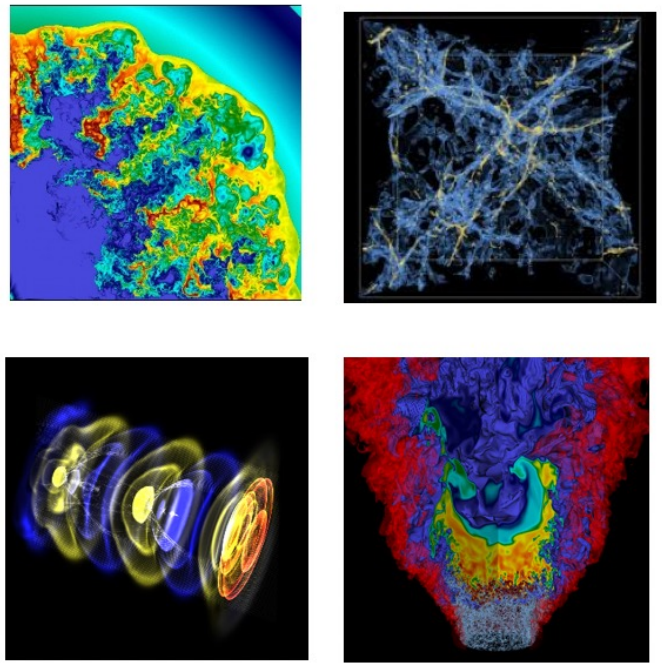
ECP EXASCALE COMPUTING PROJECT

AMReX

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

- **Capabilities**
  - Support for solution of PDEs on hierarchical adaptive mesh with particles and embedded boundary representation of complex geometry
  - Support for multiple modes of time integration
  - Support for explicit and implicit single-level and multilevel mesh operations, multilevel synchronization, particle, particle-mesh and particle-particle operations
  - Hierarchical parallelism –
    - hybrid MPI + OpenMP with logical tiling on multicore architectures
    - hybrid MPI + GPU support for hybrid CPU/GPU systems (CUDA and beyond)
  - Native multilevel geometric multigrid solvers for cell-centered and nodal data
  - Highly efficient parallel I/O for checkpoint/restart and for visualization – native format supported by Visit, Paraview, yt
  - Tutorial examples available in repository
- **Open source software**
  - Used for divers apps, including accelerator modeling, adaptive manufacturing, astrophysics, combustion, cosmology, multiphase flow, phase field modeling, …
  - Freely available on github with extensive documentation

Examples of AMReX applications



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

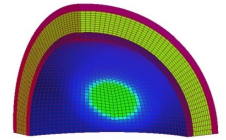
hypre

Lawrence Livermore National Laboratory

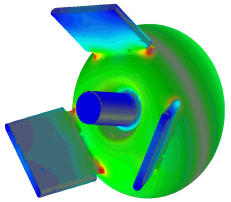
Highly scalable multilevel solvers and preconditioners. Unique user-friendly interfaces. Flexible software design. Used in a variety of applications. Freely available.

- **Conceptual interfaces**
  - Structured, semi-structured, finite elements, linear algebraic interfaces
  - Provide natural "views" of the linear system
  - Provide for efficient (scalable) linear solvers through effective data storage schemes
- **Scalable preconditioners and solvers**
  - Structured and unstructured algebraic multigrid solvers
  - Maxwell solvers, H-div solvers
  - Multigrid solvers for nonsymmetric systems: pAIR, 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

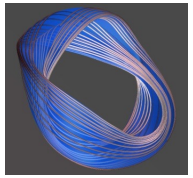
hypre high performance preconditioners



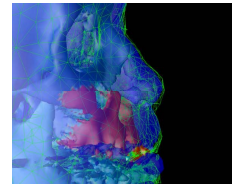
Elasticity / Plasticity



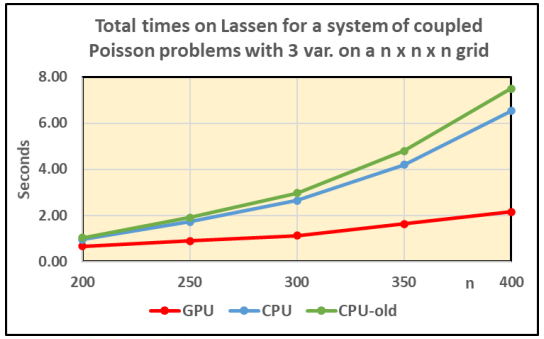
Electro-magnetics



Magneto-hydrodynamics



Facial surgery



xSDK

FASTMATH

ECP

R&D 100

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

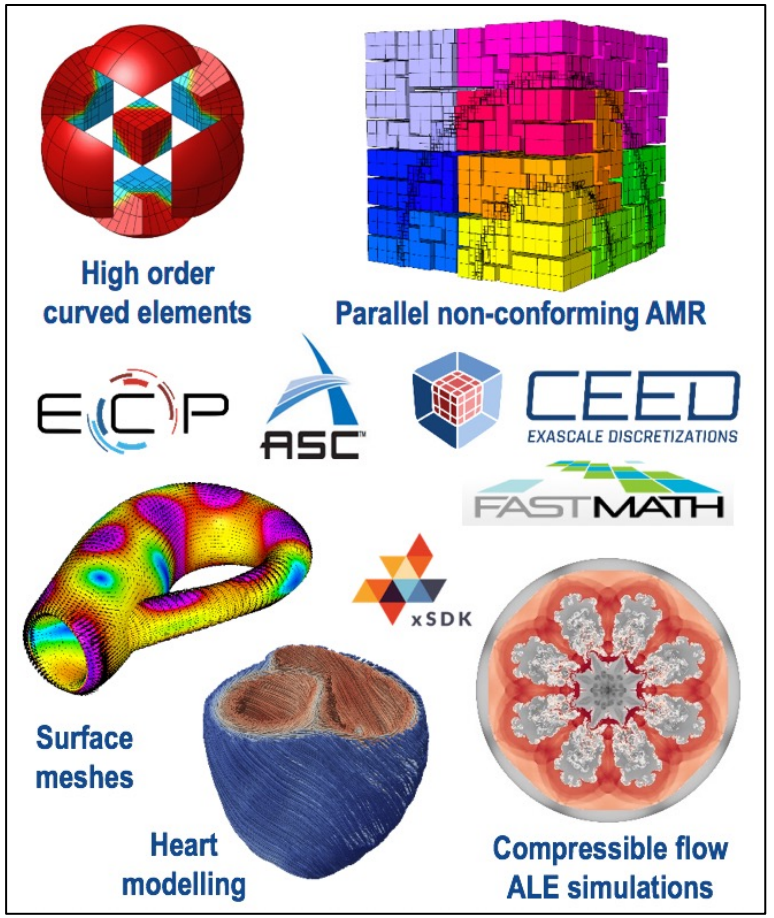
ECP EXASCALE COMPUTING PROJECT

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 H1, H(curl), H(div)- and L2 elements. Arbitrary order curvilinear meshes.
  - MPI scalable to millions of cores and includes initial GPU implementation. Enables application development on wide variety of platforms: from laptops to exascale machines.
- **Built-in solvers and visualization**
  - Integrated with: HYPRE, SUNDIALS, PETSc, SUPERLU, …
  - Accurate and flexible visualization with VisIt and GLVis
- **Open source software**
  - LGPL-2.1 with thousands of downloads/year worldwide.
  - Available on GitHub, also via OpenHPC, Spack. Part of ECP's CEED co-design center.



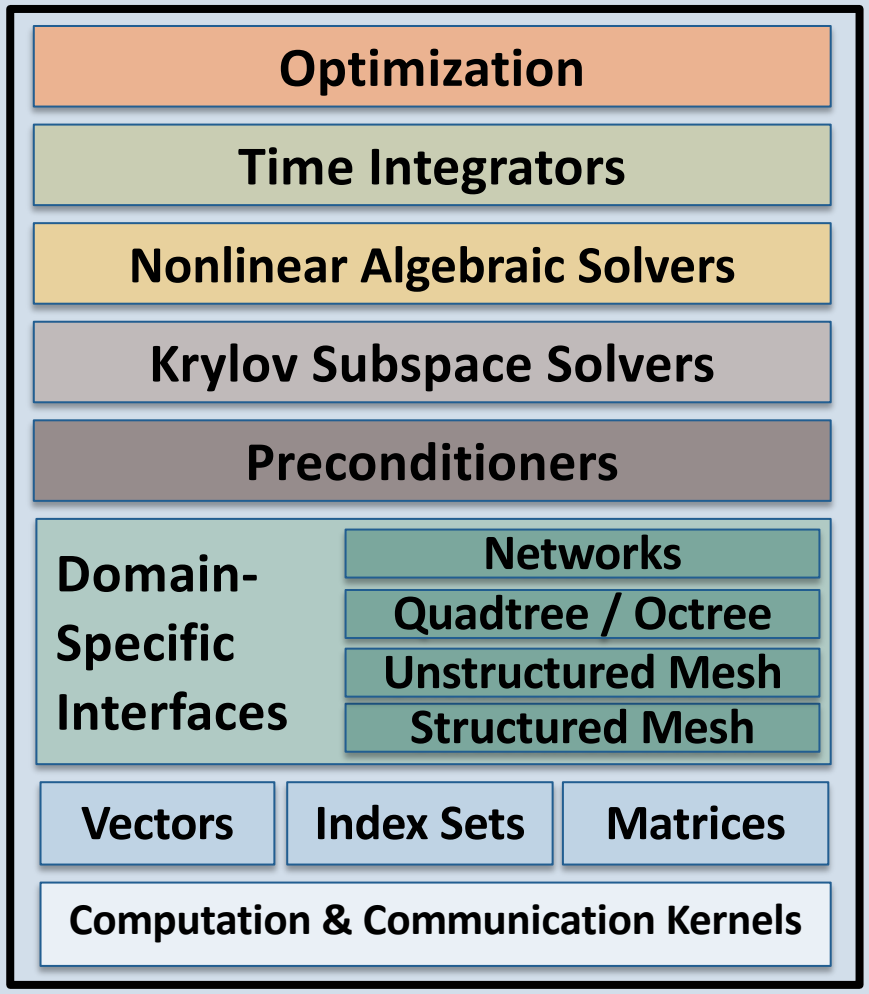
http://mfem.org

ECP EXASCALE COMPUTING PROJECT

PETSc TAO

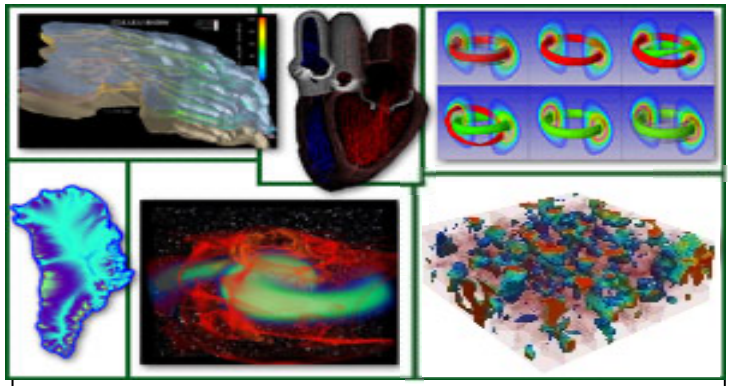
Portable, Extensible Toolkit for Scientific Computation / Toolkit for Advanced

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



- **Easy customization and composability of solvers 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

Argonne NATIONAL LABORATORY



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

ECP xSDK FASTMATH R&D 100

https://petsc.org

ECP EXASCALE COMPUTING PROJECT

Parallel Unstructured Mesh Infrastructure

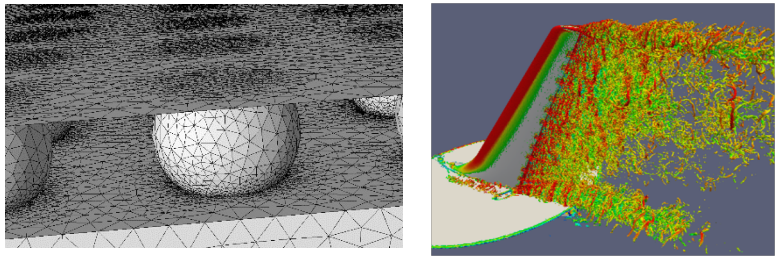
Parallel management and adaptation of unstructured meshes.
Interoperable components to support the development of unstructured mesh simulation workflows

- **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

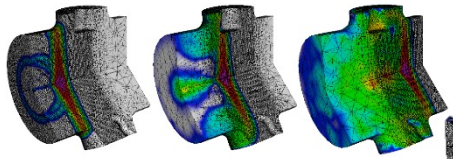
PUMI

SCOREC

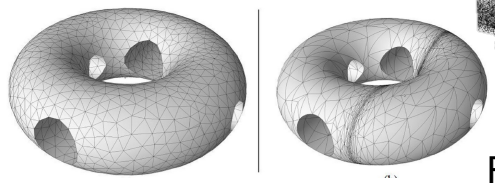
Rensselaer



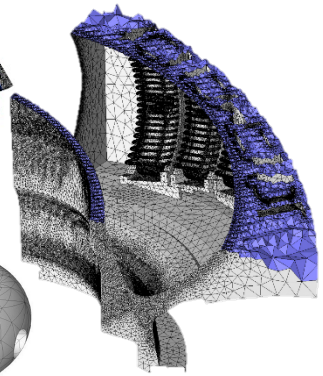
Applications with billions of elements: flip-chip (L), flow control (R)



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

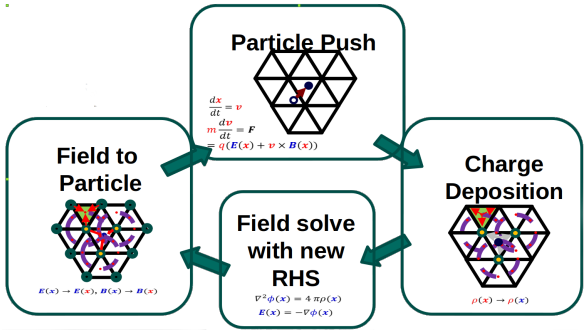
SCOREC

HBPS High-fidelity Boundary Plasma Simulation

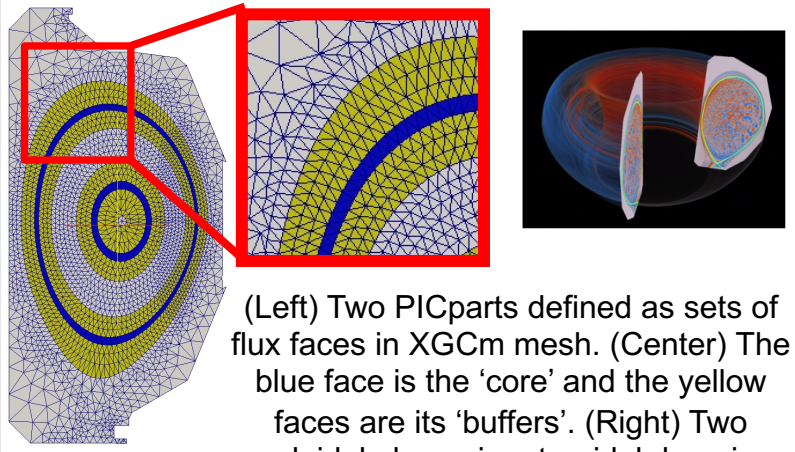
ECP

Rensselaer

FASTMATH



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

ECP EXASCALE COMPUTING PROJECT

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

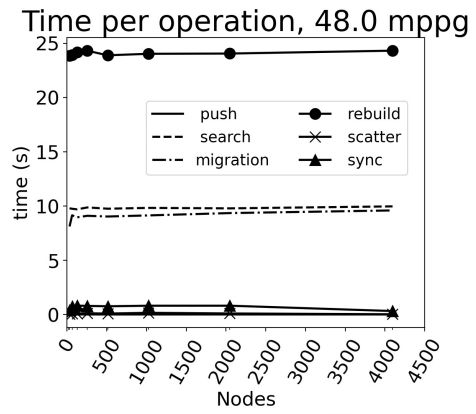
- Core and edge fusion plasma physics with ions and kinetic electrons
- Tokamak: 2D mesh partitioned into PICParts (see PUMIPic slide) based on bounding flux surfaces
- A group of processes is assigned to a PICPart and 1/Pth of the torus in the toroidal direction – group size controls particle load on 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.

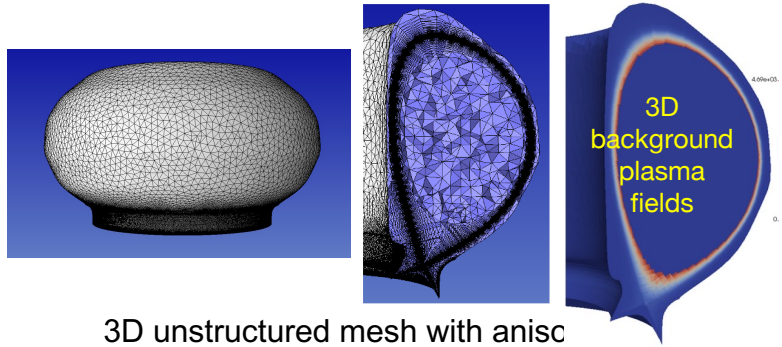
GITRm

- 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

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 anisc refinement. Less than 1% difference vs. GITR in gross erosion and deposition.

GITRm ITER test case

Contact: Mark S. Shephard
shephard@rpi.edu

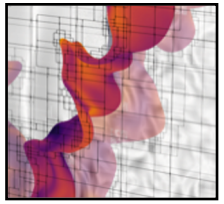
SUNDIALS

Suite of Nonlinear and Differential /Algebraic Equation Solvers

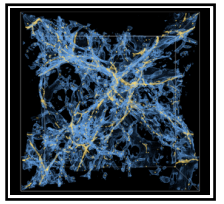
Adaptive time integrators for ODEs and DAEs and efficient nonlinear solvers
Used in a variety of applications. Freely available. Encapsulated solvers & parallelism.

- **ODE 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

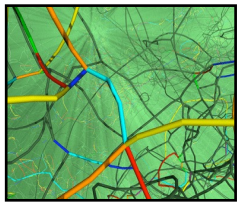
SUNDIALS is used worldwide in applications throughout research and industry



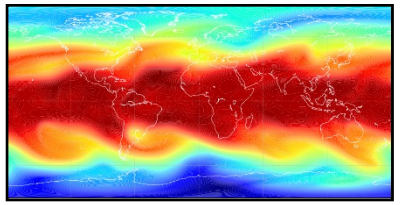
Combustion (Pele)



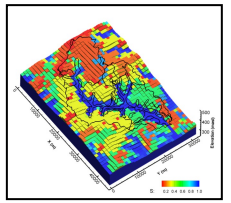
Cosmology (Nyx)



Dislocation dynamics (ParaDiS)



Atmospheric Dynamics (Tempest)



Subsurface flow (ParFlow)

Lawrence Livermore National Laboratory

ECP

FASTMATH

xSDK

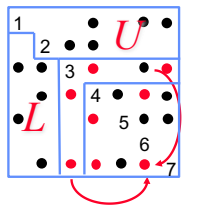
http://www.llnl.gov/casc/sundials

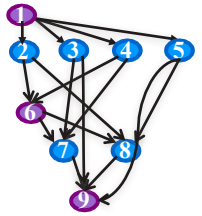
ECP EXASCALE COMPUTING PROJECT

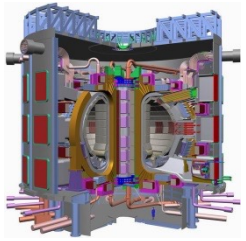
SuperLU

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

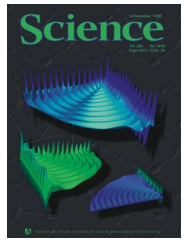
- **Capabilities**
  - Serial (thread-safe), shared-memory (SuperLU_MT, OpenMP or Pthreads), distributed-memory (SuperLU_DIST, hybrid MPI+ OpenM + CUDA/HIP).
    - Written in C, with Fortran interface
  - Sparse LU decomposition (can be nonsymmetric sparsity pattern), triangular solution with multiple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

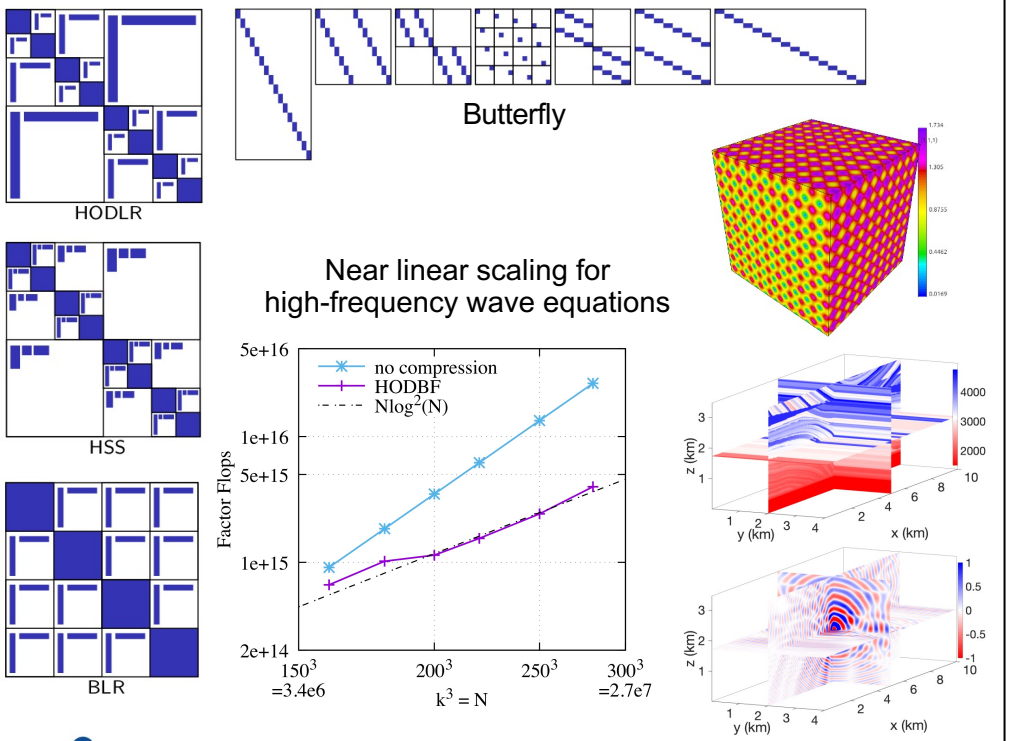
https://portal.nersc.gov/project/sparse/superlu/

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



github.com/pghysels/STRUMPACK

EXASCALE COMPUTING PROJECT

Trilinos

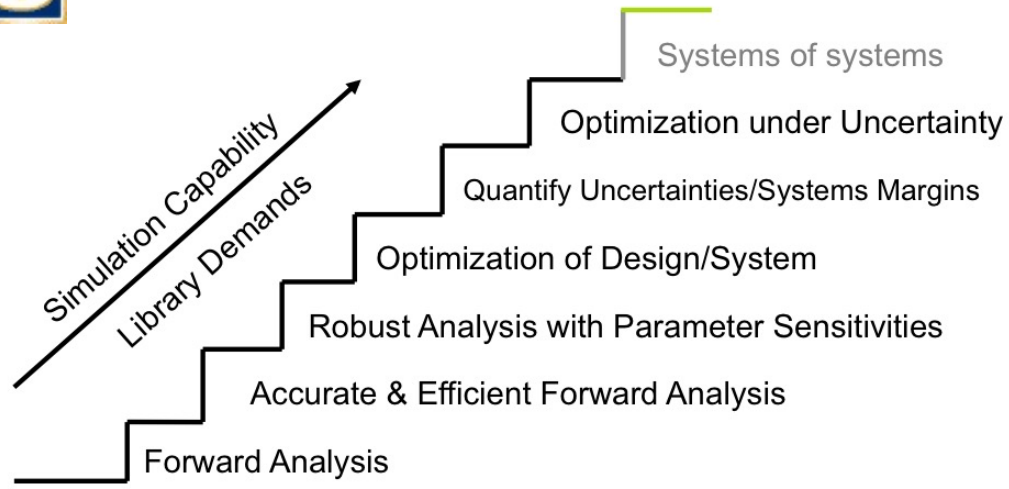
Sandia National Laboratories

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

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

R&D 100

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/

xSDK FASTMATH TRILINOS

ECP EXASCALE COMPUTING PROJECT

Trilinos/Belos

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

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

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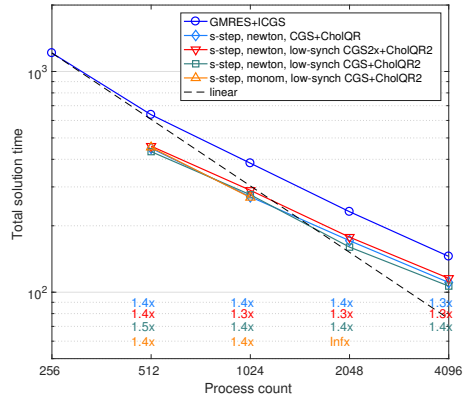
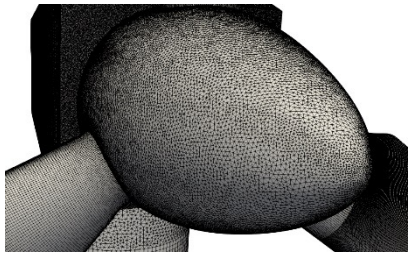


Speed-ups of various s-step Krylov methods within low Mach CFD wind-energy code Nalu-Wind.



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

Sandia National Laboratories

ASC

ECP EXASCALE COMPUTING PROJECT

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

ECP EXASCALE COMPUTING PROJECT

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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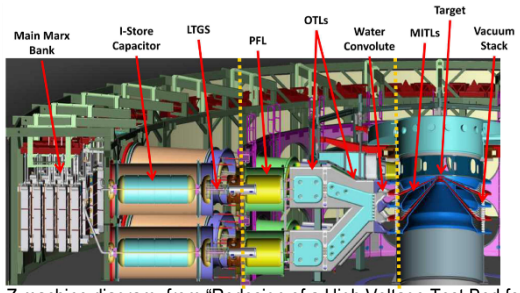
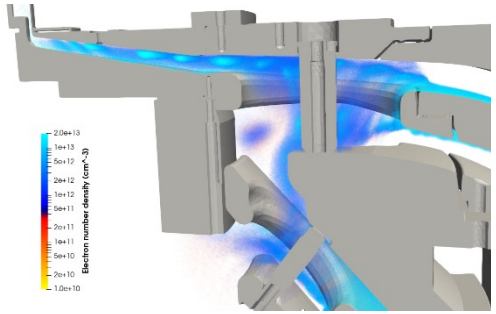


Z machine diagram, from "Redesign of a High Voltage Test Bed for Marxes on Z", W.M. White et al., 2018.

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)

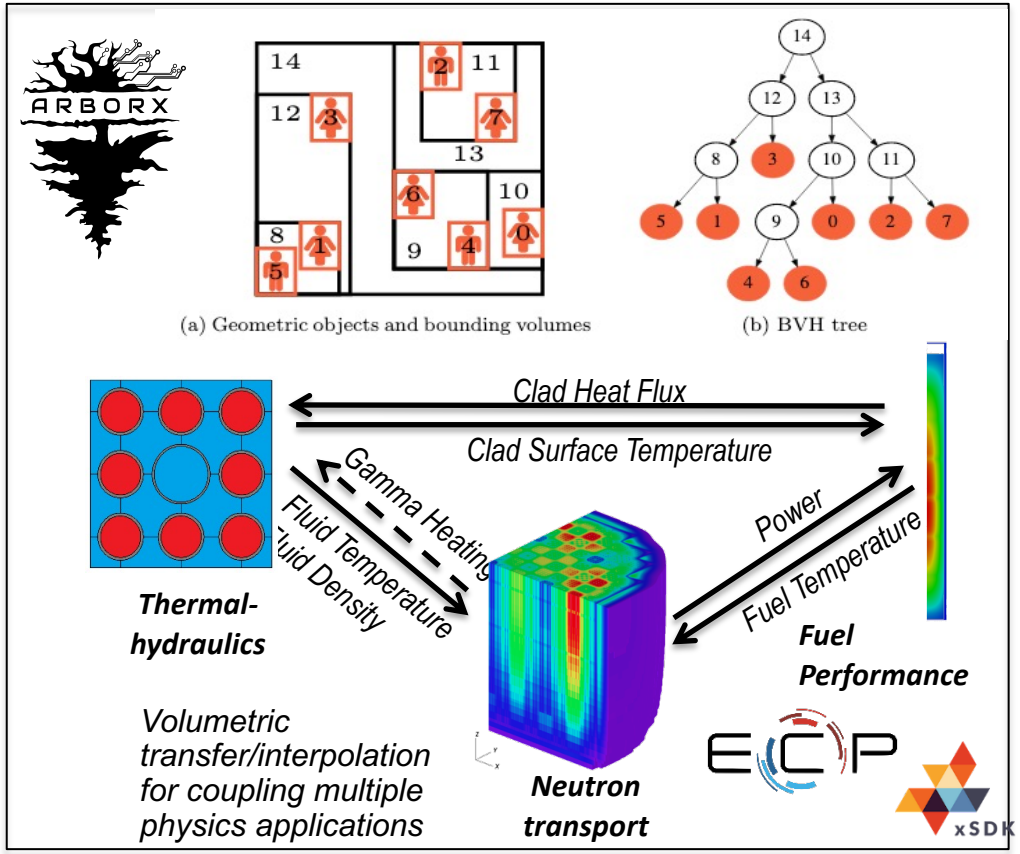
ECP EXASCALE COMPUTING PROJECT

ArborX/ DataTransferKit

OAK RIDGE National Laboratory

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



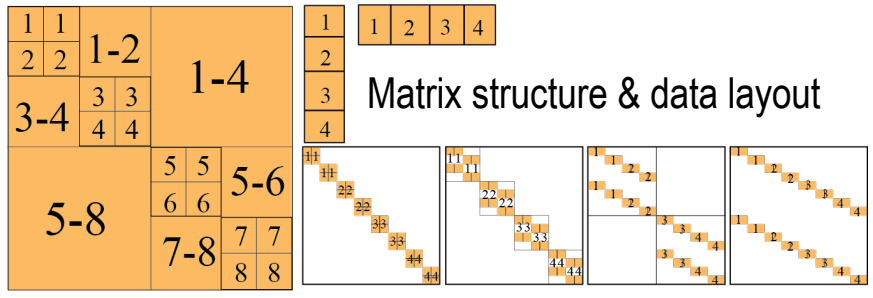
https://github.com/arborx/ArborX
https://github.com/ORNL-CEES/DataTransferKit

ECP EXASCALE COMPUTING PROJECT

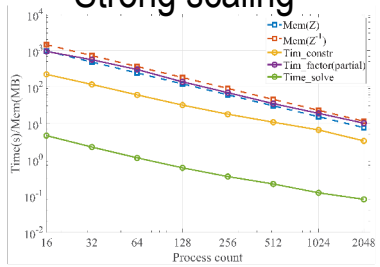
ButterflyPACK

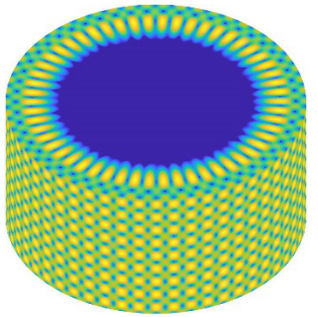
Fast direct solvers. Low-rank and butterfly compression. Distributed-memory parallel. Particularly for highly-oscillatory wave equations.

- **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



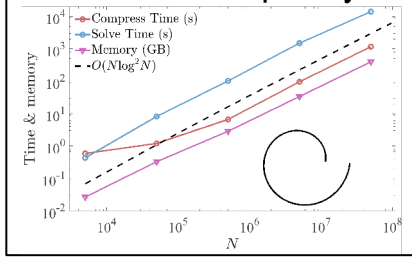
Strong scaling





Accelerator cavity

Solver complexity

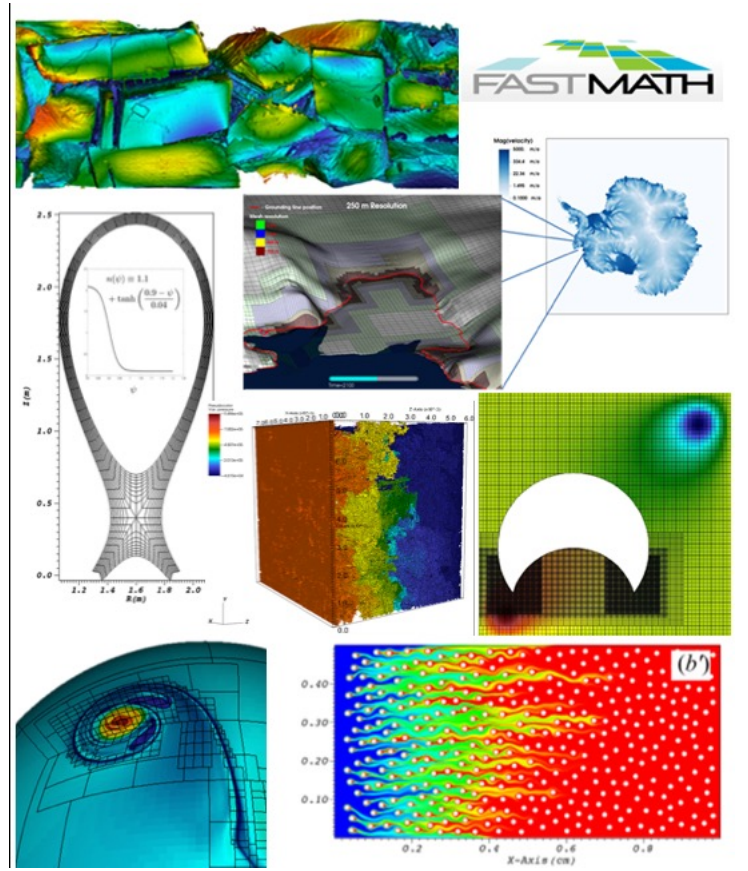


https://github.com/liuyangzhuan/ButterflyPACK

Chombo

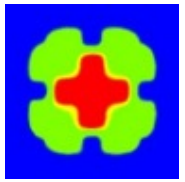
Scalable adaptive mesh refinement framework. Enables implementing scalable AMR applications with support for complex geometries.

- **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



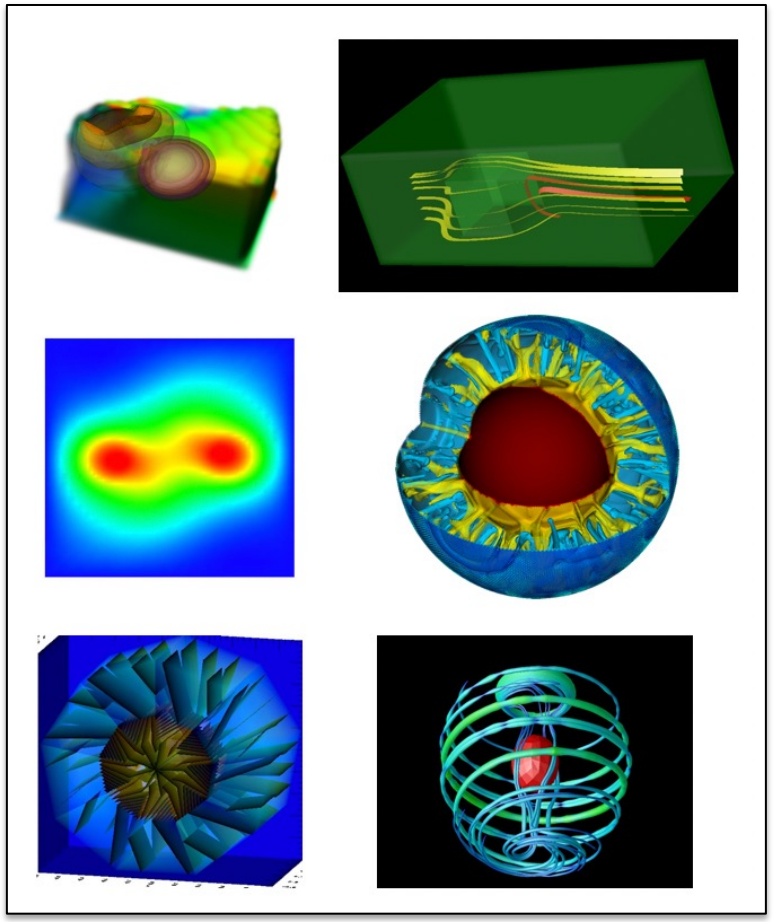
http://Chombo.lbl.gov

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

THE UNIVERSITY OF TENNESSEE KNOXVILLE

KIT Karlsruhe Institute of Technology

UJI

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

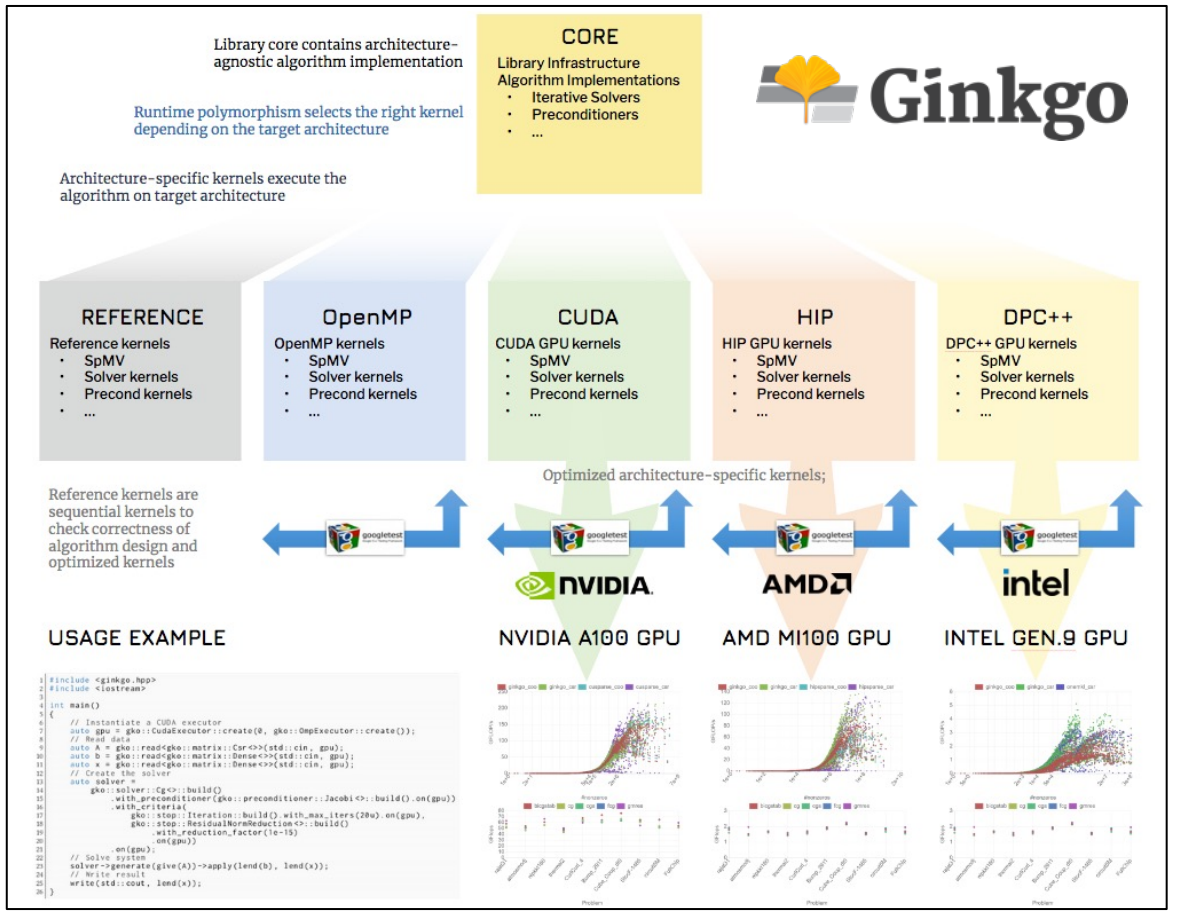
- **High performance sparse linear algebra**
  - Linear solvers: BiCG, BiCGSTAB, CG, CGS, FCG, GMRES, IDR;
  - Advanced preconditioning techniques: ParILU, ParILUT, SAI;
  - Mixed precision algorithms: adaptive precision Jacobi, FSPAI;
  - Decoupling of arithmetic precision and memory precision;
  - *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**;

ECP

E4S

xSDK

deal.II



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

ECP EXASCALE COMPUTING PROJECT

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:

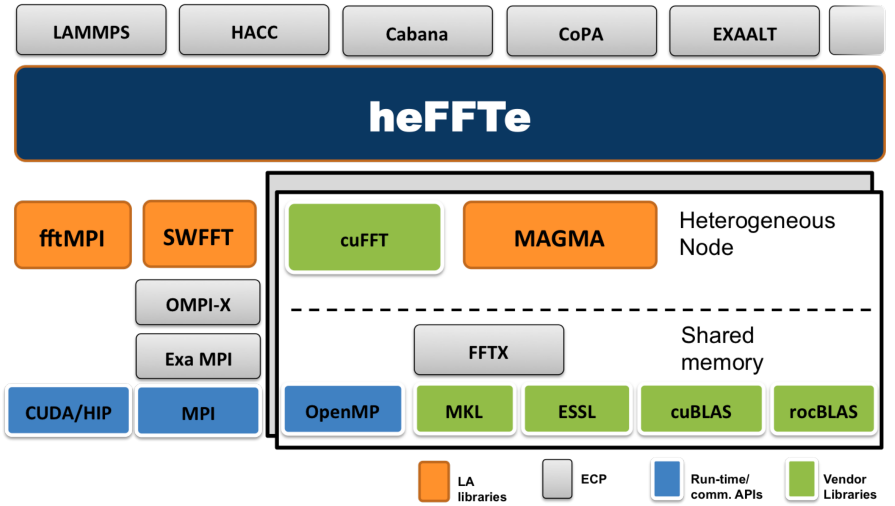
- **Summit @ OLCF (Nvidia GPUs), Poplar (AMD GPUs), and others**
- **In progress: Intel GPU**

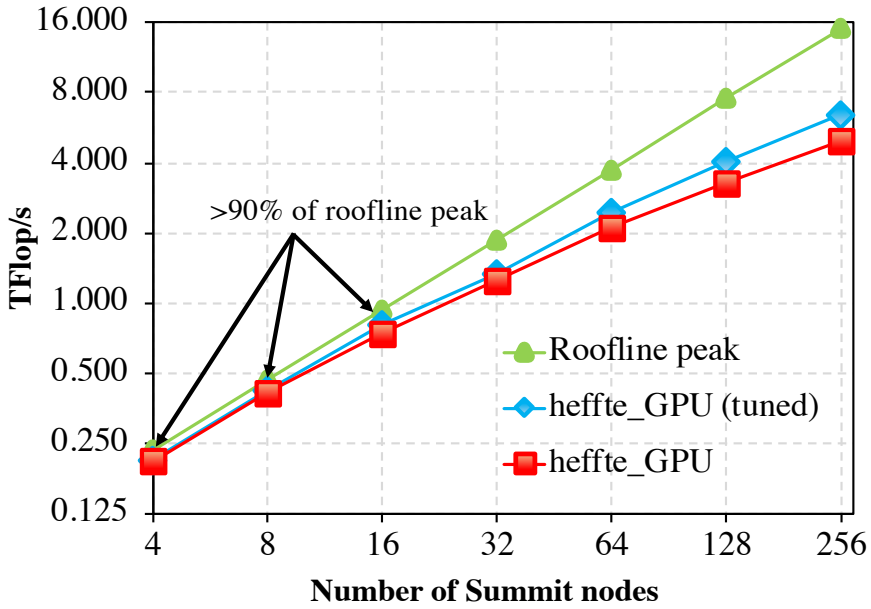
Current status:

- 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

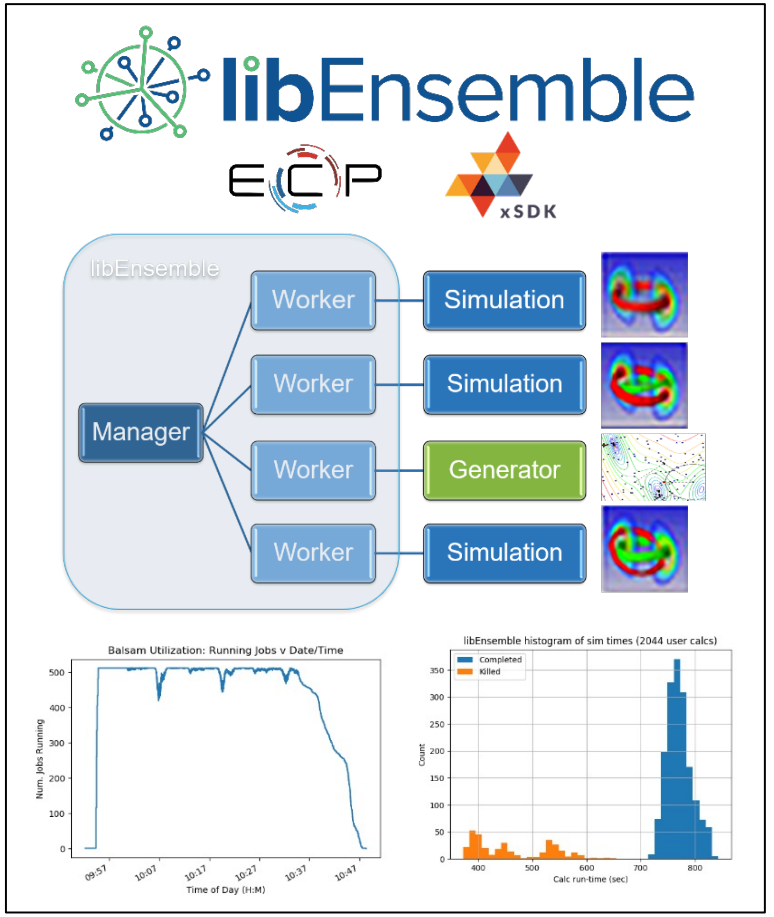
Argonne NATIONAL LABORATORY

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

ECP EXASCALE COMPUTING PROJECT

INNOVATIVE COMPUTING LABORATORY

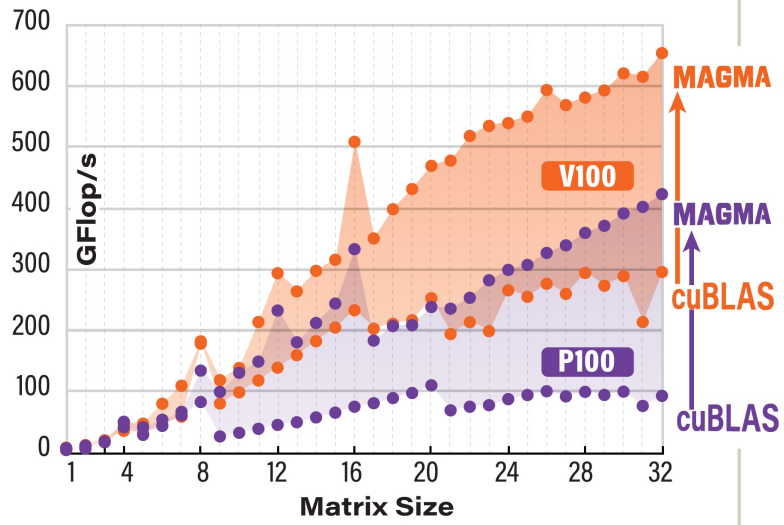
MAGMA

Matrix Algebra on GPU and Multicore Architectures

- 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, SPMM (CSR, ELL, … etc.)

PERFORMANCE OF BATCHED LU

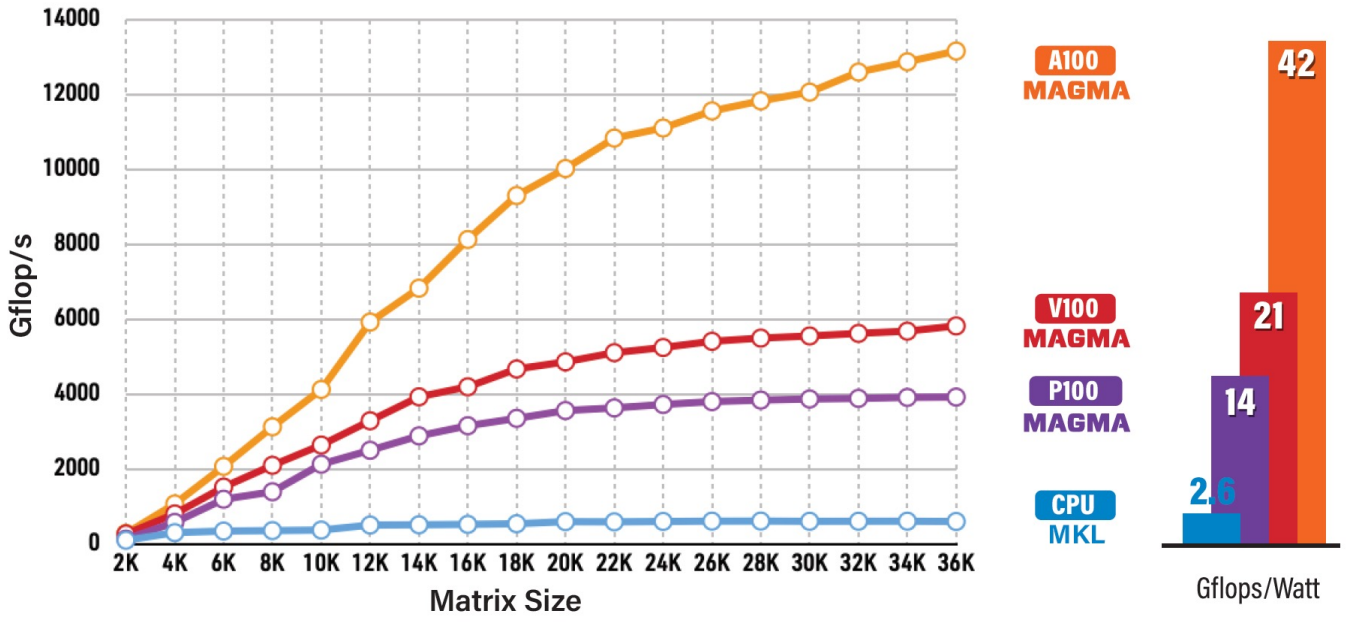
in double-precision arithmetic on 1 million matrices



PERFORMANCE & ENERGY EFFICIENCY

MAGMA LU factorization in double-precision arithmetic

CPU	P100	V100	A100
Intel Xeon E5-2650 v3 (Haswell)	NVIDIA Pascal GPU	NVIDIA Volta GPU	NVIDIA Ampere GPU
2 x 10 cores @ 2.30 GHz	56 SMs x 64 @ 1.19 GHz	80 SMs x 64 @ 1.37 GHz	108 SMs x 64 @ 1.41 GHz



- Support CUDA and ROCM/HIP
- https://icl.utk.edu/magma

IN COLLABORATION WITH

Berkeley · University of Colorado Denver · U.S. Department of Defense · U.S. Department of Energy · AMD · intel · Inria · KAUST · ECP · National Science Foundation · MathWorks · NVIDIA

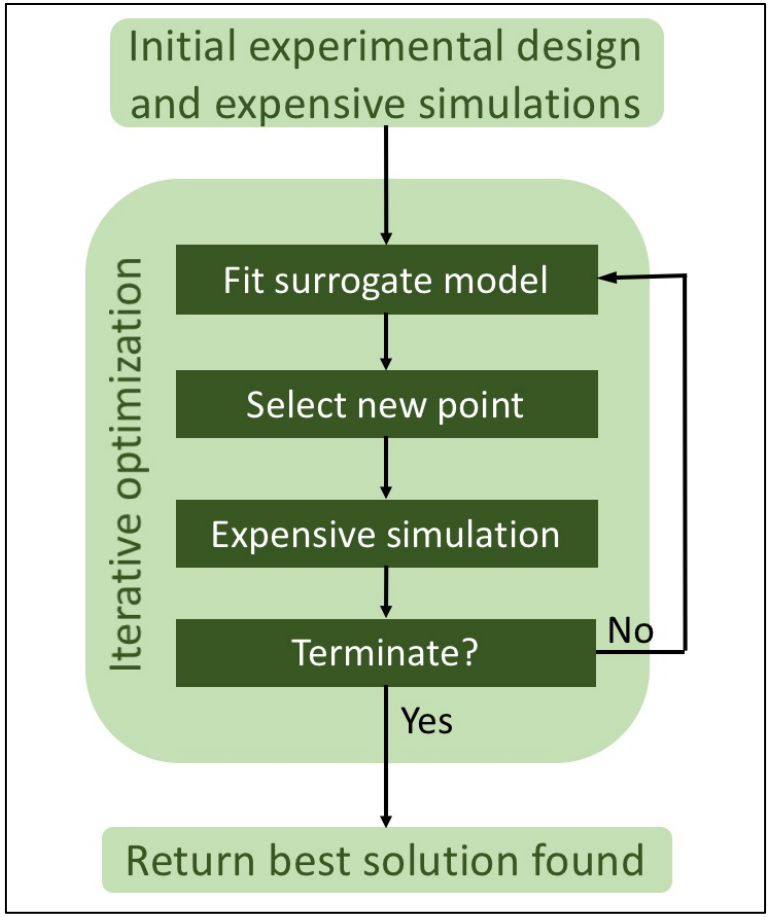
SPONSORED

MATSuMoTo

MATLAB Surrogate Model Toolbox

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

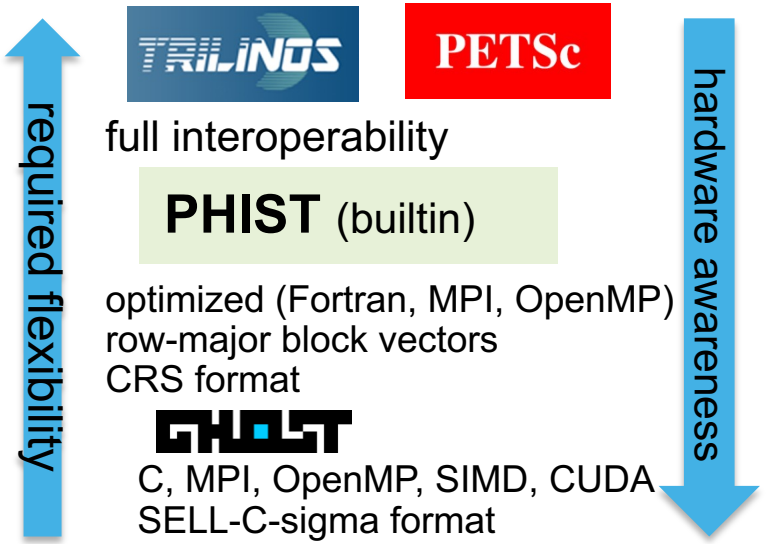
PHIST

Pipelined, Hybrid-parallel Iterative Solver Toolkit

Hybrid-parallel Iterative Sparse Eigenvalue and linear solvers
Integration with different linear algebra backends and preconditioners

- **Sparse Eigenvalue Solver: Block Jacobi-Davidson QR**
  - Hermitian or non-Hermitian matrices
  - Generalized problems $\boldsymbol{A}x = \lambda \boldsymbol{B}x$ (for Hermitian pos. def. matrix $\mathbf{B}$)
  - Blocked iterative linear solvers like GMRES, BiCGStab and CGMN
  - Can be accelerated by preconditioning
  - Matrix-free interface
  - Supported data types: D, Z, S, C
- **Algorithmic Building Blocks**
  - block orthogonalization
  - Eigenvalue counting (kernel polynomial method/KPM)
  - Fused basic operations for better performance
- **Various interfaces**
  - C, C++, Fortran 2003, Python

Can choose from several backends at compile time



Funded by the DFG project ESSEX
SPPEXA

https://bitbucket.org/essex/phist

ECP EXASCALE COMPUTING PROJECT

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

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

```
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 native libraries for vendor-level on-device performance

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);
}
```

SLATE

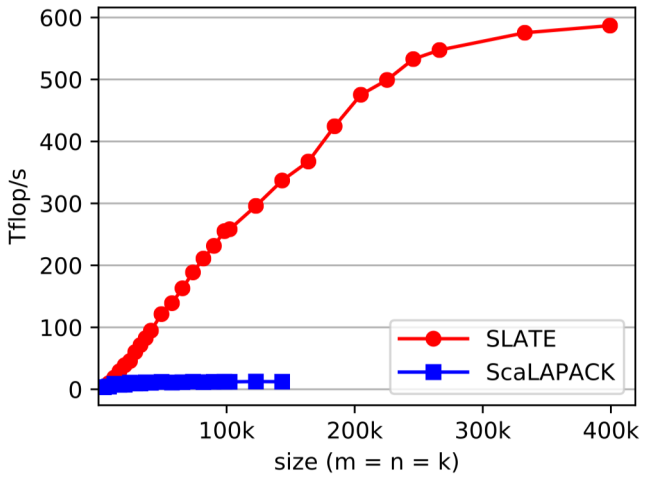
Software for Linear Algebra Targeting Exascale

THE UNIVERSITY OF TENNESSEE KNOXVILLE

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 ≈ b): QR, LQ
  - Eigenvalue (Ax = λx)
  - SVD (A = UΣVH)
- **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/

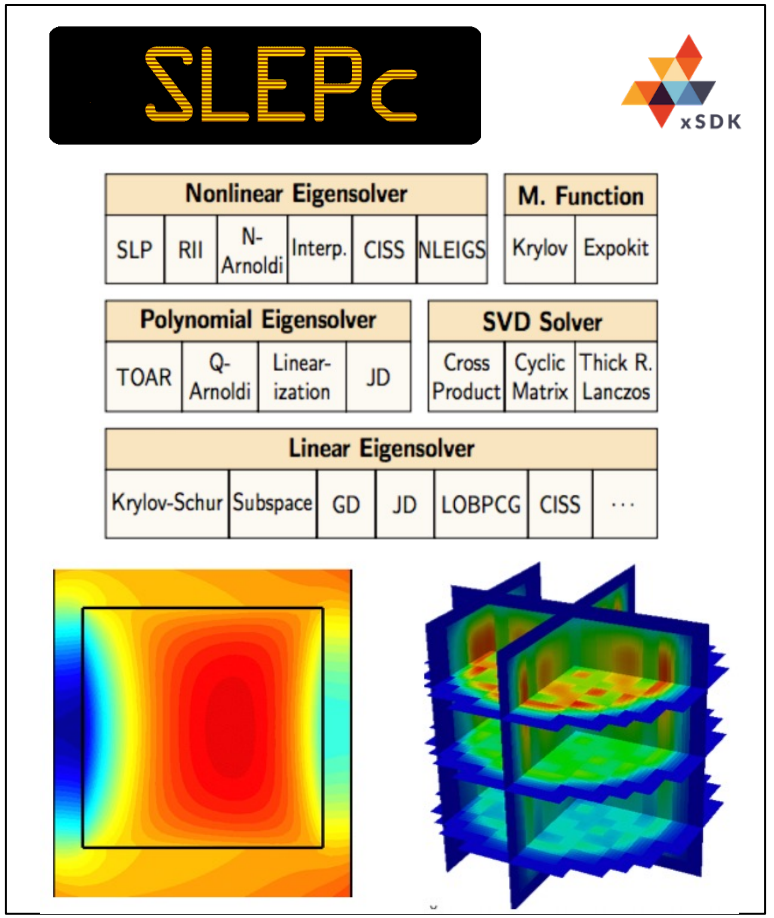
EXASCALE COMPUTING PROJECT

SLEPc

UNIVERSITAT POLITÈCNICA DE VALÈNCIA

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

- **Linear eigenvalue problems and SVD**
  - Standard and generalized eigenproblem, $Ax=\lambda x$, $Ax=\lambda Bx$; singular values $Au=\sigma v$
  - Easy selection of target eigenvalues, shift-and-invert available for interior ones
  - Many solvers: Krylov, Davidson, LOBPCG, contour integral, …
- **Nonlinear eigenvalue problems**
  - Polynomial eigenproblem $P(\lambda)x=0$, for quadratic or higher-degree polynomials
  - Solvers: Krylov with compact basis representation; Jacobi-Davidson
  - General nonlinear eigenproblem $T(\lambda)x=0$, for any nonlinear function incl. rational
- **Matrix functions**
  - Parallel Krylov solver to evaluate $y=f(A)v$
  - Support for matrix exponential, square root, etc. and combinations thereof
- **Extension of PETSc**
  - Runtime customization, portability and performance, C/C++/Fortran/python
  - Can use any PETSc linear solvers and preconditioners



http://slepc.upv.es

EXASCALE COMPUTING PROJECT

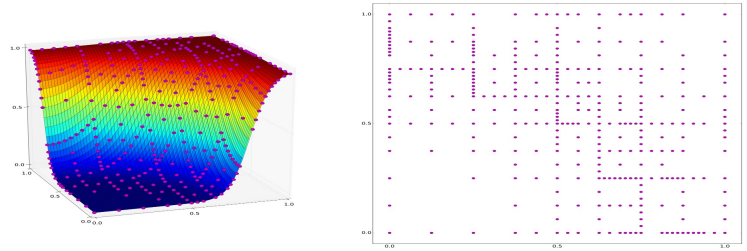
Tasmanian

OAK RIDGE National Laboratory

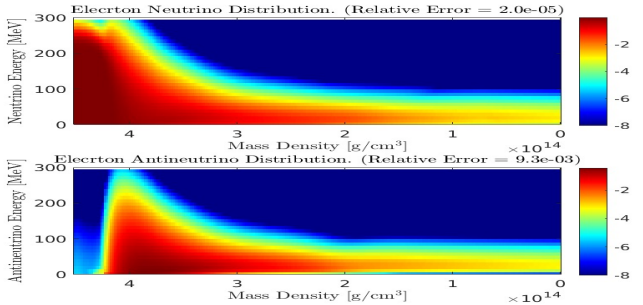
Toolkit for Adaptive Stochastic Modeling and Non-Intrusive ApproximatioN. Open Source Library for Uncertainty Quantification, surrogate modeling, data compression, Bayesian inference, and optimization.

- **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 anaisotropy
- **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

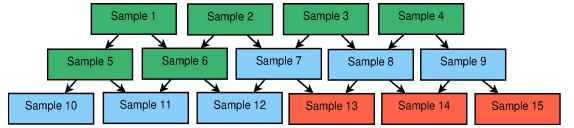
Adaptive Sparse Grid Sampling



Multiphysics simulation of Neutrino Radiation



Dynamic Adaptive Sampling



xSDK

ECP

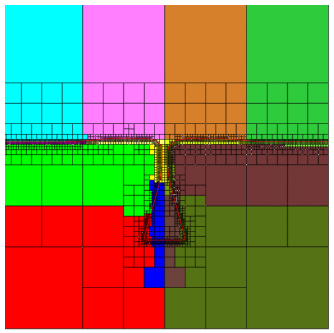
https://github.com/ORNL/TASMANIAN

ECP EXASCALE COMPUTING PROJECT

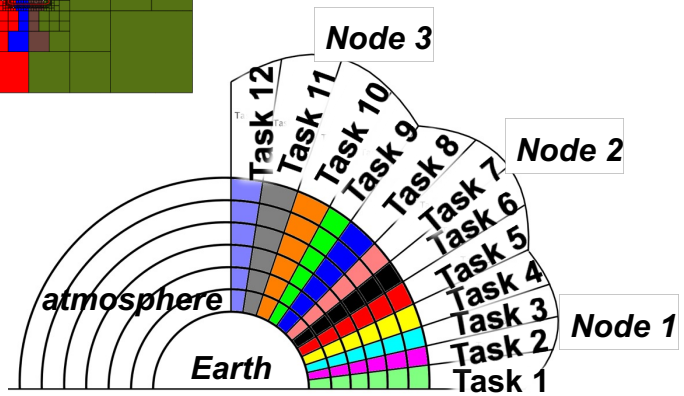
Zoltan/Zoltan2

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

- **Partitioning & load-balancing support many applications**
  - Fast geometric methods maintain spatial locality of data (e.g., for adaptive finite element methods, particle methods, crash/contact simulations)
  - Graph and hypergraph methods explicitly account for communication costs (e.g., for electrical circuits, finite element meshes, social networks)
  - Single interface to popular partitioning TPLs: XtraPuLP (SNL, RPI); ParMA (RPI); PT-Scotch (U Bordeaux); ParMETIS (U Minnesota)
  - MPI+X geometric partitioning using Kokkos for GPU and multicore
- **Architecture-aware MPI task placement reduces application communication time**
  - Places interdependent MPI tasks on "nearby" nodes in network
  - Reduces communication time and network congestion
- **Graph algorithms for coloring, ordering, connectivity**
- **Use as a stand-alone library or as a Trilinos component**



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



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

Sandia National Laboratories

FASTMATH

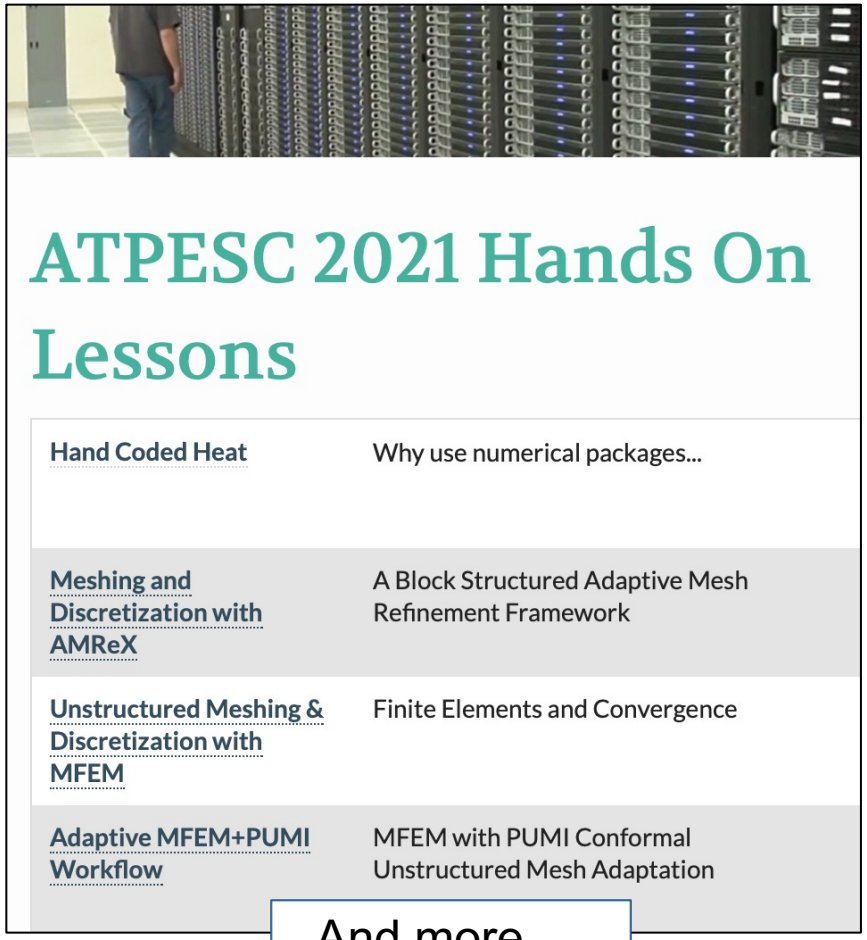
ASC

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

ECP EXASCALE COMPUTING PROJECT

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



And more …

Github pages site:

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

ECP EXASCALE COMPUTING PROJECT

Hello World
(for numerical packages)

Alp Dener

Mathematics and Computer Science

Argonne National Laboratory

with special thanks to Mark Miller, LLNL

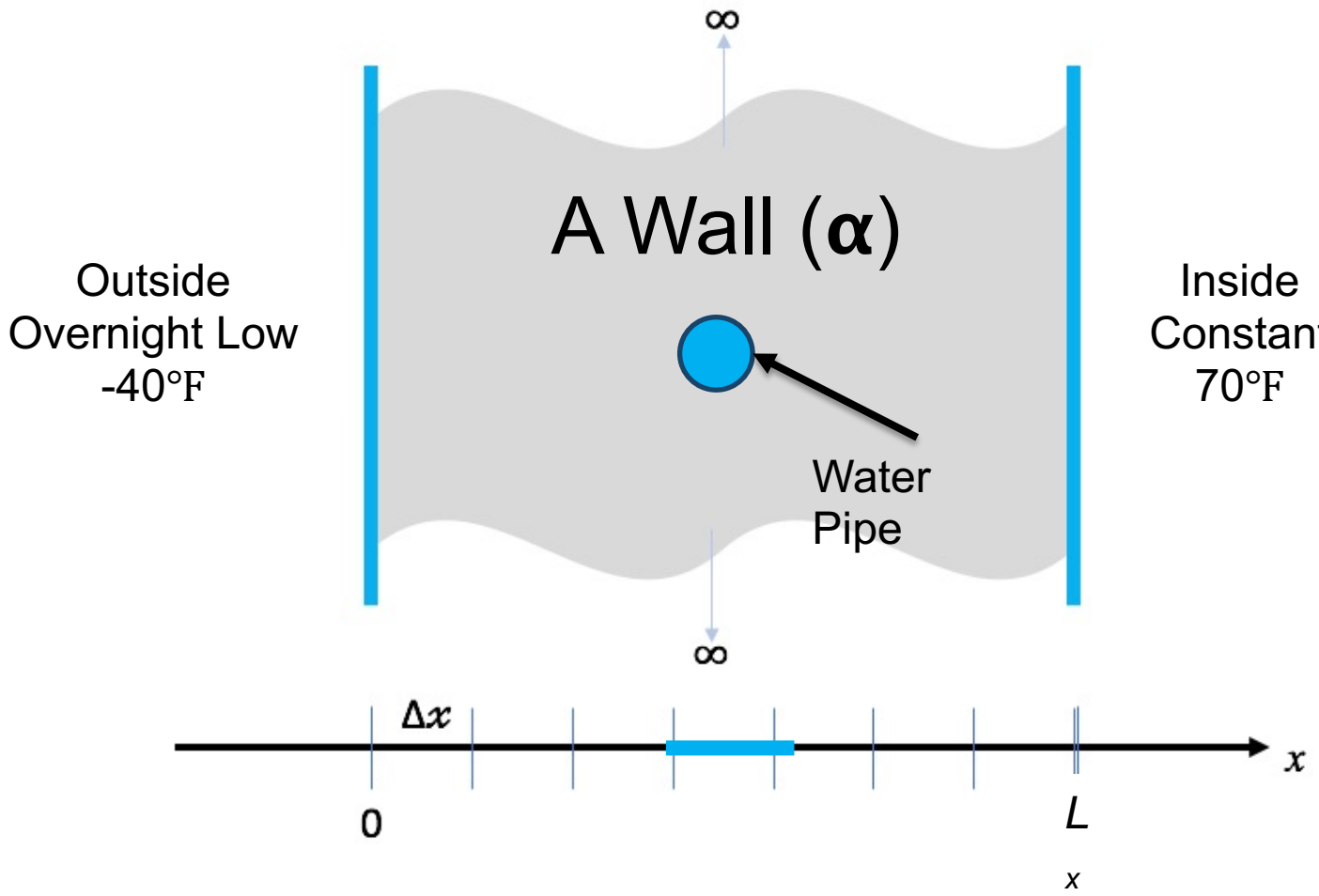
U.S. DEPARTMENT OF ENERGY | Office of Science

ATPESC Numerical Software Track

EXASCALE COMPUTING PROJECT

Argonne NATIONAL LABORATORY · BERKELEY LAB · Sandia National Laboratories · Rensselaer · SMU

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



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

ECP EXASCALE COMPUTING PROJECT

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)

ECP EXASCALE COMPUTING PROJECT

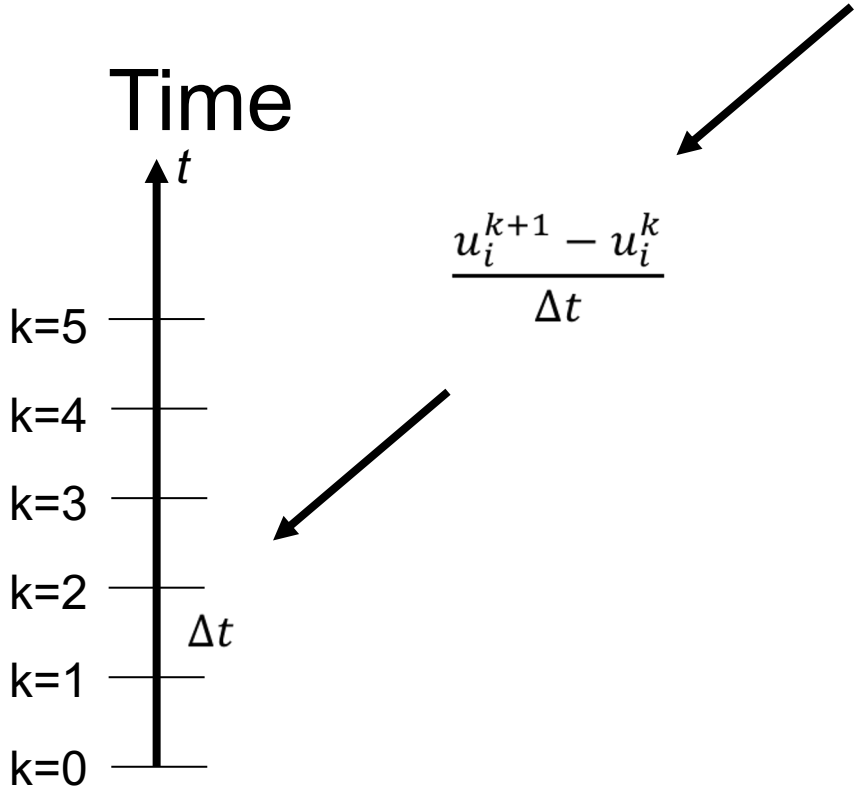
Discretize: Continuous Discrete

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

EXASCALE COMPUTING PROJECT

Discretize: Continuous □ Discrete

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



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

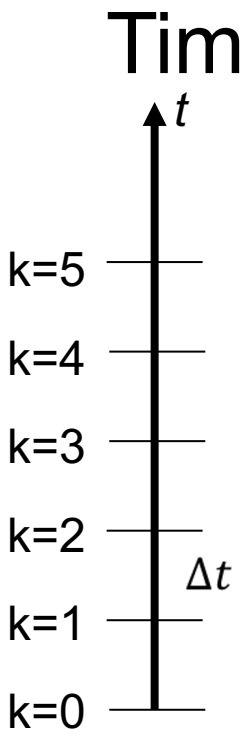
ECP EXASCALE COMPUTING PROJECT

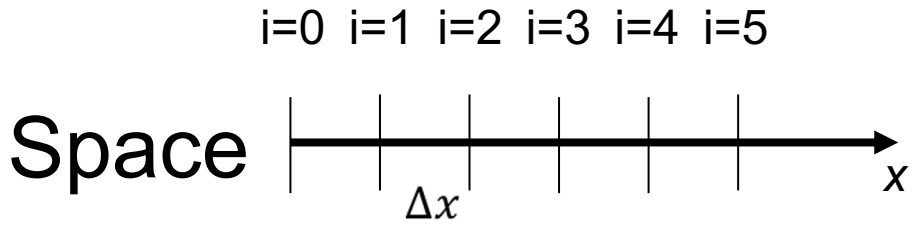
Discretize: Continuous Discrete

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

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

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



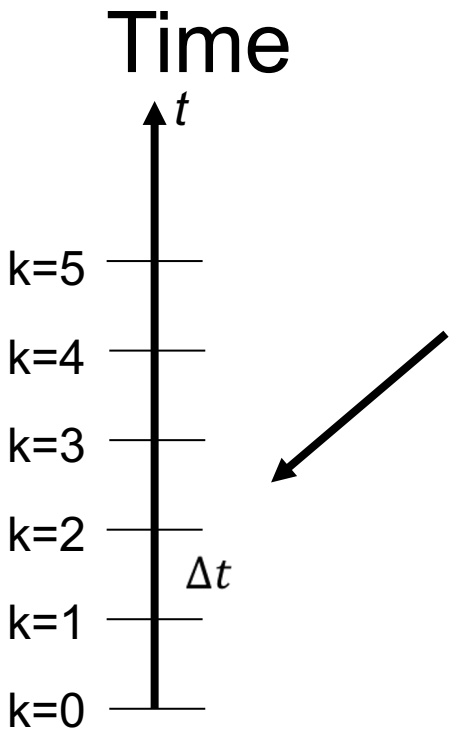


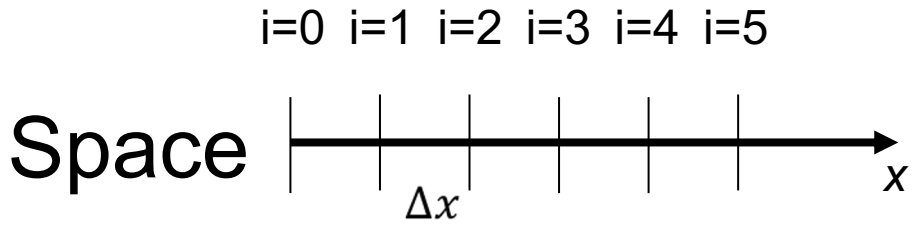
ECP EXASCALE COMPUTING PROJECT

Discretize: Continuous Discrete

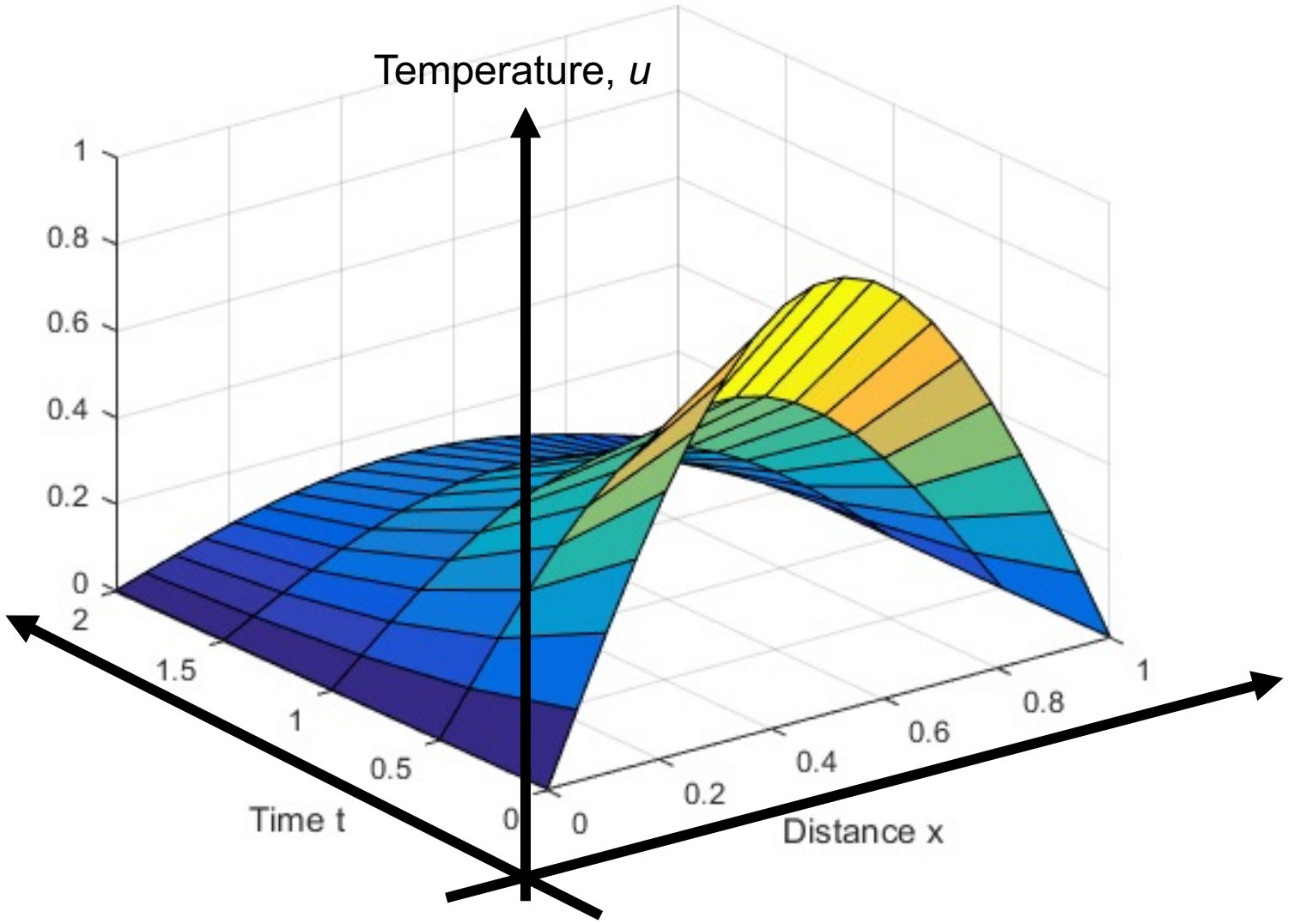
$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

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





ECP EXASCALE COMPUTING PROJECT



ECP EXASCALE COMPUTING PROJECT

A numerical, iterative solution algorithm

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

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

- *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 $r > \frac{1}{2}$

ECP EXASCALE COMPUTING PROJECT

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
{




}
```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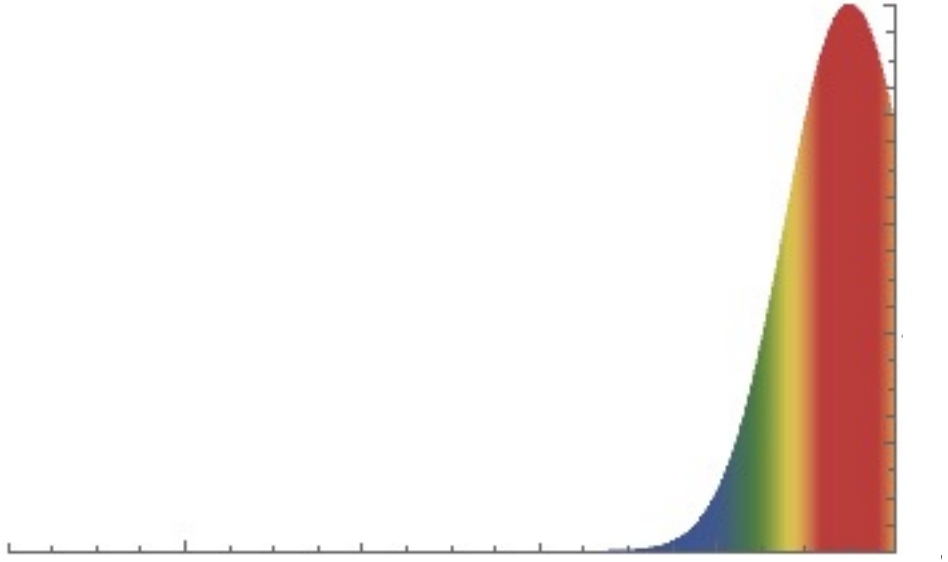
Exercise #2 (1 min)
Build and test the application

```
% 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

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Exercise #3 (2 mins):
Run the application to model a problem of interest

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

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

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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?

ECP EXASCALE COMPUTING PROJECT

Simplifications hide challenges of math package software engineering

- **Challenges in numerical algorithms**
  - Discretizations: Dimensions, geometries, material interfaces, etc
  - Solvers: Implicit, explicit, iterative, direct, preconditioners, etc.
  - Time Integrators: Adaptive, faster convergence, efficiencies, etc.
  - Optimization: Outer loops, nonintrusive, reduced-order models, etc.
  - Validation & verification: Vetted, trusted results, community accepted
- **Challenges in software development**
  - Time and space performance
  - Scalability & performance portability
  - Encapsulation, interfaces & interoperability
  - Documentation, ease of installation, ease of use
  - Sustainable open source, supported with regular updates, bug tracking/fixing
  - Support for user-defined customization and extensibility

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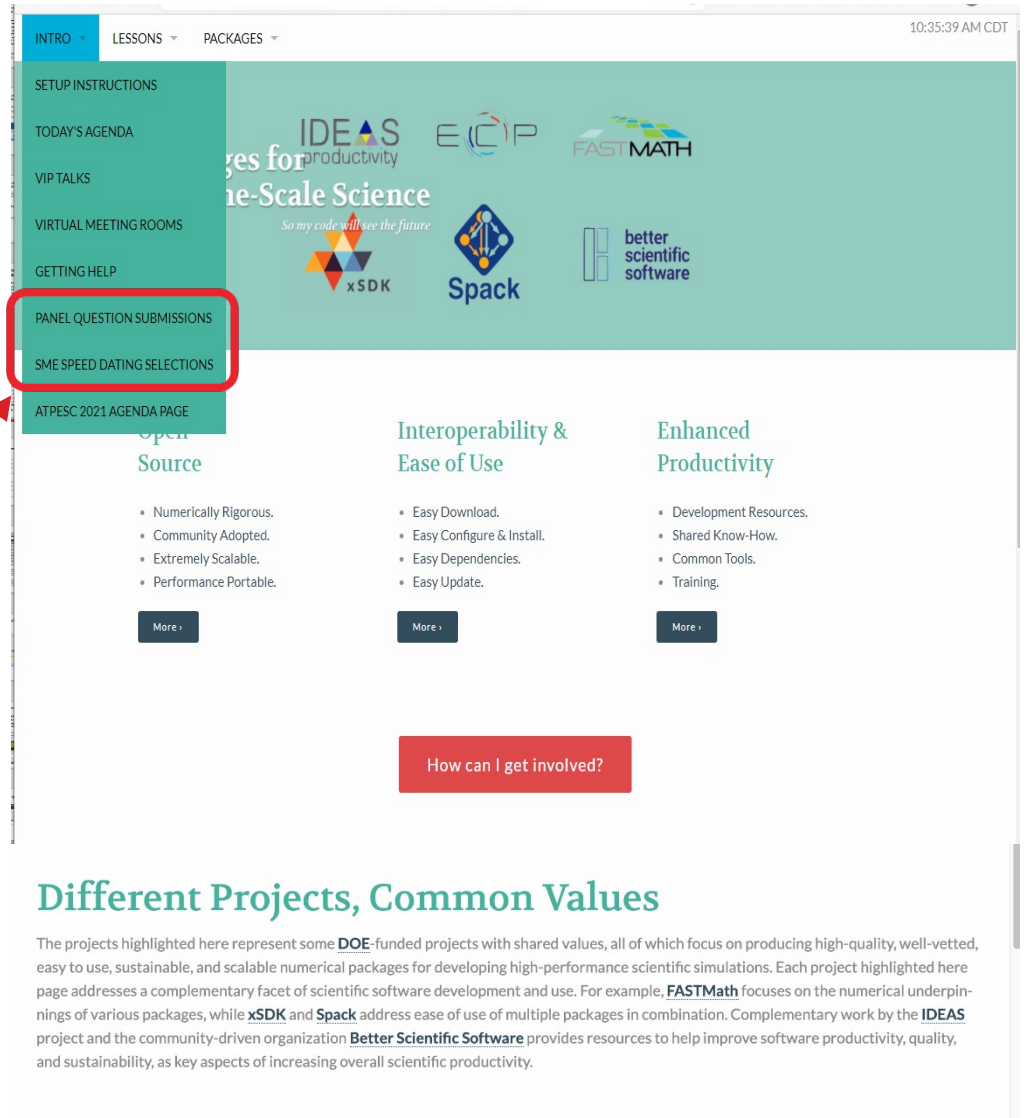
Next steps

- **Attend parallel sessions**
  - **10:30 CDT and 11:45 CDT**
  - **Access Zoom rooms via**

    https://xsdk-project.github.io/MathPackagesTraining2021/
- **During breaks and lunch**
  - **Sign up for discussions with numerical software developers** (optional)
    - Your email address
    - Select 1st, 2nd, and 3rd priorities
    - Brief description of interests
    - Complete by 4:30 pm CDT
  - **Submit questions for panelists** (optional)
- **Panel session: 1:45 pm CDT**



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)	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 Peter 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 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 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 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)

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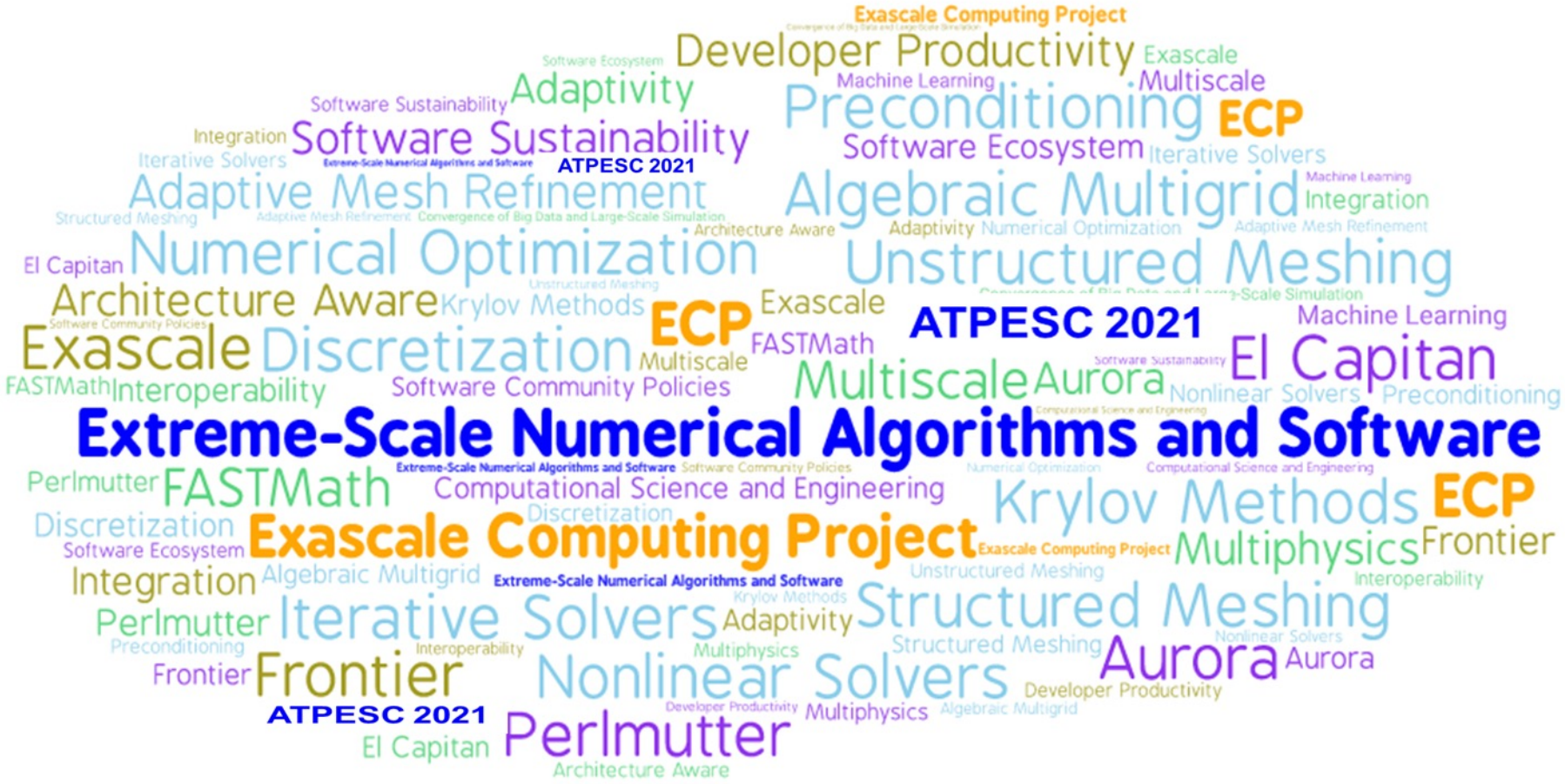
Addendum … ATPESC afternoon sessions



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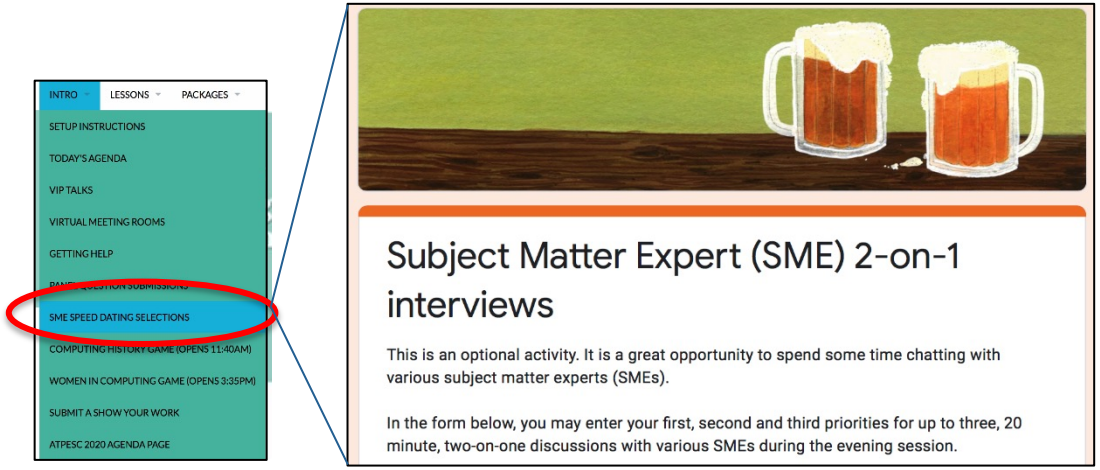
Next steps: Extreme-Scale Numerical Algorithms and Software

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

- **Panel session: Main Room @ 1:45 pm CDT**
- **During breaks and lunch**
  - **Sign up for discussions with numerical software developers** (optional)
    - Your email address
    - Select 1st, 2nd, and 3rd priorities
    - Brief description of interests
    - Complete by 3:30 pm CDT



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

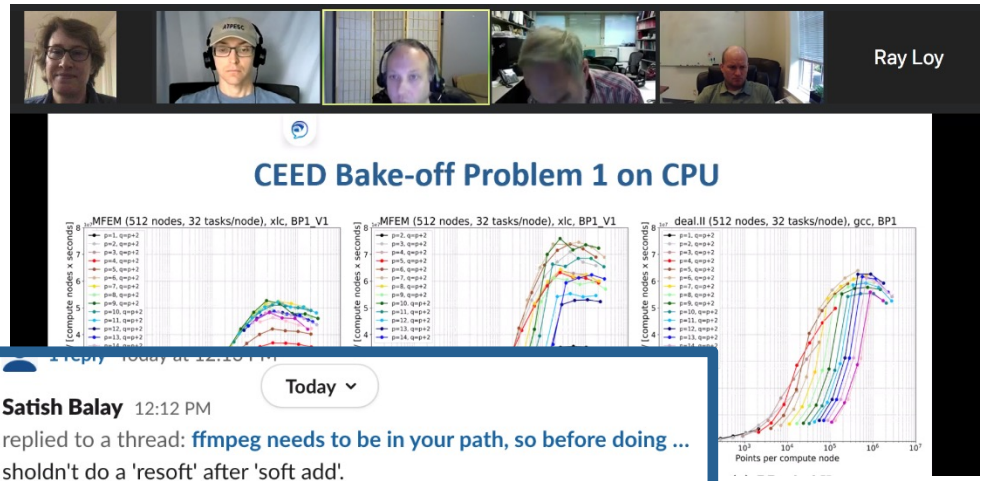
Not shown:
- Ann Almgren
- Aaron Fisher
- Richard Mills

The ATPESC Team 2021 on Zoom

EXASCALE COMPUTING PROJECT

Parallel morning sessions

A few highlights



track-5-aurora-breakout
track-5-elcapitan-breakout
track-5-frontier-breakout
track-5-numerical
track-5-perlmutter-breakout

Sarah Osborn 12:43 PM
Welcome to Session 2: Iterative Solvers & Algebraic Multigrid (with hypre) of Track 5 - Numerical Algorithms and Software for Extreme-Scale Science. Ulrike Yang (Lawrence Livermore National Laboratory) will begin presenting at 11:45am CDT.

The hands-on instructions are here: https://xsdk-project.github.io/MathPackagesTraining2020/lessons/krylov_amg_hypre/

Session organization notes are listed below:

ask

Today

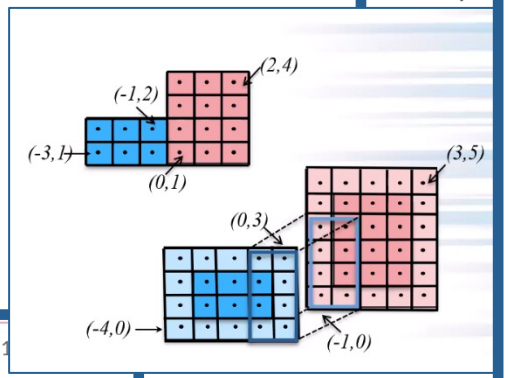
Satish Balay 12:12 PM
replied to a thread: **ffmpeg needs to be in your path, so before doing ...**
sholdn't do a 'resoft' after 'soft add'.
resoft is used after modifying ~/.soft.cooley

Ann Almgren 12:15 PM
just checking in ... everyone doing ok?
2 replies Last reply today at 12:16 PM

Muaaz Awan 12:17 PM
`soft add` needs to be done in the login node?
2 replies Last reply today at 12:19 PM

Don Willcox 12:17 PM
I can do it on the compute node and it seems to wo

Ligia Diana Amorim 12:20 PM
Yes
3 replies Last reply today at 12:23 PM



Ligia Diana Amorim 1
Thank you!

Kevin Green 1:49 PM
Thank you

New

Mark C Miller 1:02 PM
Reminder to everyone, don't pass up this (optional) activity to meet one-on-one with subject matter experts (SMEs) after the end of the regular agenda...

Today

Pieter Ghysels 12:21 PM
Please follow along with the SuperLU hands on, and post any questions/comments here.
We are monitoring this. (edited)

Lois Curfman McInnes 12:31 PM
Friendly reminder: Next parallel sessions begin at 11:45 am CDT, see info and Zoom links here: – https://xsdk-project.github.io/MathPackagesTraining2020/agenda

> **ATPESC 2020 Math Packages Training**
> Numerical Packages Agenda
> Software Carpentry Style Lessons for Math Packages

New

Thomas Linker 12:37 PM
Thanks this was great!

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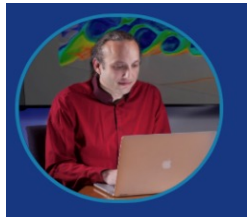
Panel: Contributing to the Numerical Software Community

1:45 pm CDT, Main Room in Zoom

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

- Panelists

Ann Almgren, LBL


Aaron Fisher, LLNL

Richard Mills, ANL

Cameron Smith, RPI

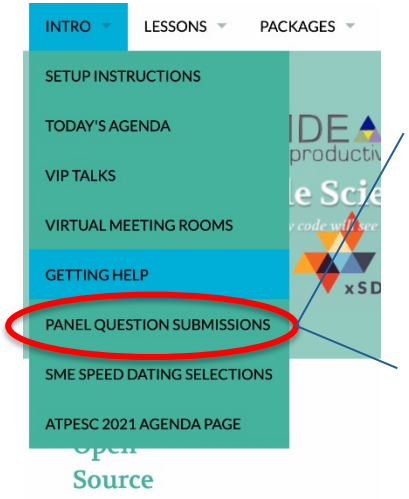
Dan Reynolds, SMU

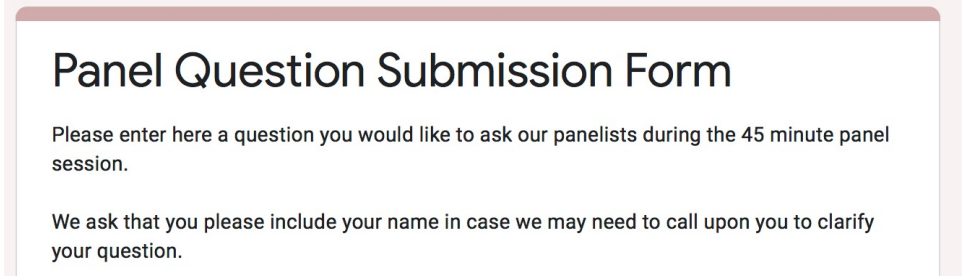
Christian Glusa, SNL

- Moderator

Alp Dener, ANL

Lois Curfman McInnes, ANL





Afternoon agenda

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

Nonlinear Solvers (with PETSc)

Slides

We will begin with a quick overview of iterative solvers for nonlinear systems, and then take a deeper look into Newton-Krylov methods and how to use them via the PETSc Scalable Nonlinear Equation Solvers (SNES) component. We will do some hands-on exploration with a classic computational fluid dynamics benchmark, the lid-driven cavity prob
end by looking at how nonlinear composition and preconditioning can be us
wide array of nonlinear solvers from the algorithmic building blocks in SNE
strate how these techniques can handle particularly difficult nonlinearities.

Time Integration (with SUNDIALS)

Slides

In this lecture we will discuss the role and impact of high order, adaptive, and flexible time integration libraries in solution accuracy and computational efficiency of large-scale simulations. Due to the wide variety of backgrounds among ATPESC participants, we will briefly discuss

- the location of time integrators in the HPC landscape, and their reliance on scalable nonlinear and linear solver libraries,
- the different categories of time integration methods (explicit/implicit/IMEX),
- properties of time integration methods (order of accuracy, linear
- daptivity for improving accuracy and efficiency,
- ime integration packages.

ately half of the time period in lecture, followed by hands-on exer-
ity, accuracy, temporal adaptivity, and the role of problem-specific
e hands-on exercises focus on time-dependent PDEs, and use the
rary for time integration, along with the AMReX library for spatial

Optimization (with TAO)

Slides

This lecture will provide an introduction to numerical optimization with a theoretical focus on simulation-based problems. We will introduce the user interfaces for the Toolkit for Advanced Optimization (TAO) package within the PETSc library and exercise several gradient-based algorithms on scalable synthetic test problems. We will observe and discuss the relative convergence of different classes of algorithms and sensitivity analysis methods in a parallel environment.

02:35	50	**Parallel Session Three**		
		Nonlinear Solvers (with PETSc)	Richard Tran Mills	Frontier
		Optimization (with TAO)	Alp Dener	Aurora
		Time Integration (with SUNDIALS)	Dan Reynolds	Perlmutter
		Iterative Solvers & Algebraic Multigrid (with HYPRE)	Ulrike Yang Sarah Osborn	El-Capitan
03:25	15	**Break** *SME Selections Due*		
03:40	50	**Parallel Session Four**		
		Nonlinear Solvers (with PETSc)	Richard Tran Mills	Frontier
		Optimization (with TAO)	Alp Dener	Aurora
		Time Integration (with SUNDIALS)	Dan Reynolds	Perlmutter
		Direct Solvers (with SuperLU/Strumpack)	Sherry Li Pieter Ghysels	El-Capitan
04:30	5	Telecon Transition		
04:35	25	Working with Numerical Packages in Practice	Ann Almgren	Main-room
		END OF OFFICIAL AGENDA		
05:00	15	**Break**		
05:15	80	SME Speed Dating OPTIONAL ACTIVITY		

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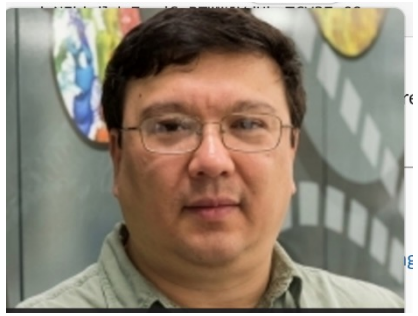
Thank you to all ATPESC staff



Special thanks to Ray Loy and Yasaman Ghadar

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

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

From Ligia Diana Amorim to Everyone:
And the great tutorials like the ones here at ATPESC also help a lot!

From Mark C. Miller to Everyone:
Ditto

From Neil Mehta to Everyone:
Thank you!

From Valeria Barra to Everyone:
I also want to add that I really appreciated the website put together for today's tutorials. Thanks for the nice work!

From Ligia Diana Amorim to Everyone:
Thank you all for the great sessions today! Yes, indeed, the website was great to follow all the hands on

From Zhi Jackie Yao to Everyone:
Thank you!

From Juan Colmenares to Everyone:
yes

From Kevin Green to Everyone:
Thanks for all of the hands on material today! Was a lot of info to take in a once, but I'm looking forward to slowly digesting it all over the next evenings :)

From Mukund Raj to Everyone:
Thanks all for the presentation and great materials!

Some Zoom and Slack chats during sessions on extreme-scale numerical algorithms and software

Severin Diederichs 3:53 PM
How well does the adaptive time step selection work with multi step methods like a 5th order Adams-Bashforths integrator?
1 reply Today at 3:57 PM

Komal Kumari 4:04 PM
Unstable?
1

Zac Johnston 4:05 PM
about 21?

Juan Diego Colmenares Fernandez 4:05
yeah around 22

Aaron Fisher 3:23 PM
There are Python bindings for MFEM (edited)

Kevin Green 3:23 PM
Doesn't scipy interface to SuperLU?

Sherry Li 3:24 PM
@Kevin Green Indeed! I think they wrote the Python interface, it's not in superlu release.
2 replies Last reply today at 3:27 PM

Kevin Green 3:27 PM
Thanks panelists
9

Bruce A. Perry 5:34 PM
Thanks for the presentation!

Daniel R. Reynolds 5:34 PM
You're welcome!

Hugo Brunie 5:34 PM
Thanks, great tutorial

Philippe Blain 5:35 PM
Thanks Dan, very nice presentation! (edited)

CASC

Center for Applied Scientific Computing

Lawrence Livermore National Laboratory

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