

Track 4: Numerical Algorithms and Software for Extreme-Scale Science

Presented to
ATPESC 2017 Participants

Lois Curfman McInnes
Senior Computational Scientist
Mathematics and Computer Science Division
Argonne National Laboratory

Q Center, St. Charles, IL (USA)
Date 08//07/2017



ATPESC Numerical Software Track



Track 4: Goals

Numerical Algorithms and Software for Extreme-Scale Science

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)

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

Track 4: Numerical Algorithms and Software for Extreme-Scale Science

TUESDAY, August 1

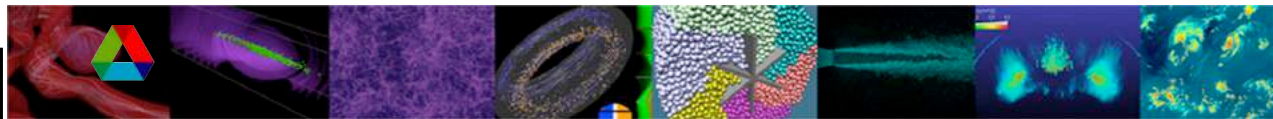
Time	Title of presentation	Lecturer
4:30 pm	Algorithmic Adaptations to Extreme Scale	David Keyes, KAUST

THURSDAY, August 3

Time	Title of presentation	Lecturer
4:45 pm	Communication-Avoiding Algorithms for Linear Algebra	Jim Demmel, UC Berkeley

MONDAY, August 7

Time	Title of presentation	Lecturer
8:35 am	Adaptive Linear Solvers and Eigensolvers	Jack Dongarra, U. Tennessee-Knoxville, ORNL



continue

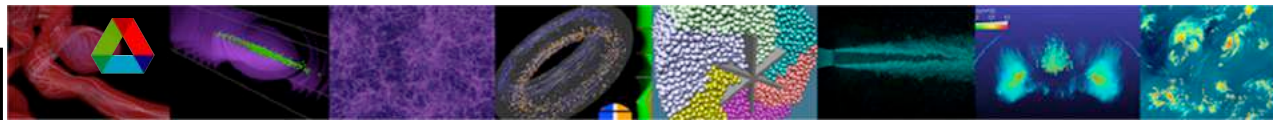


Introduction to the Sessions

Track 4: Numerical Algorithms and Software for Extreme-Scale Science

MONDAY, August 7

Time	Title of presentation	Lecturer
9:30 am	Numerical Software: Foundational Tools for HPC Simulations	Lori Diachin, LLNL
... with hands-on sessions throughout the day for various topics		
11:00 am	Structured Mesh Technologies	Ann Almgren, LBNL
11:45 am	Unstructured Mesh Technologies	Tzanio Kolev, LLNL and Mark Shephard, RPI
12:30 pm	Lunch	
1:30 pm	Panel: Heterogeneity and Performance Portability	Mark Miller, LLNL (Moderator)
2:15 pm	Time Integration	Carol Woodward, LLNL
3:00 pm	Nonlinear Solvers and Krylov Methods	Barry Smith, ANL
3:35 pm	Break	
4:05 pm	Sparse Direct Solvers	Sherry Li, LBNL
4:35 pm	Algebraic Multigrid	Ulrike Yang, LLNL
5:05 pm	Introducing the xSDK and Spack	Lois Curfman McInnes and Barry Smith, ANL



+ Hands-on

Track 4: Numerical Algorithms and Software for Extreme-Scale Science

MONDAY, August 7

Time	Title of presentation	Lecturer
5:30 pm	Dinner + Panel: Extreme-Scale Algorithms and Software	Mark Miller, LLNL (Moderator)
6:30 pm	Conforming and Nonconforming Adaptivity for Unstructured Meshes	Tzanio Kolev, LLNL and Mark Shephard, RPI
7:00 pm	Open hands-on time	All
7:30 pm	Enabling Optimization Using Adjoint Software	Hong Zhang, ANL
8:00 pm	Open hands-on time	All
8:30 pm	One-on-one discussions with ATPESC participants	
9:30 pm	Adjourn	

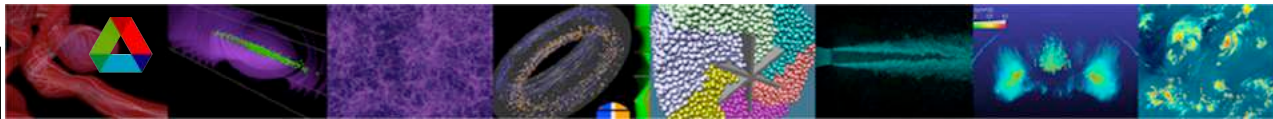
Hands-on Lead: Mark Miller (LLNL)

Additional contributors to lectures and hands-on lessons:

Satish Balay (ANL), Aaron Fisher (LLNL), David Gardner (LLNL), Lois Curfman McInnes (ANL)

Additional contributors to Gallery of Highlights:

Karen Devine (SNL), Mike Heroux (SNL), Dan Martin (LBNL)



+ Hands-on