The Argonne Training Program on Extreme-Scale Computing

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The Argonne Training Program in Extreme-Scale Computing (ATPESC) provides training on the key skills, approaches, and tools necessary to design, implement, and execute Computational Science and Engineering (CS&E) applications on current high-end systems
– and the leadership-class systems expected to be available in 2017 and beyond.

The training features lectures by leading computer and computational scientists in the topics covered and

Extensive hands-on exercises on leadership-class computers.

http://extremecomputingtraining.anl.gov
Motivation for the ATPESC

- With the challenges posed by the architecture and software environments of today’s most powerful supercomputers -- and even greater complexity on the horizon from next-generation and exascale systems -- there is a critical need for specialized, in-depth training for the scientists poised to facilitate breakthrough science and engineering using these computational resources.
Computational research at the high end requires expertise in many areas

- The architecture and software environments of today's most powerful systems - including those at the Argonne Leadership Computing Facility and at the Oak Ridge Leadership Computing Facility - pose new and unique challenges to their users.

- Technology trends indicate that the next generation of systems, circa 2017, and the exascale systems projected for 2022 will feature far greater parallelism and complexity of architectures.

- Computational research projects tackle ever more complex projects.
Scope of the Argonne Training Program

- The ATPESC covers many of the key skills that computational scientists and engineers need to carry out their research on leadership-class systems.
- In two weeks it is not possible to present detailed material on all topics; in some cases we aim to make participants of the existence of certain approaches, methods, and tools.
  - E.g., PGAS languages, software engineering tools.
High-level view of curriculum

- Computer architectures, mathematical models and numerical algorithms
- Programming methodologies that are effective across a variety of today’s supercomputers and that are expected to be applicable to exascale systems
- Multiple approaches on unifying concepts and levels of abstraction that provide migration paths and performance portability among current and future architectures
- Approaches to building community codes for HPC systems, and methodologies and tools relevant for Big Data applications
Curriculum tracks and their leaders

- Architectures – Pete Beckman
- Programming models and languages – Rusty Lusk, Rajeev Thakur
- Mathematical algorithms and software -- Lois McInnes, Lori Diachin
- Software engineering in scientific computing – Katherine Riley, Anshu Dubey
- Performance and debugging tools – Kalyan Kumaran, Scott Parker
- Visualization and Data Analysis – Mike Papka
- Data-intensive computing – Rob Ross and Rob Latham
- Community codes– Katherine Riley and Anshu Dubey
- Application case studies– Katherine Riley and Anshu Dubey
Logistics

- The training program is held at the Pheasant Run Resort in St. Charles, Illinois
  - Lodging and all meeting rooms are at the same facility
  - Moderately priced: we use the old conference center

- Participants pay no registration fee

- Domestic airfare, meals, and lodging are provided for the participants
Program Schedule

- **Daily schedule**
  - 08:30 – 10:30 Lectures
  - 10:30 – 11:00 Break
  - 11:00 – 12:00 Lectures
  - 12:00 – 13:00 Lunch and Hands-on exercises
  - 13:00 – 15:00 Lectures
  - 15:00 – 15:30 Break
  - 15:30 – 17:30 Lectures
  - 17:30 – 18:30 Dinner and dinner talk
  - 18:30 – 21:30 Hands-on exercises and lectures

- **Program begins mid-afternoon on a Sunday**
- **Free time in middle week-end: Saturday afternoon and Sunday**
- **Program ends noon second Friday**
Qualifications of Applicants

- **Target participants are**
  - doctoral students,
  - postdocs, and
  - computational scientists.

- **Developers of programming models, algorithms, and tools for leading-edge systems may also apply.**

- **This program provides advanced training. Therefore, successful applicants must**
  - Have substantial experience in MPI and/or OpenMP programming
  - have used at least one HPC system for a reasonably complex application and
  - are planning to conduct CS&E research on large-scale computers.

- **~60 participants are selected.**
Application and selection process

- **Applicants submit through a website:**
  - Letter written by applicant stating purpose for attending the training program and description of computing experience.
  - Curriculum Vitae.
  - One letter of recommendation from an advisor or supervisor.

- **In 2013 we received 160 applications**

- **A committee of five people selected 63 participants, based on candidates having**
  - Substantial MPI and/or OpenMP programming experience
  - Used an HPC system for a reasonably complex application
  - Having conducted or are preparing to conduct computational science and engineering research on large-scale computers
**ATPESC 2013 Participant Distribution**

<table>
<thead>
<tr>
<th>Category</th>
<th>Count</th>
</tr>
</thead>
<tbody>
<tr>
<td>Undergraduate student</td>
<td>1</td>
</tr>
<tr>
<td>Graduate student</td>
<td>32</td>
</tr>
<tr>
<td>Postdoc</td>
<td>12</td>
</tr>
<tr>
<td>Assistant professor</td>
<td>2</td>
</tr>
<tr>
<td>Research staff academia</td>
<td>4</td>
</tr>
<tr>
<td>Research staff US government labs</td>
<td>7</td>
</tr>
<tr>
<td>Research staff foreign labs</td>
<td>2</td>
</tr>
<tr>
<td>Industry</td>
<td>3</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>63</strong></td>
</tr>
</tbody>
</table>
## Other ATPESC 2013 Participant Profiles

| US Government laboratory affiliation: | 7 research staff  
| Argonne (3)  
| Army Research Laboratory  
| Geophysical Fluid Dynamics Laboratory  
| LANL (3)  
| LLNL  
| NCAR  
| National Energy Technology Laboratory | 4 postdocs |
| Foreign institution affiliation: | 2 graduate students  
| Brazil (Brazil Nat Lab)  
| Germany (Juelich, Aachen)  
| Italy (CMCC, University of Salento)  
| Singapore (National University Hospital)  
| Greece (National Technical U of Athens) | 1 assistant professor  
| 2 research staff  
| 2 postdocs |
| Gender | 54 Male  
| 9 Female (11 were selected but 2 did not accept the invitation due to changes in their schedules) |
ATPESC main lecture hall
Access to ATPESC 2013 Lectures

- Slides for all lectures can be downloaded from the 2013 agenda page:
- Videos of the talks will be online soon
ATPESC 2013 Lectures
Supercomputing Architecture Trends

- *Architecting for Exascale* -- Tryggve Fossum (Intel Corp.)
- *An Introduction to Parallel Supercomputing* -- Pete Beckman (ANL)
- *PIM & Memory: The Need for a Revolution in Architecture* -- Peter Kogge (U. of Notre Dame)
- *Macro Architecture for Exascale* -- Pavan Balaji (ANL)
- *Micro Architecture for Exascale* -- Tryggve Fossum (Intel Corp.)
ATPESC 2013 Lectures
Programming Models for HPC

- Programming Models for HPC -- Marc Snir (ANL)
- MPI for Scalable Computing -- Bill Gropp (U. of Illinois), Rusty Lusk (ANL), Rajeev Thakur (ANL)
- Using OpenMP for Intranode Parallelism, OpenMP 4.0 and the Future of OpenMP -- Bronis de Supinski (LLNL)
- Writing Parallel Programs that Work -- Paul Petersen (Intel)
- Multi-resolution Global-View Programming in Chapel -- Brad Chamberlain (Cray)
- Partitioned Global Address Space Programming -- Kathy Yelick (LBNL and UC Berkeley)
- Programming with Parallel Migratable Objects -- Sanjay Kale (U. of Illinois)
ATPESC 2013 Lectures
Accelerator and GPU Programming

- High Performance with Accelerator Programming – Jeff Vetter (ORNL) and Bronson Messer (ORNL)
- An Introduction to OpenACC -- Jeff Vetter (ORNL) and Bronson Messer (ORNL)
- The Evolution of GPU Accelerated Computing -- Steve Parker (NVIDIA Corp.)
- Scientific Computing on GPUs -- Nick Frontiere (ANL)
- MPI and Hybrid Programming Models – Bill Gropp (U. of Illinois)
ATPESC 2013 Lectures
Mathematical Software and Numerical Algorithms

Lecturers
- Mark Adams (LBNL)
- Jim Demmel (UC Berkeley)
- Lori Diachin (LLNL)
- Jack Dongarra (UT and ORNL)
- Robert Falgout (LLNL)
- Glen Hansen (SNL)
- David Keyes (KAUST)
- Mark Miller (LLNL)
- Mark Shepard (RPI)
- Barry Smith (ANL)
- Cameron Smith (RPI)
- Tim Tautges (ANL)
- Carol Woodward (LLNL)

Topics
- Architectural adaptation of algorithms
- Algebraic solvers
- PETSc toolkit
- Preconditioners
- Nonlinear and differential/algebraic equation solvers
- AMR technologies
- Parallel adaptive unstructured mesh simulations
- Communication-avoiding algorithms
- Adaptive linear solvers and eigensolvers
ATPESC 2013 Lectures
Tookits and Frameworks

- Scott Parker (ANL)
- Mike Brim (ORNL)
- David Lecomber (Allinea Software Ltd.)
- Allen Malony (U. of Oregon)
- John Mellor-Crummey (Rice U.)
- Mike Wilde (ANL)
ATPESC 2013 Lectures
Community Codes and Application Case Studies

- Salman Habib (ANL)
- Sean Couch (U. of Chicago)
- Jeff Hammond (ANL)
- Hal Finkel (ANL)
- Anshu Dubey (LBNL)
- Jim Phillips (U. of Illinois)
ATPESC 2013 Lectures
Visualization and Data Analysis

- Mike Papka (ANL)
- Tom Peterka (ANL)
- Frank Childs (LBNL and U. of Oregon)
- Mark Hereld (ANL)
- Joseph Insley (ANL)
- Venkat Vishwanath (ANL)
- David DeMarle (Kitware, Inc.)
ATPESC 2013 Lectures
Data Intensive Computing and I/O

- Rob Ross (ANL)
- Rob Latham (ANL)
- Quincey Koziol (The HDF Group)
- Steve Tuecke (U. of Chicago)
The Lecture and Hands-on Exercises Room
Hands-on sessions

- The ATPESC provides extensive access to leadership-class computers for extensive hands-on sessions.

- The 2013 ATPESC provided access to:
  - Vesta: IBM Blue Gene/Q with 32K cores
  - Mira: IBM Blue Gene/Q with 768K cores
  - Tukey: visualization and analysis cluster at ALCF
  - Titan: Cray XK7 with 299,008 cores and 18,688 GPUs
  - Keeneland KIDS: a heterogeneous HP SL-390 (Ariston) cluster with 120 nodes, 240 CPUs and 360 GPUs.

- In addition, during evening hands-on sessions, lecturers and their assistants provide individualized help and tutoring to the participants.
Evening hands-on exercises
Rusty Lusk provides one-on-one training
Working into the late evening
Dinner talks

- Purpose: present additional topics that will probably be relevant to the participants’ research at some point in their career – or are interesting
Dinner Talks in 2013

- **Grid, Cloud, and Beyond: what have we learned about computing on demand?** -- Ian Foster (Argonne and U. of Chicago)
- **Petascale Post-doctoral Computing or: How I Learned to Stop Worrying and Blow Up Stars** -- Sean Couch (U. of Chicago)
- **Large-Scale Visual Analysis** -- Chris Johnson (U. of Utah)
- **Scientific Computing while Supercomputing: Software Carpentry** -- Aron Ahmadia (Continuum Analytics)
- **Perspectives on Teaming from the DOE National Labs** -- Lori Diachin (LLNL)
- **Dawn of the Era of Quantum Computation** -- Bob Lucas (USC-ISI)
- **Urban Center for Computation and Data** -- Charlie Catlett (Argonne)
- **Argonne National Laboratory: Innovative Research in the National Interest** -- Mark Peters (Argonne)
- **Big Data + Extreme-scale time to compute -> Actionable Insights** -- Alok Choudhary (Northwestern U.)
Chris Johnson delivering an evening lecture
ATPESC Student Snapshot, Jordan Musser

- Jordan works as research engineer in the DOE’s National Energy Technology Laboratory’s (NETL) Computational and Basic Sciences Division where he is a user and developer of MFIX, an open-source reacting multiphase CFD software.

- “My primary goal for applying to attend ATPESC was to gain knowledge that will help me refine MFIX so we can fully utilize the NETL-SBEUC, a 24K-core system used for energy-related simulations. I intend to incorporate many of the strategies I learned at ATPESC into my regular development activities.”
ATPESC Student Snapshot: Jeff Amelang

- Jeff is a fourth year Ph.D. candidate in Mechanical Engineering at the California Institute of Technology studying coarse-grained molecular dynamics, specifically the atomistic to continuum transition through the quasicontinuum method. His work includes a heavy emphasis on the application of high-performance computing to systems of engineering interest.

- “I study an area of physics that would be out of reach without HPC. I applied for the program because I love HPC, program HPC systems all day, taught an HPC class, and yet I hadn’t had formal training in it for lack of opportunity and availability. The class was exactly what I was looking for: background and foundational knowledge, how to leverage the current state of the art, and a glimpse at what the future of HPC looks—all from leaders in the field. It was invaluable.”
Fredrik is a second year Ph.D. student in Computer Science at MIT CSAIL, where he is a member of the D-TEC X-Stack project at work on declarative and operational programming model constructs and compiler techniques to support practical higher-level, tunable and performance-portable programming on extreme-scale machines.

“As a computer scientist, the Programming Model and Application tracks were extremely helpful in giving me a greater understanding of how the algorithms used on extreme-scale machines fit together, and what the challenges of implementing them using contemporary programming models are. I plan to use what I learned at ATPESC to inform my research and to work to transfer the knowledge to the MIT X-Stack team. I hope this will help us develop technologies that solve real problems faced by the HPC community.”
Argonne Training Program on Extreme-Scale Computing: 2013 participants
Training

Argonne Training Program on
EXTREME-SCALE COMPUTING
July 28 – August 9, 2013

2014 dates:
August 3-15

- ALCF Outreach
  - Workshops
    - Tutorials
    - Lectures
    - Hands-on
    - One-on-one with ALCF experts
      - Benchmark, scale up, tune your application
  - Webinars
    - Mira Performance Bootcamp
    - Getting Started
    - Leap to Petascale
Acknowledgments

- The ATPESC is funded by DOE-SC/ASCR
- The FASTMath and SDAV SciDAC institutes presented major portions of the curriculum
- The Argonne and Oak Ridge Leadership Computing Facilities and the Keeneland National Institute for Experimental Computing provided access to their systems for hands-on exercises
- ALCF staff provided many lecturers and support for all aspects of the the program
- Rusty Lusk, Rajeev Thakur, and Pete Beckman (Argonne MCS Division) participated in the organizing committee