

# *High Performance Software Tools to Fast-Track The Development of Scalable and Sustainable Applications*

The DOE Advanced Computational Software Collection (ACTS)

Eleventh DOE  
ACTS Collection Workshop  
Berkeley, California, August 17-20, 2010

**Tony Drummond**  
Computational Research Division  
Lawrence Berkeley National Laboratory



# OUTLINE

- HPC Tutorial Agenda
- Motivation
- Hardware Trend
- HPC Software Stack
- The DOE ACTS Collection
  - ACTS Functionality
- Summary

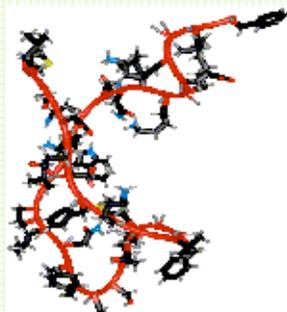
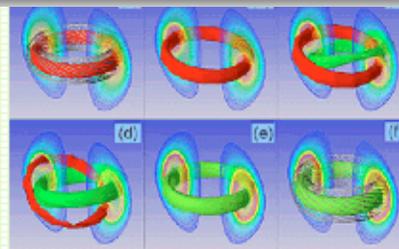
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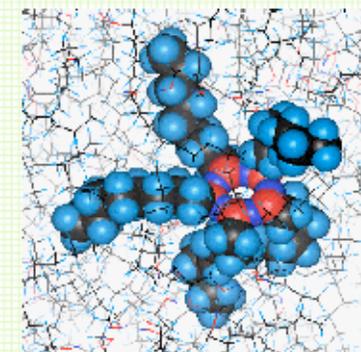
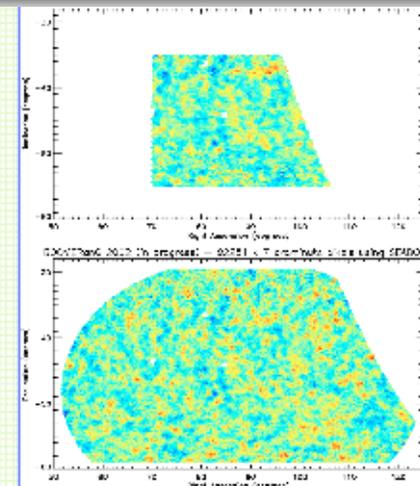


# Motivation - HPC Applications

- Accelerator Science
- Astrophysics
- Biology
- Chemistry
- Earth Sciences
- Materials Science
- Nanoscience
- Plasma Science
- 
- 



OmniSP is a parallel distributed memory code intended for the modeling and analysis of accelerator cavities, which requires the solution of generalized eigenvalue problems. A parallel exact shift-invert eigenvalue based on PARDYAC and SuperLU, has allowed in the solution of a problem of order 7.5 million with 204 million unknowns.



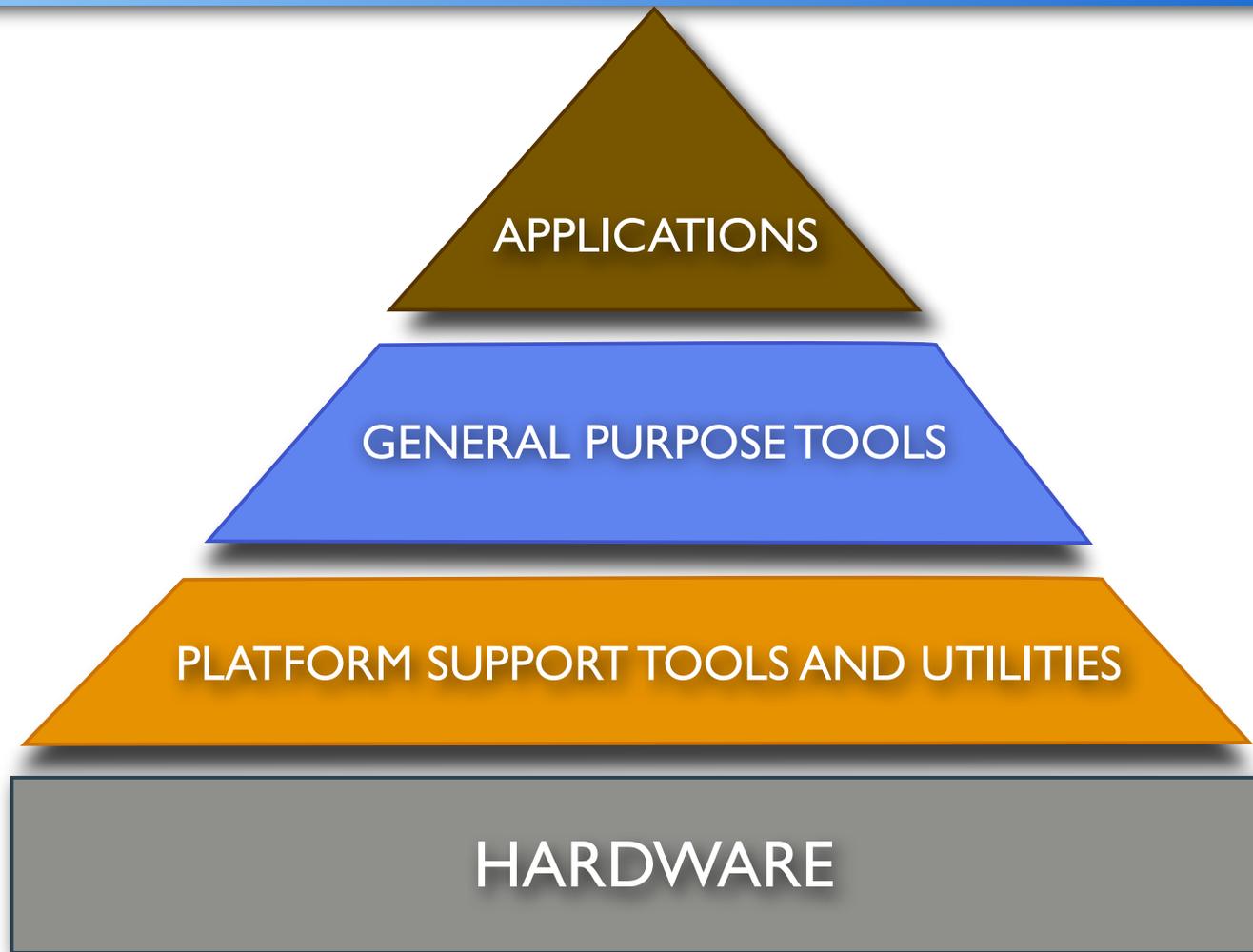
## Commonalities:

- Major advancements in Science
- Increasing demands for computational power
- Rely on available computational systems, languages, and software tools

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# HPC Software Stack

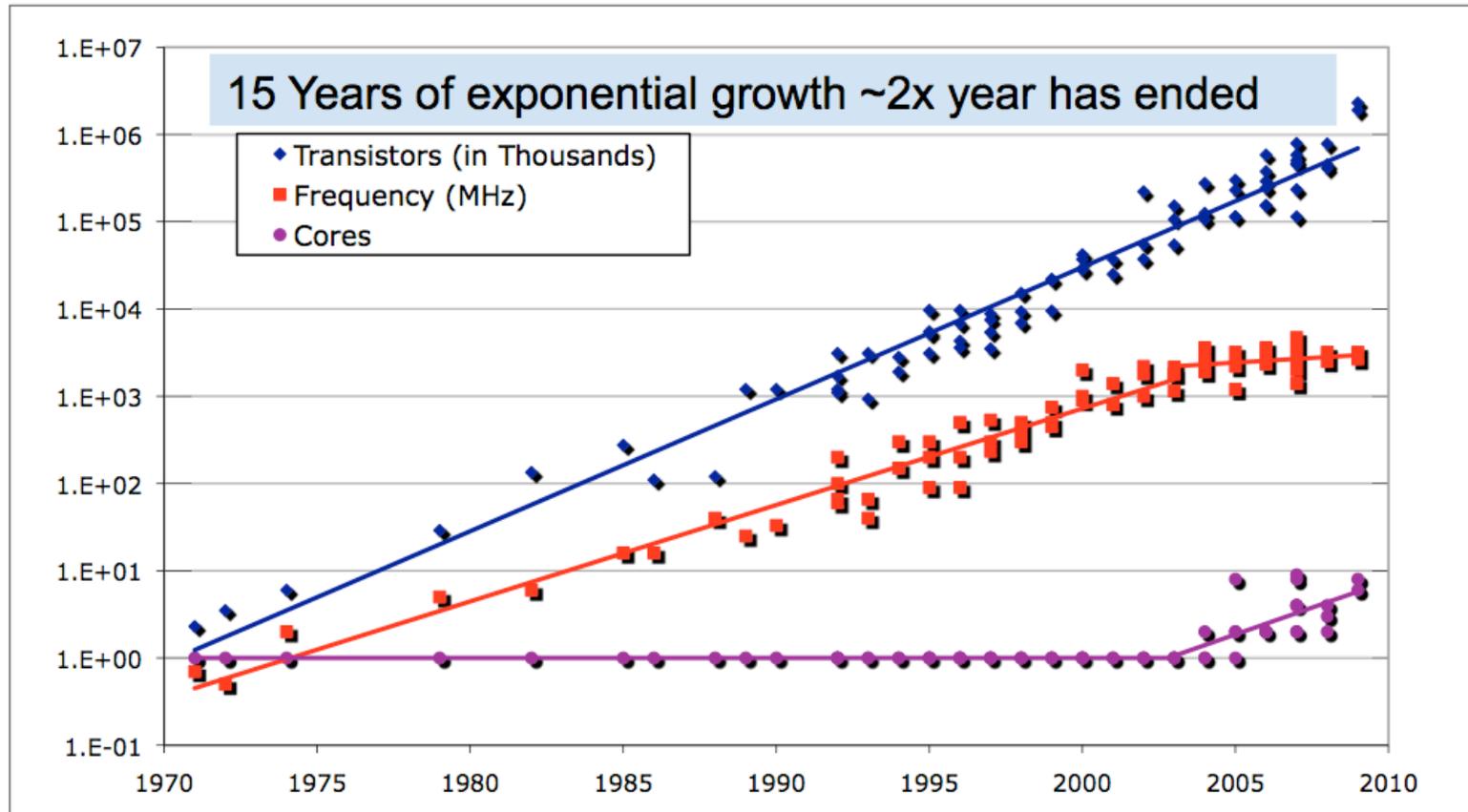


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# Hardware Trend



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# Hardware Trend

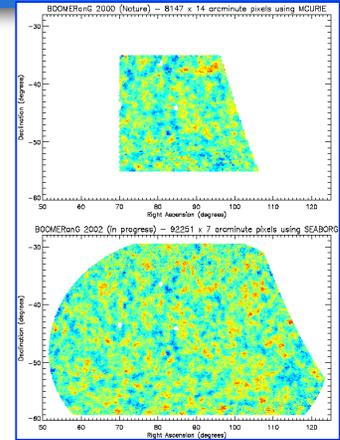
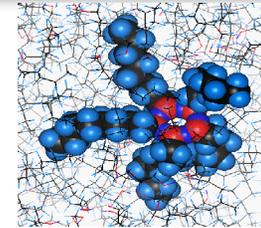
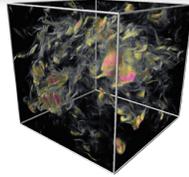
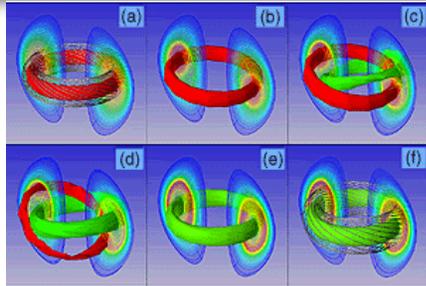
## Multicore:

- Current trajectory is to use the fastest multicore process in the market (AMD Barcelona, Shang-Hai, Intel Nehalem, etc. )
- Duplicate the number of cores per processes every +/- 18 months

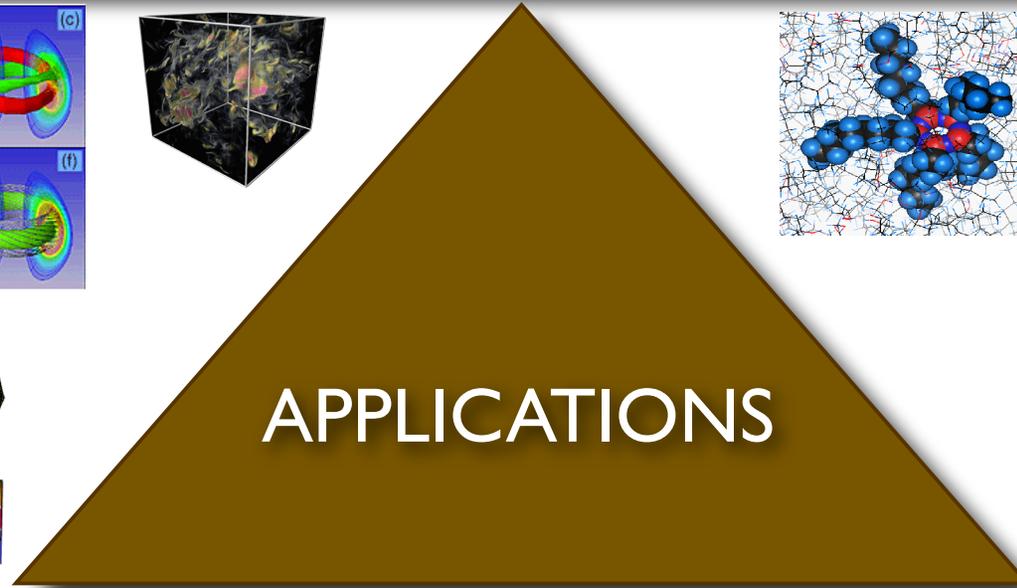
## Manycore:

- Simplified the core technology: shorter pipelines, slower clocks, reduce, etc. . (Nvidia G80, Cell SPE, Cisco Tensilica Metro)
- Better energy consumption
- Better factor of computing capacity per area

# HPC Software Stack

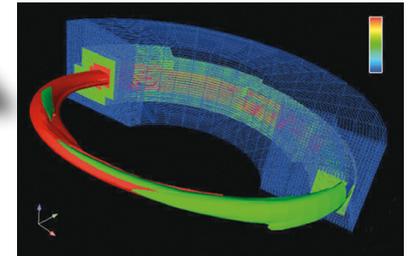


Omega3P is a parallel distributed-memory code intended for the modeling and analysis of accelerator cavities, which requires the solution of generalized eigenvalue problems. A parallel exact shift-invert eigensolver based on PARPACK and SuperLU has allowed for the solution of a problem of order 7.5 million with 304 million nonzeros.



GENERAL PURPOSE TOOLS

PLATFORM SUPPORT TOOLS AND UTILITIES

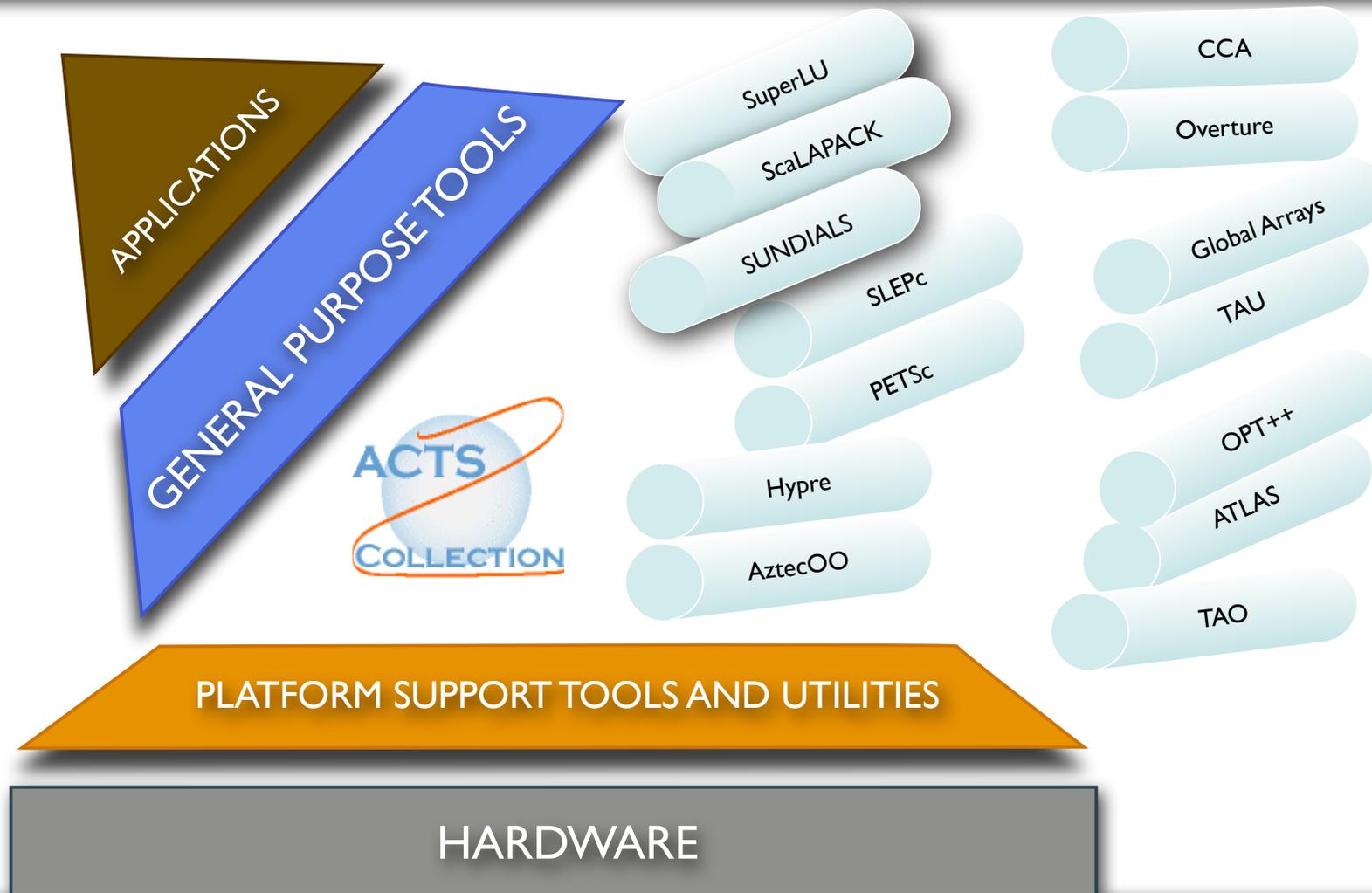


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# HPC Software Stack

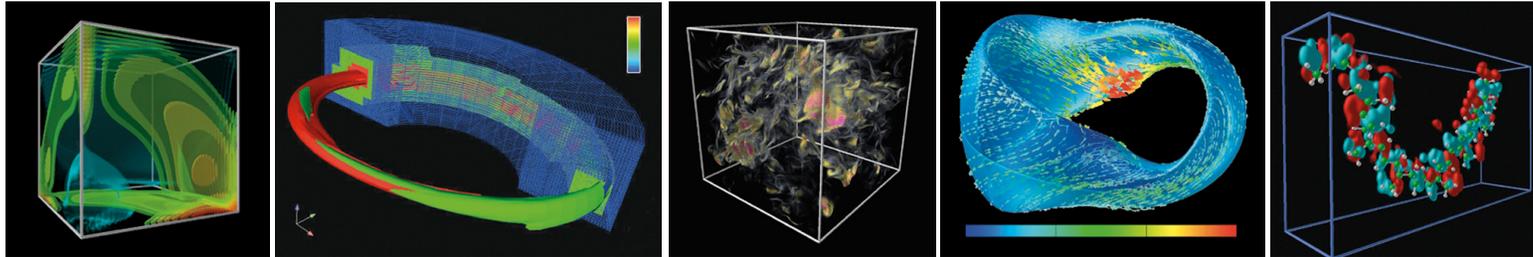


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# The DOE ACTS Collection



**Goal:** The Advanced Computational Software Collection (ACTS) makes reliable and efficient software tools more widely used, and more effective in solving the nation's engineering and scientific problems.

## **References:**

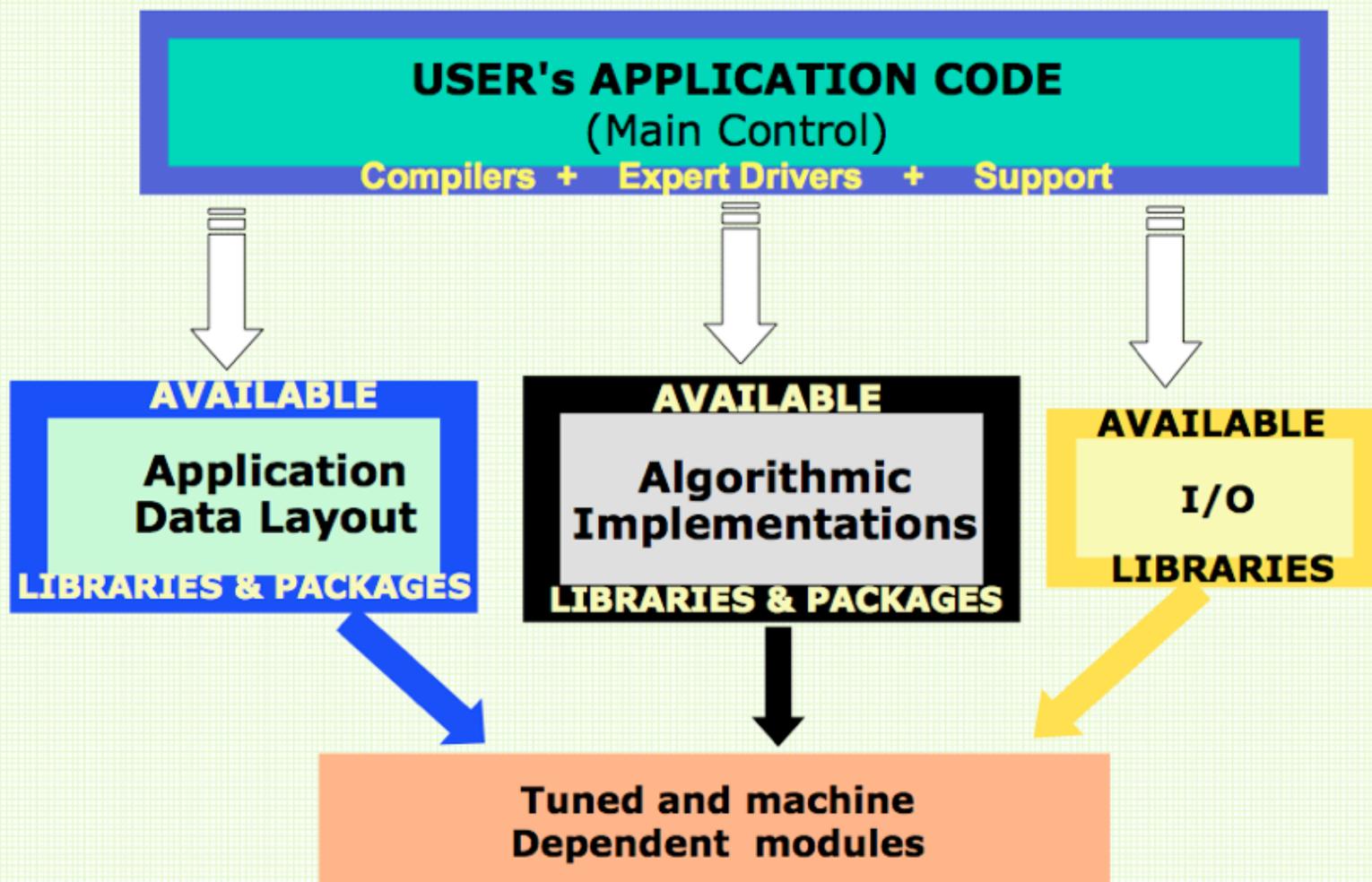
- L.A. Drummond, O. Marques: An Overview of the Advanced Computational Software (ACTS) Collection. ACM Transactions on Mathematical Software Vol. 31 pp. 282-301, 2005
- <http://acts.nersc.gov>

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# Speeding-Up Software Development



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# The DOE ACTS Collection

Category	Tool	Functionalities
Numerical	AztecOO	Scalable linear and non-linear solvers using iterative schemes.
	Hypre	A family of scalable preconditioners.
	PETSc	Scalable linear and non-linear solvers and additional support for PDE related work.
	OPT++	Object-oriented nonlinear optimization solvers.
	SUNDIALS	Solvers for the solution of systems of ordinary differential equations, nonlinear algebraic equations, and differential-algebraic equations.
	ScaLAPACK	High performance parallel dense linear algebra.
	SLEPc	Scalable algorithms for the solution of large sparse eigenvalue problems.
	SuperLU	Scalable direct solution of large, sparse, nonsymmetric linear systems of equations.
	TAO	Large-scale optimization software.
Code Development	Global Arrays	Supports the development of parallel programs.
	Overture	Supports the development of computational fluid dynamics codes in complex geometries.
Run Time Support	TAU	Portable and scalable performance analyzes and tracing tools for C, C++, Fortran and Java programs.
Library Development	ATLAS	Automatic generation of optimized numerical dense algebra for scalar processors.

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# The DOE ACTS Collection

SuperLU

General-purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations.

ScaLAPACK

Most complete library for High-Performance Dense Linear Algebra.

PETSc

Supports the solution of PDEs that require solving large-scale, sparse linear and nonlinear systems of equations.

Hypre

Supports iterative solution of large sparse linear Systems of equation using scalable preconditioners.

AztecOO

A package in the Trilinos framework. Algorithms for the iterative solution of large sparse linear systems.

*For more information visit [acts.nersc.gov](http://acts.nersc.gov)*

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# The DOE ACTS Collection

TAO

Library for solving large scale non-linear optimization problems.

OPT++

Object Oriented non-linear optimization library.

SUNDIALS

Family of solvers for ordinary differential, nonlinear algebraic, and differential-algebraic equations.

SLEPC

High Performance Library for the solution of large sparse eigenproblems.

Overture

Library for solving computational fluid dynamics and combustion problems in complex geometries

ATLAS

Automatic generation of optimized numerical software for modern computer architectures and compilers.

*For more information visit [acts.nersc.gov](http://acts.nersc.gov)*

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# The DOE ACTS Collection

TAU

Tuning and Analysis Utilities

Global Arrays

The Global Arrays (GA) toolkit is a library for writing parallel programs that use large arrays distributed across processing nodes

*For more information visit [acts.nersc.gov](http://acts.nersc.gov)*

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations	Direct Methods	LU Factorization	ScaLAPACK(dense) SuperLU (sparse)
		Cholesky Factorization	ScaLAPACK
		LDL <sup>T</sup> (Tridiagonal matrices)	ScaLAPACK
		QR Factorization	ScaLAPACK
		QR with column pivoting	ScaLAPACK
		LQ factorization	ScaLAPACK

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations (cont..)	Iterative Methods	Conjugate Gradient	AztecOO (Trilinos) PETSc
		GMRES	AztecOO PETSc Hypre
		CG Squared	AztecOO PETSc
		Bi-CG Stab	AztecOO PETSc
		Quasi-Minimal Residual (QMR)	AztecOO
		Transpose Free QMR	AztecOO PETSc

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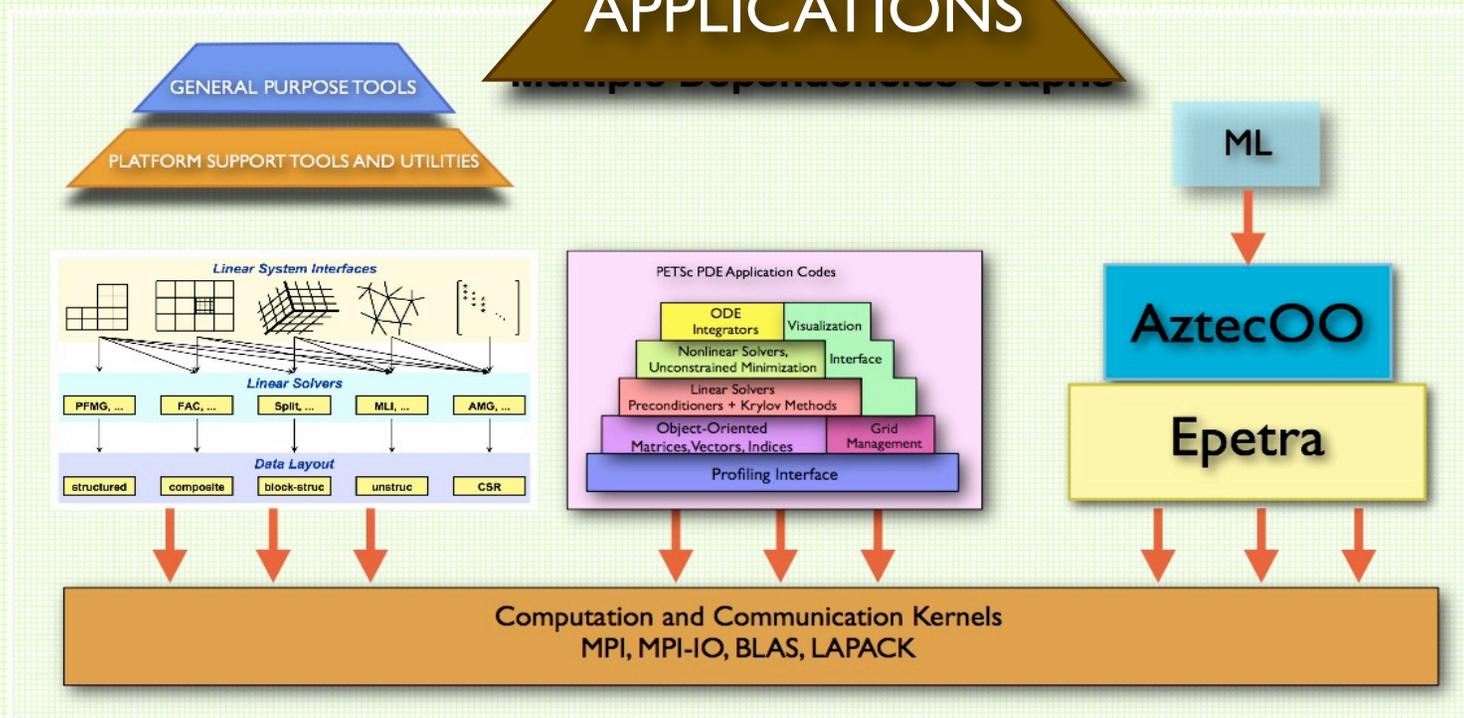
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# Overlapping Functionality

Iterative Schemes for  
Linear and Non-Linear Solvers

APPLICATIONS



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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations (cont..)	Iterative Methods	Conjugate Gradient	AztecOO (Trilinos) PETSc
		GMRES	AztecOO PETSc Hypre
		CG Squared	AztecOO PETSc
		Bi-CG Stab	AztecOO PETSc
		Quasi-Minimal Residual (QMR)	AztecOO
		Transpose Free QMR	AztecOO PETSc

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations ( <i>cont..</i> )	Iterative Methods ( <i>cont..</i> )	SYMMLQ	PETSc
		Precondition CG	AztecOO PETSc Hypre
		Richardson	PETSc
		Block Jacobi Preconditioner	AztecOO PETSc Hypre
		Point Jacobi Preconditioner	AztecOO
		Least Squares Polynomials	PETSc

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithms	Library
Systems of Linear Equations (cont..)	Iterative Methods (cont..)	SOR Preconditioning	PETSc
		Overlapping Additive Schwartz	PETSc
		Approximate Inverse	Hypre
		Sparse LU preconditioner	AztecOO PETSc Hypre
		Incomplete LU (ILU) preconditioner	AztecOO
		Least Squares Polynomials	PETSc
	MultiGrid (MG) Methods	MG Preconditioner	PETSc Hypre
		Algebraic MG	Hypre
		Semi-coarsening	Hypre

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Linear Least Squares Problems	Least Squares	$\min_x \  b - Ax \ _2$	ScaLAPACK
	Minimum Norm Solution	$\min_x \  x \ _2$	ScaLAPACK
	Minimum Norm Least Squares	$\min_x \  b - Ax \ _2$ $\min_x \  x \ _2$	ScaLAPACK
Standard Eigenvalue Problem	Symmetric Eigenvalue Problem	$Az = \lambda z$ For $A=A^H$ or $A=A^T$	ScaLAPACK (dense) SLEPc (sparse)
Singular Value Problem	Singular Value Decomposition	$A = U\Sigma V^T$ $A = U\Sigma V^H$	ScaLAPACK (dense) SLEPc (sparse)
Generalized Symmetric Definite Eigenproblem	Eigenproblem	$Az = \lambda Bz$ $ABz = \lambda z$ $BAz = \lambda z$	ScaLAPACK (dense) SLEPc (sparse)

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Non-Linear Equations	Newton Based	Line Search	PETSc
		Trust Regions	PETSc
		Pseudo-Transient Continuation	PETSc
		Matrix Free	PETSc

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# Functionality in The DOE ACTS Collection

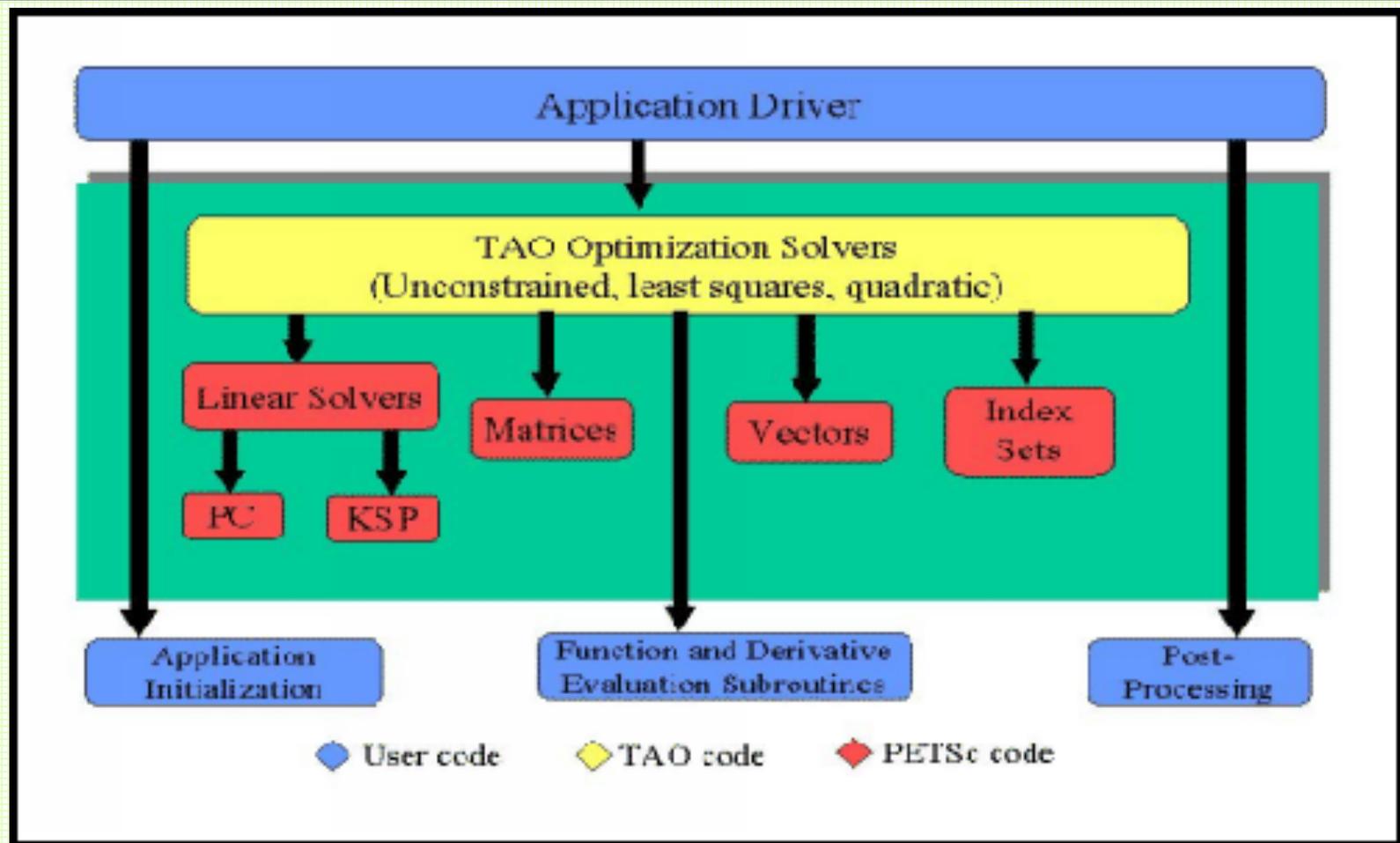
Computational Problem	Methodology	Algorithm	Library
Non-Linear Optimization	Newton Based	Newton	OPT++ TAO
		Finite-Difference Newton	OPT++ TAO
		Quasi-Newton	OPT++ TAO
		Non-linear Interior Point	OPT++ TAO
	CG	Standard Non-linear CG	OPT++ TAO
		Limited Memory BFGS	OPT++
		Gradient Projections	TAO
	Direct Search	No derivate information	OPT++

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# TAO Interface Reusing PETSc



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# Functionality in The DOE ACTS Collection

- Four major classes of problems available
  - *NLFO*(*ndim*, *fcn*, *init\_fcn*, *constraint*)
    - Basic nonlinear function, no derivative information available
  - *NLFI*(*ndim*, *fcn*, *init\_fcn*, *constraint*)
    - Nonlinear function, first derivative information available
  - *FDNLFI*(*ndim*, *fcn*, *init\_fcn*, *constraint*)
    - Nonlinear function, first derivative information approximated
  - *NLF2*(*ndim*, *fcn*, *init\_fcn*, *constraint*)
    - Nonlinear function, first and second derivative information available

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Non-Linear Optimization	Newton Based	Newton	OPT++ TAO
		Finite-Difference Newton	OPT++ TAO
		Quasi-Newton	OPT++ TAO
		Non-linear Interior Point	OPT++ TAO
	CG	Standard Non-linear CG	OPT++ TAO
		Limited Memory BFGS	OPT++
		Gradient Projections	TAO
	Direct Search	No derivate information	OPT++

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# Functionality in The DOE ACTS Collection

Computational Problem	Methodology	Algorithm	Library
Non-Linear Optimization (cont..)	Semismoothing	Feasible Semismooth	TAO
		Unfeasible semismooth	TAO
Ordinary Differential Equations	Integration	Adam-Moulton (Variable coefficient forms)	CVODE (SUNDIALS) CVODES
	Backward Differential Formula	Direct and Iterative Solvers	CVODE CVODES
Nonlinear Algebraic Equations	Inexact Newton	Line Search	KINSOL (SUNDIALS)
Differential Algebraic Equations	Backward Differential Formula	Direct and Iterative Solvers	IDA (SUNDIALS)

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# Functionality in The DOE ACTS Collection

Computational Problem	Support	Techniques	Library
Writing Parallel Programs	Distributed Arrays	Shared-Memory	Global Arrays
		Grid Generation	OVERTURE
		Structured Meshes	Hypre OVERTURE PETSc
		Semi-Structured Meshes	Hypre OVERTURE

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# Functionality in The DOE ACTS Collection

Computational Problem	Support	Technique	Library
Profiling	Algorithmic Performance	Automatic instrumentation	PETSc
		User Instrumentation	PETSc
	Execution Performance	Automatic Instrumentation	TAU
		User Instrumentation	TAU
Code Optimization	Library Installation	Linear Algebra Tuning	ATLAS

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# User Interfaces

```
CALL BLACS_GET( -1, 0, ICTXT )
CALL BLACS_GRIDINIT( ICTXT, 'Row-major', NPROW, NPCOL )
:
CALL BLACS_GRIDINFO( ICTXT, NPROW, NPCOL, MYROW, MYCOL )
:
:
CALL PDGESHV( N, NRHS, A, IA, JA, DESCA, IPIV, B, IB, JB, DESCB,
$            INFO )
```

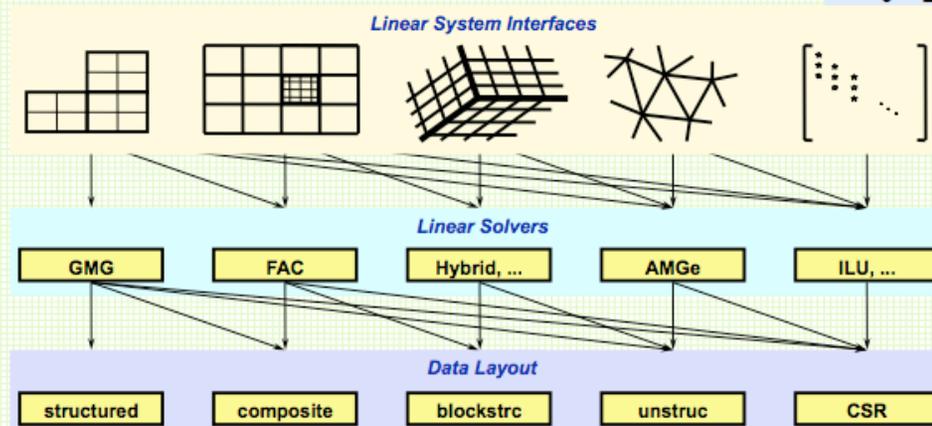
## Command lines

## Library Calls

- `-ksp_type` [cg,gmres,bcgs,tfqmr, ...]
- `-pc_type` [lu,ilu,jacobi,sor,asm, ...]

### More advanced:

- `-ksp_max_it` <max\_iters>
- `-ksp_gmres_restart` <restart>
- `-pc_asm_overlap` <overlap>

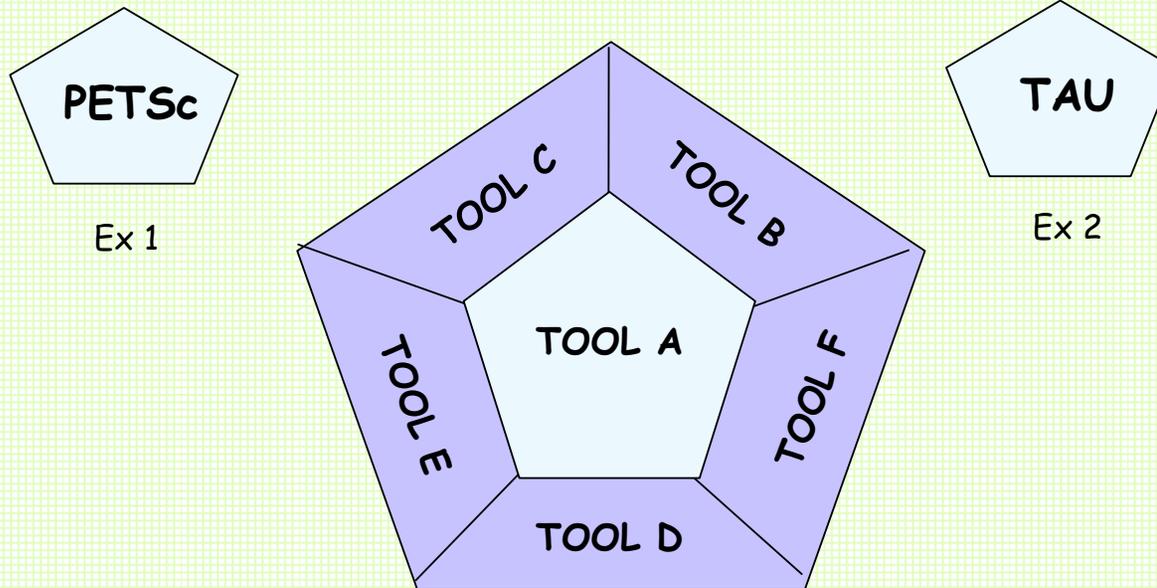


## Problem Domain

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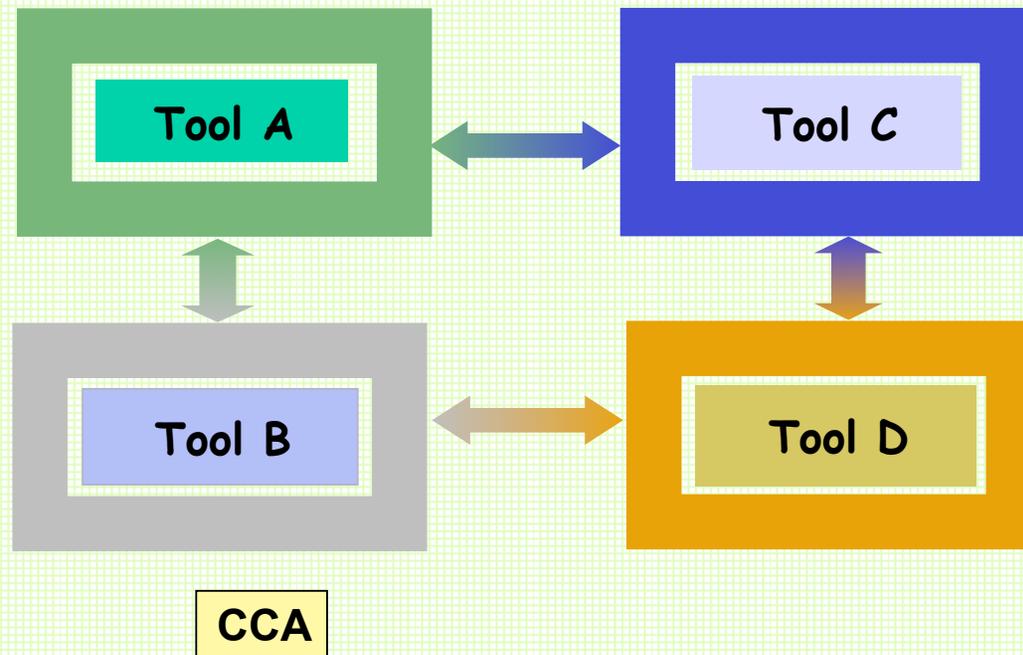
# Interoperability



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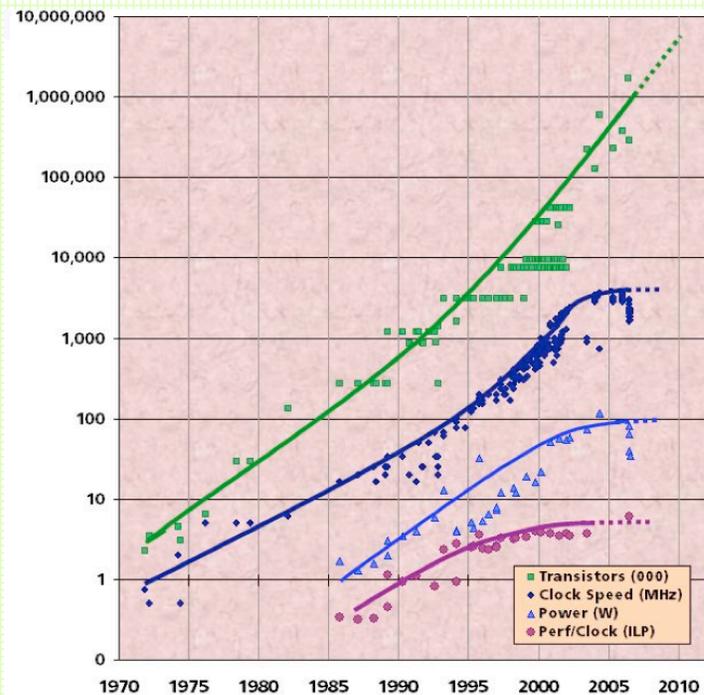
# Interoperability



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# Scalability and Sustainability



K. Olukotun et. al.,

- Number of cores per node will continue to increase.
- Memory per node is not increasing at the same rate

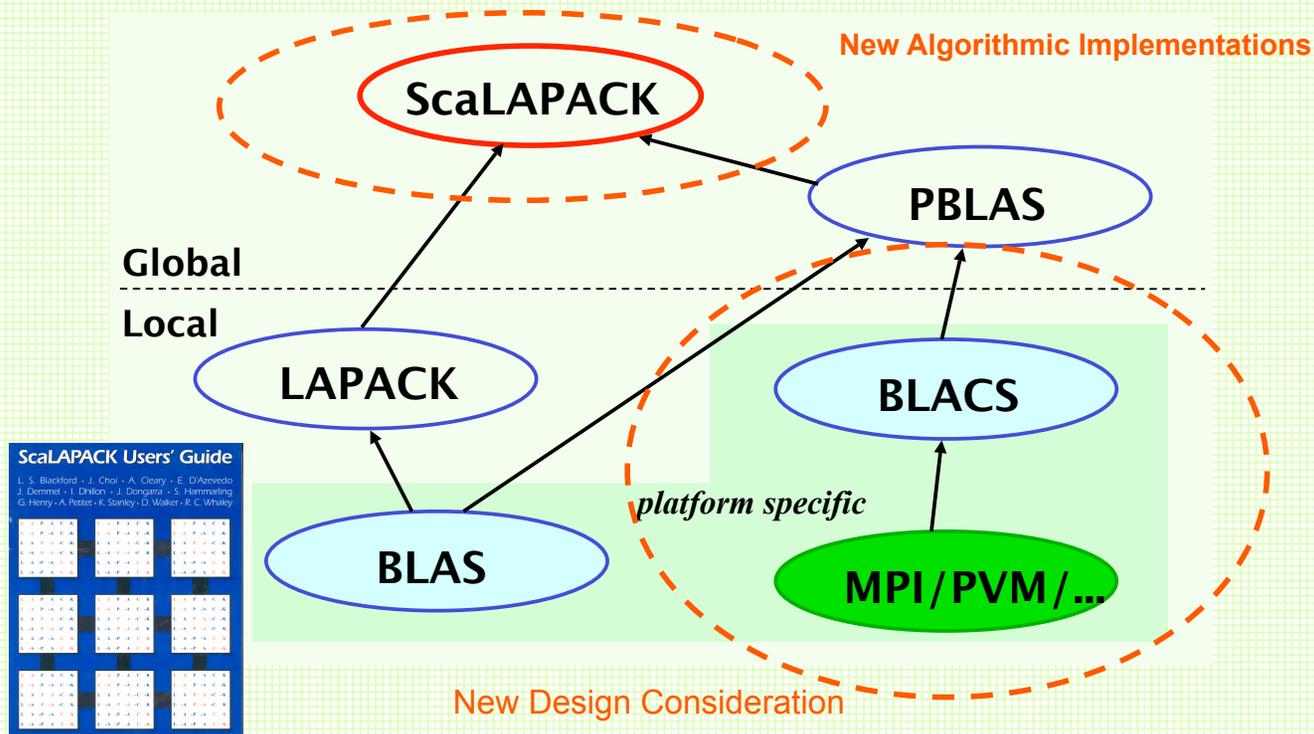
*Looking back in history. ..*

- Processor speed increased at faster rate than memory speed.
- Memory bandwidth relevant to overall performance

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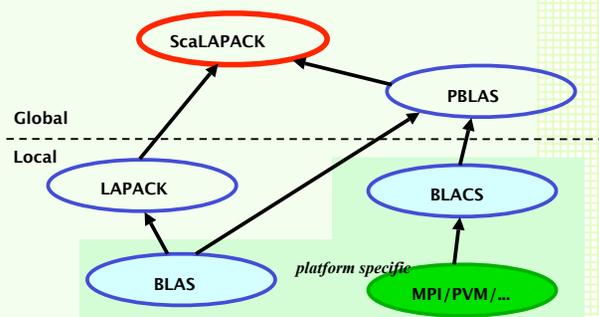
# Scalability and Sustainability



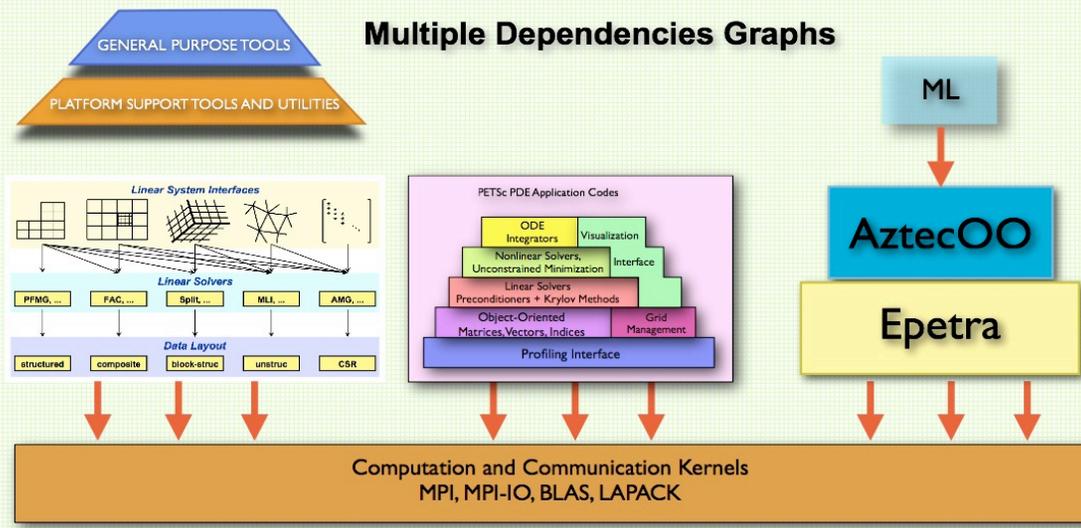
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# Software Dependency Graph



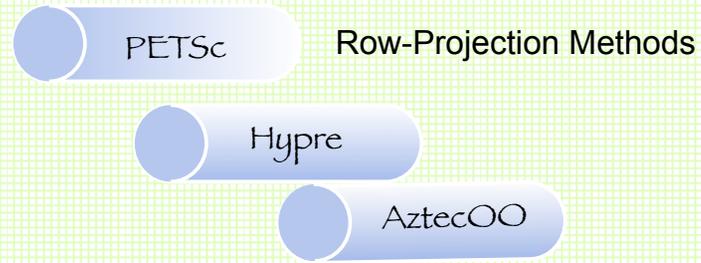
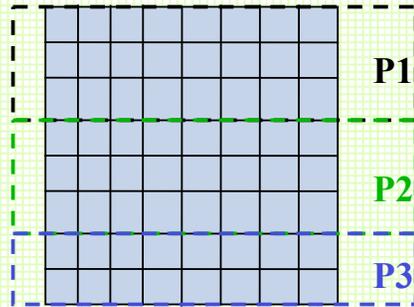
- Identify key common kernels
- Identify parameters that drive performance
- Profile and test (bottom-up)



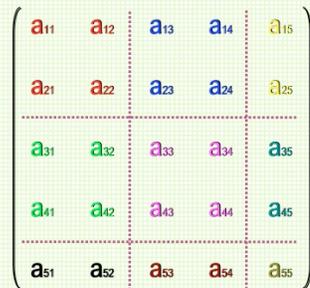
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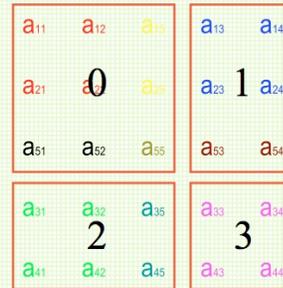
# Kernel Optimization



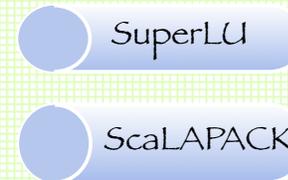
5x5 matrix partitioned in 2x2 blocks



2x2 process point of view



Dense Linear Algebra



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# Kernel Optimization

$$Ax = b \text{ or } AX = B$$

$$Hx = b'$$

$$\min_x \|b - Ax\|_2$$

$$\min_x \|x\|_2$$

$$\min_x \|b - Ax\|_2$$

$$\min_x \|x\|_2$$

$$Az = \lambda z$$

$$A = U\Sigma V^T$$

$$A = U\Sigma V^H$$

$$Az = \lambda Bz$$

$$ABz = \lambda z$$

$$BAz = \lambda z$$

## Exploit concurrency :

(in and out a node)

- Hybrid programming (MPI+threads)
- NUMA Aware operations

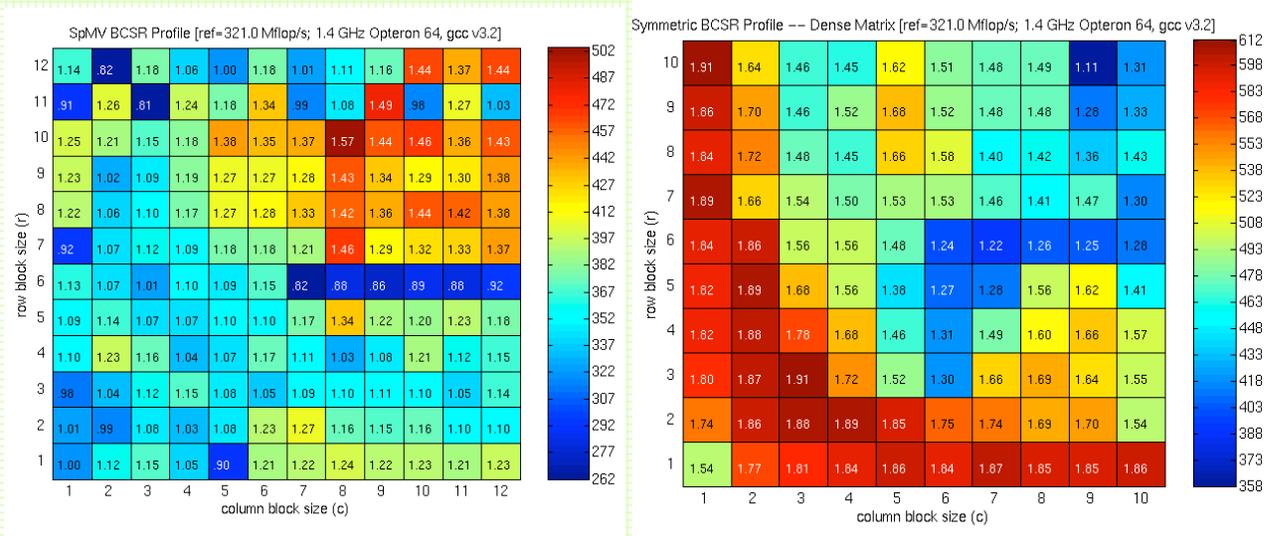
## Kernel reusability:

- Bottom-Up automatic optimization
- Identify key parameters in the algorithm
- Run-time parameter control

# Functionality in The DOE ACTS Collection

OSKI

Symmetric peak = 612 MFlops



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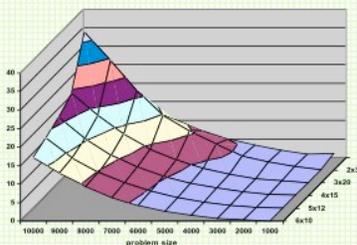
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# ACTS Software Sustainability Cycle

## Profiling and Tracing Tools: TAU

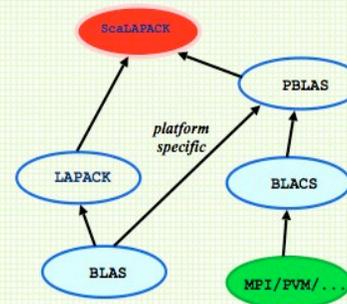
Execution time of PDPOSV for various grid shapes



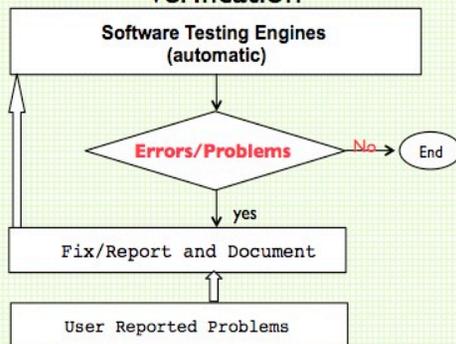
## Performance and Scalability



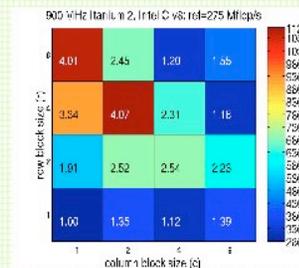
## Software Dependency Graph



## Automatic Testing and Verification



## Auto-Tuning (OSKI, ATLAS,)



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Berkeley, California, August 17-20, 2010



# Summary

**min**[*time\_to\_first\_solution*] (prototype)

**min**[*time\_to\_solution*] (production)

- Outlive Complexity
  - Increasingly sophisticated models
  - Model coupling
  - Interdisciplinary
- Sustained Performance
  - Increasingly complex algorithms
  - Increasingly diverse architectures
  - Increasingly demanding applications

(Software Evolution)

(Long-term deliverables)

**min**[*software-development-cost*]

**max**[*software\_life*] and **max**[*resource\_utilization*]

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# This Week at The Workshop

Tuesday	Wednesday	Thursday	Friday
<i>Registration</i> 7:45 AM	<i>Doors Open</i> 8:00 AM	<i>Doors Open</i> 8:00 AM	<i>Doors Open</i> 8:00 AM
<i>Welcome Remarks and Introduction</i> <b>T. Drummond</b> 08:30 - 09:30	<i>PETSc</i> <b>M. Knepley</b> 08:30 - 10:30	<i>Trilinos</i> <b>J. Hu</b> 08:30 - 09:30	<i>Zoltan</i> <b>M. Wolf</b> 08:30 - 09:30
<i>ScaLAPACK</i> <b>T. Drummond</b> 09:30 - 10:30		<i>Invited Talk</i> <b>H. Simon</b> CRD Div. Director 09:30 - 10:30	<i>TAU</i> <b>S. Shende</b> 08:30 - 09:30
<b>Break</b> 10:30 - 11:00	<b>Break</b> 10:30 - 11:00	<b>Break</b> 10:30 - 11:00	<b>Break</b> 10:30 - 11:00
<i>SUNDIALS</i> <b>C. Woodward</b> 11:00 - 12:00	<i>SuperLU</i> <b>S. Li</b> 11:00 - 12:30	<i>Hypre</i> <b>R. Falgout</b> 11:00 - 12:30	<i>CCA</i> <b>CCA Team*</b> 11:00 - 12:30
<i>LiveDVD and Hands-On Sessions</i> <b>T. Drummond</b> <b>S. Shende</b> 12:00 - 12:30			
<b>Lunch</b> 12:30 - 13:30	<b>Lunch</b> 12:30 - 13:30	<b>Lunch</b> 12:30 - 13:30	<b>Lunch</b> 12:30 - 13:30

High Performance Software Tools to Fast-Track  
The Development of Scalable and Sustainable Applications

Eleventh DOE ACTS Collection Workshop  
Berkeley, California, August 17-20, 2010



# This Week at The Workshop

Tuesday	Wednesday	Thursday	Friday
<i>Mesquite</i> <b>L. Freitag-Diachin</b> 13:30 – 14:30	<i>TAO</i> <b>J. Sarich</b> 13:30 – 14:30	<i>Overture</i> <b>B. Henshaw</b> 13:30 – 14:30	<i>Zoltan</i> <i>Hands-On</i> <b>M. Wolf</b> 13:30 – 14:30
<i>Global Arrays</i> <b>B. Palmer</b> 14:30 – 15:30	<i>ADIC 2.0</i> <b>S. Narayanan</b> 14:30 – 15:30	<b>Break</b> 14:30 - 14:45	<i>TAU</i> <i>Hands-On</i> <b>S. Shende</b> 14:30 – 15:30
<b>Break</b> 15:30 - 15:45	<b>Break</b> 15:30 - 15:45	<i>Overture</i> <i>Hands-On</i> <b>B. Henshaw</b> 14:45 – 15:45	<b>Break</b> 15:30 - 15:45
<i>ScaLAPACK</i> <i>Hands-On</i> <b>T. Drummond</b> 15:45 – 16:45	<i>PETSc</i> <i>Hands-On</i> <b>S. Balay</b> 15:45 – 16:45	<i>Trilinos</i> <i>Hands-On</i> <b>J. Hu</b> 15:45 - 17:45	<i>CCA</i> <i>Hands-On</i> <b>CCA TEAM*</b> 15:45 – 17:45
<i>Global Arrays</i> <i>Hands-On</i> <b>M. Krishnan</b> <b>B. Palmer</b> 16:45 – 17:45	<i>TAO</i> <i>Hands-On</i> <b>S. Sarich</b> 16:45 – 17:45		
<b>Welcome Dinner</b> 19:00 - 21:00			<b>Workshop Ends</b>

\* **CCA TEAM:**  
 David Bernholdt  
 Wael Elwasif  
 Dietmar Ebner  
 Sameer Shende

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 The Development of Scalable and Sustainable Applications

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# This Week at The Workshop

## Two Accounts:

- Computer Lab Accounts
- NERSC Accounts (login to [carver.nersc.gov](http://carver.nersc.gov))
  - Return computer policy form

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The Development of Scalable and Sustainable Applications

Eleventh DOE ACTS Collection Workshop  
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# Acknowledgments

- National Energy Research Scientific Computing Center (NERSC) for the use of their I Linux Cluster (magellan)
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- Valerie Heatlie for travel support
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- DOE Office of Science
- U of Oregon and ParaTools for their support creating the ACTS Collection LiveDVDs