

A Workshop on the ACTS Collection

**Robust and High Performance
Tools for Scientific Computing**

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How can ACTS work for you?

- Computational problems at hand.
- A sample of scientific applications.
- Why do we need all these tools?
- Agenda for the Workshop.

ScaLAPACK

Aztec/Trilinos

SuperLU

$$Ax = b$$

$$Az = \lambda z$$

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

$$\min \left\{ \frac{1}{2} \|r(x)\|^2 : x_l \leq x \leq x_u \right\}$$

PDEs

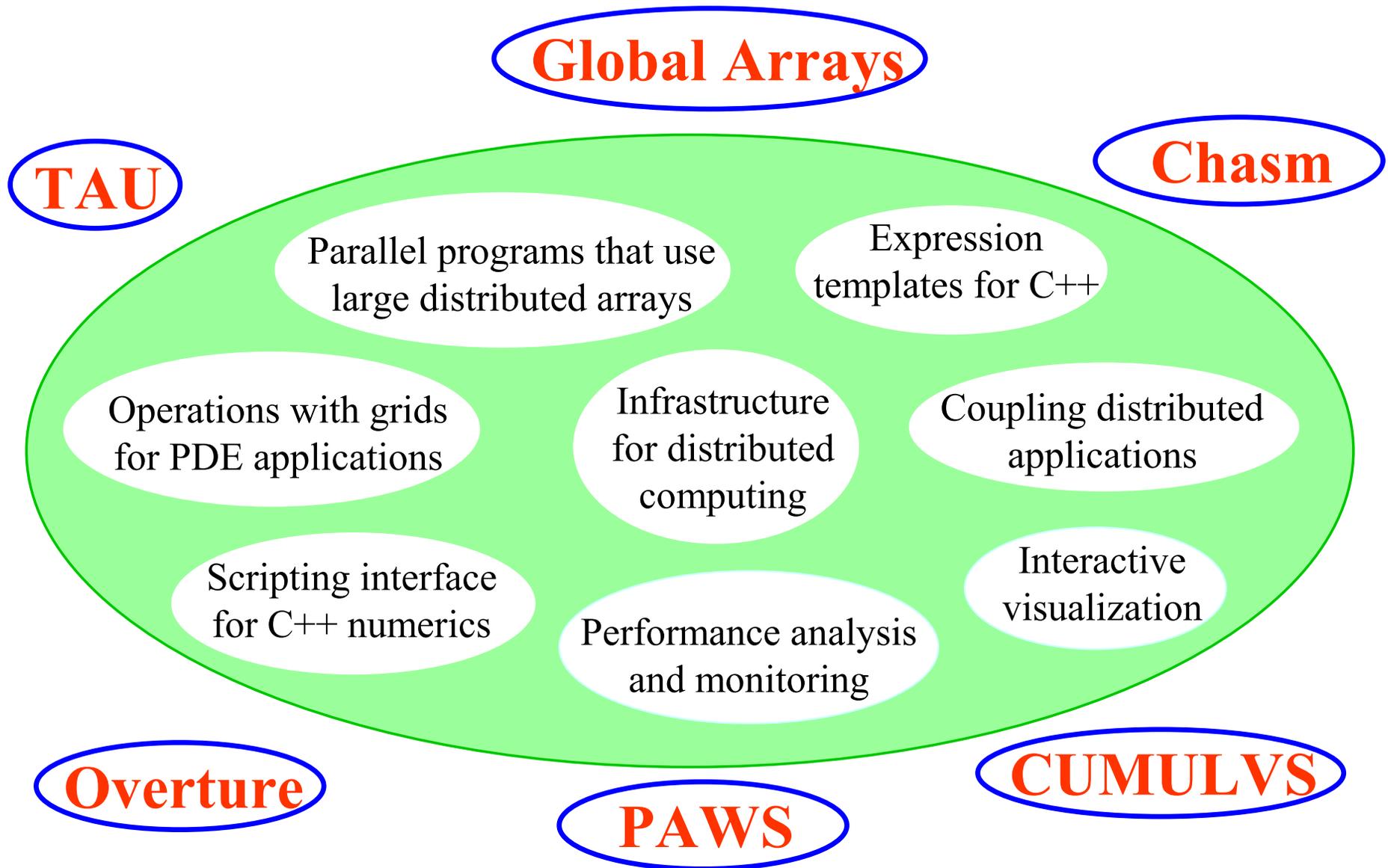
ODEs

PETSc

PVODE

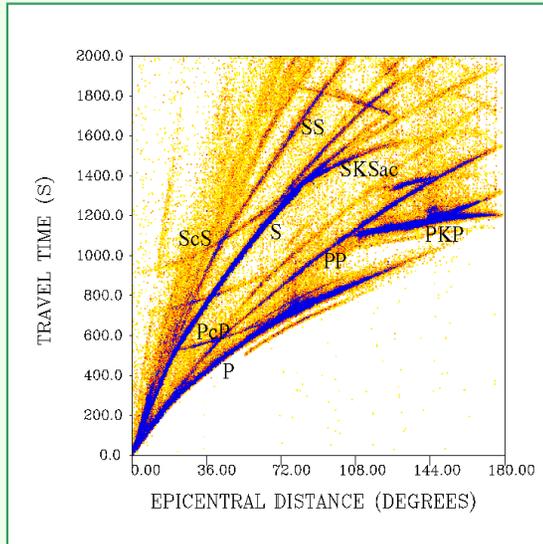
TAO

Hypre



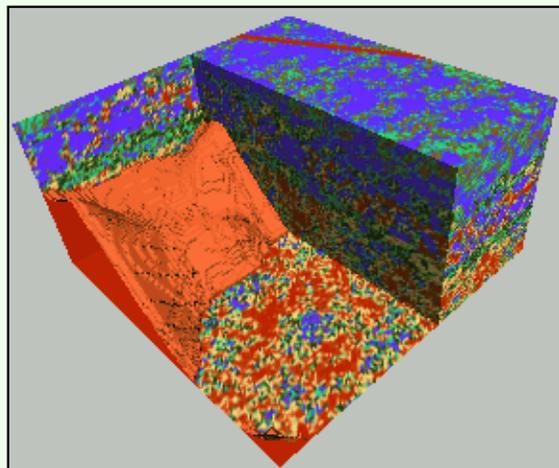
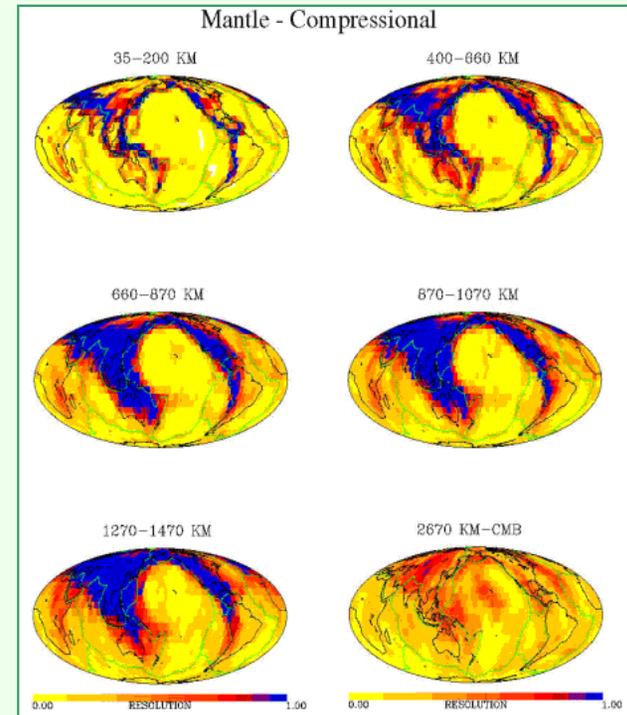
Data: travel times of sound waves generated by earthquakes used to infer structure in the entire Earth (crust, mantle and core).

Goal: model for the internal structure of the Earth



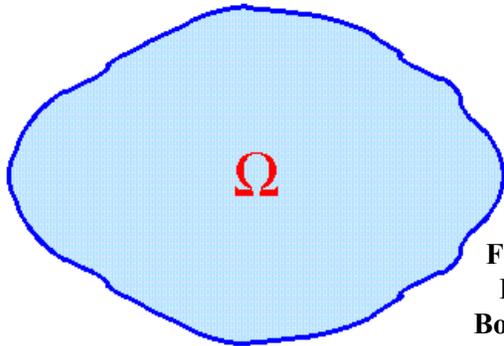
more than 1×10^6 data points and 2×10^5 parameters

ScaLAPACK used for the solution of eigenvalue problems.



PVODE used in the ParFlow ground-water flow project to solve three-dimensional models of fluid flow and chemical transport through heterogeneous porous media (LLNL).

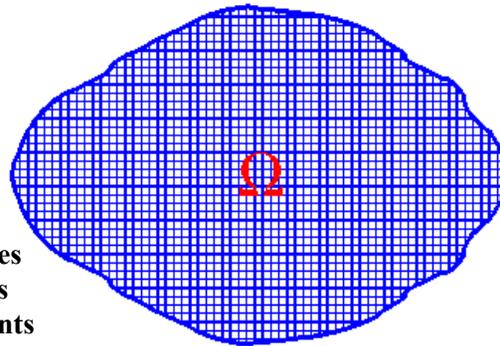
continuous problem



grid



discrete problem

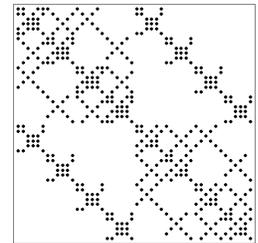


Finite Differences
Finite Elements
Boundary Elements
Fourier
⋮

$$m \frac{d^2 x}{dt^2} + c \frac{dx}{dt} + kx = f(t)$$

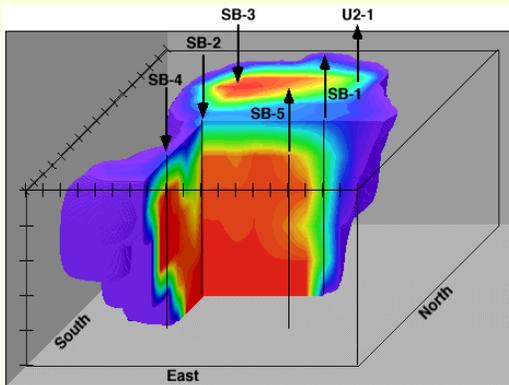
$$\frac{\partial v}{\partial t} = -v \frac{\partial v}{\partial x} + \Gamma \frac{\partial^2 v}{\partial x^2}$$

$$\vdots$$

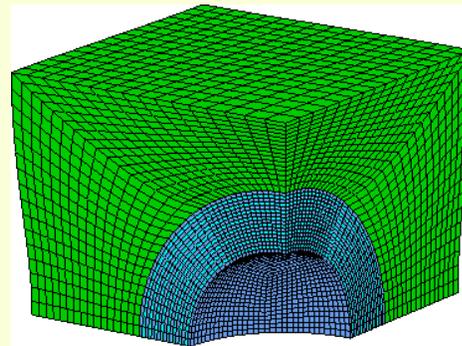


= A

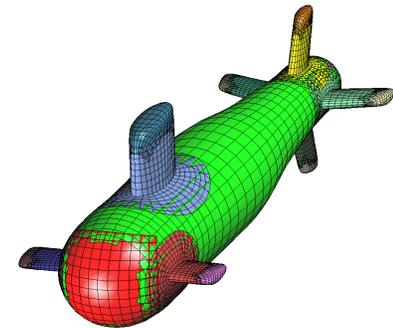
(sparse matrix)



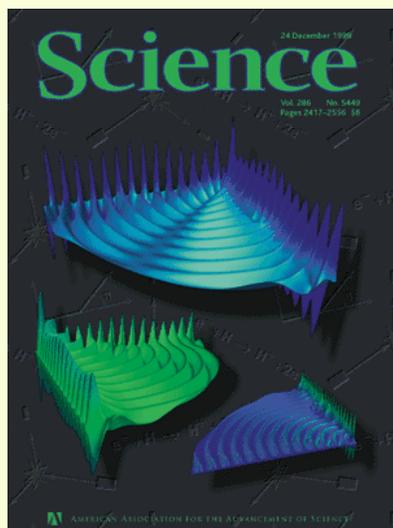
Multiphase flow using *PETSc*, 4 million cell blocks, 32 million DOF, over 10.6 Gflops on an IBM SP (128 nodes), entire simulation runs in less than 30 minutes (Pope, Gropp, Morgan, Seperhrnoori, Smith and Wheeler).



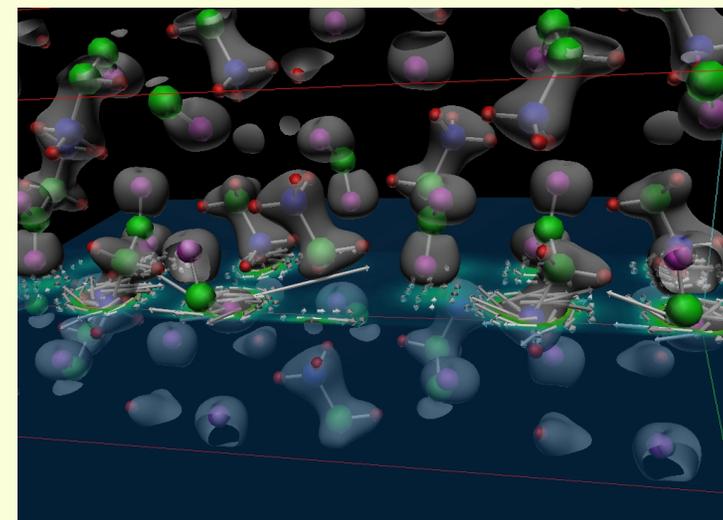
Model of a "hard" sphere included in a "soft" material, 26 million d.o.f. (Adams and Demmel, Prometheus and *PETSc*, unstructured meshes in solid mechanics).



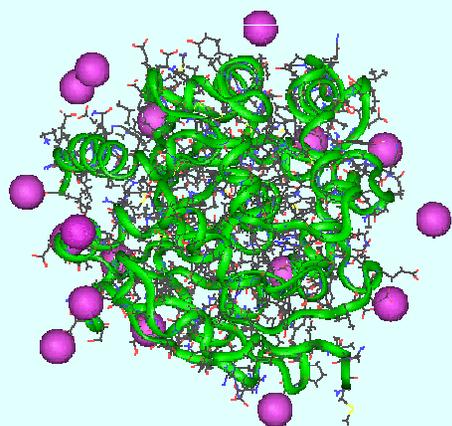
3D overlapping grid for a submarine produced with *Overture's* module *ogen*.



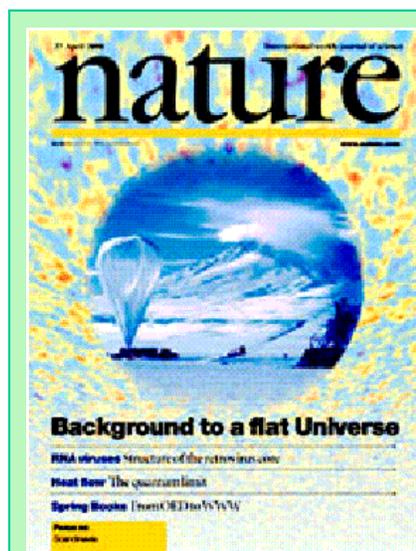
Collaborators at the LBNL, LLNL and the UC Davis obtained a complete solution of the ionization of a hydrogen atom by collision with an electron, the simplest nontrivial example of the long-standing unsolved problem of scattering in a quantum system of three charge particles. The images show representative wave functions of the problem (Rescigno, Baertschy, Isaacs and McCurdy, Dec. 24, 1999). *SuperLU* was used to build preconditioners for complex, unsymmetric and ill-conditioned sparse linear systems of order up to 2 million.



Induced current (white arrows) and charge density (colored plane and gray surface) in crystallized glycine due to an external field (Louie, Yoon, Pfrommer and Canning), eigenvalue problems solved with *ScaLAPACK*.

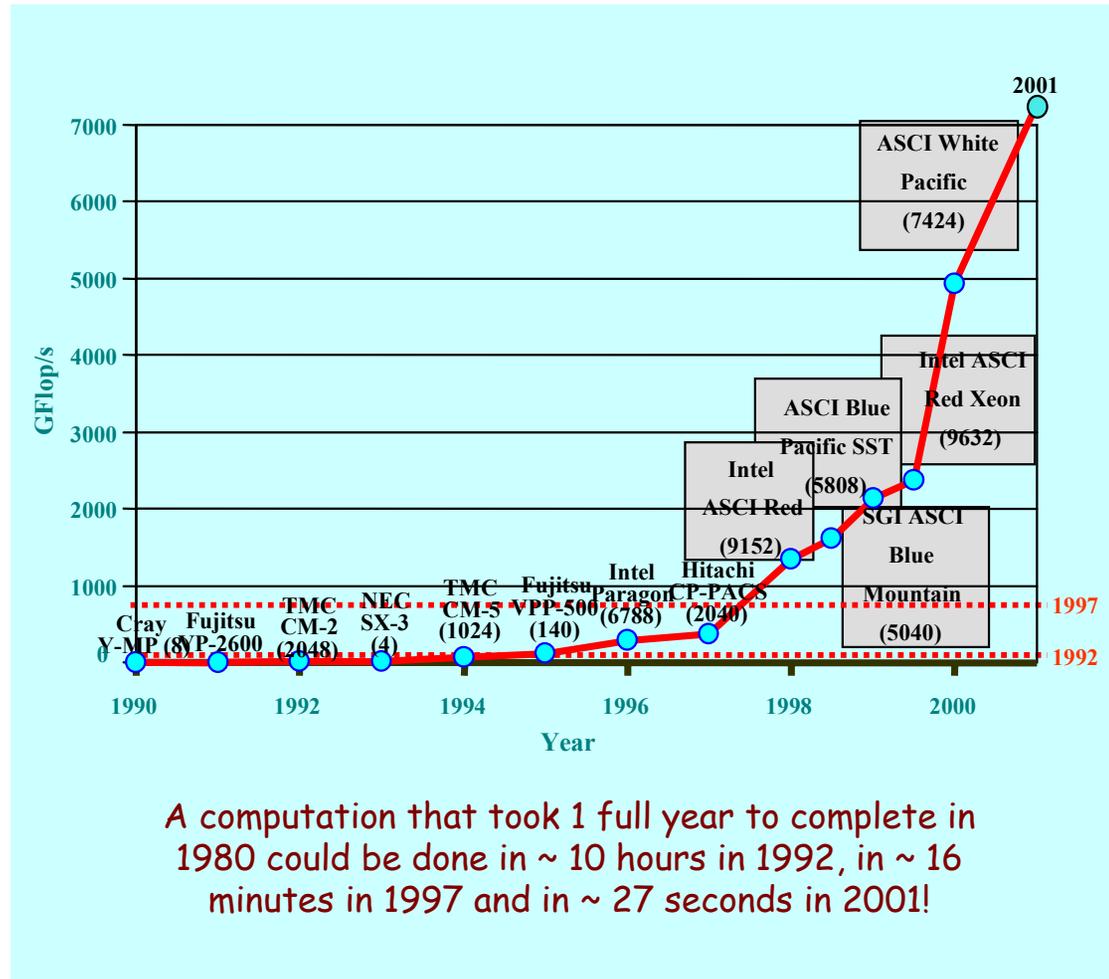


Molecular dynamics simulation of a haloalkane dehalogenase enzyme performed by a molecular dynamics code developed by T. Straatsma at PNNL, and using *Global Arrays*.



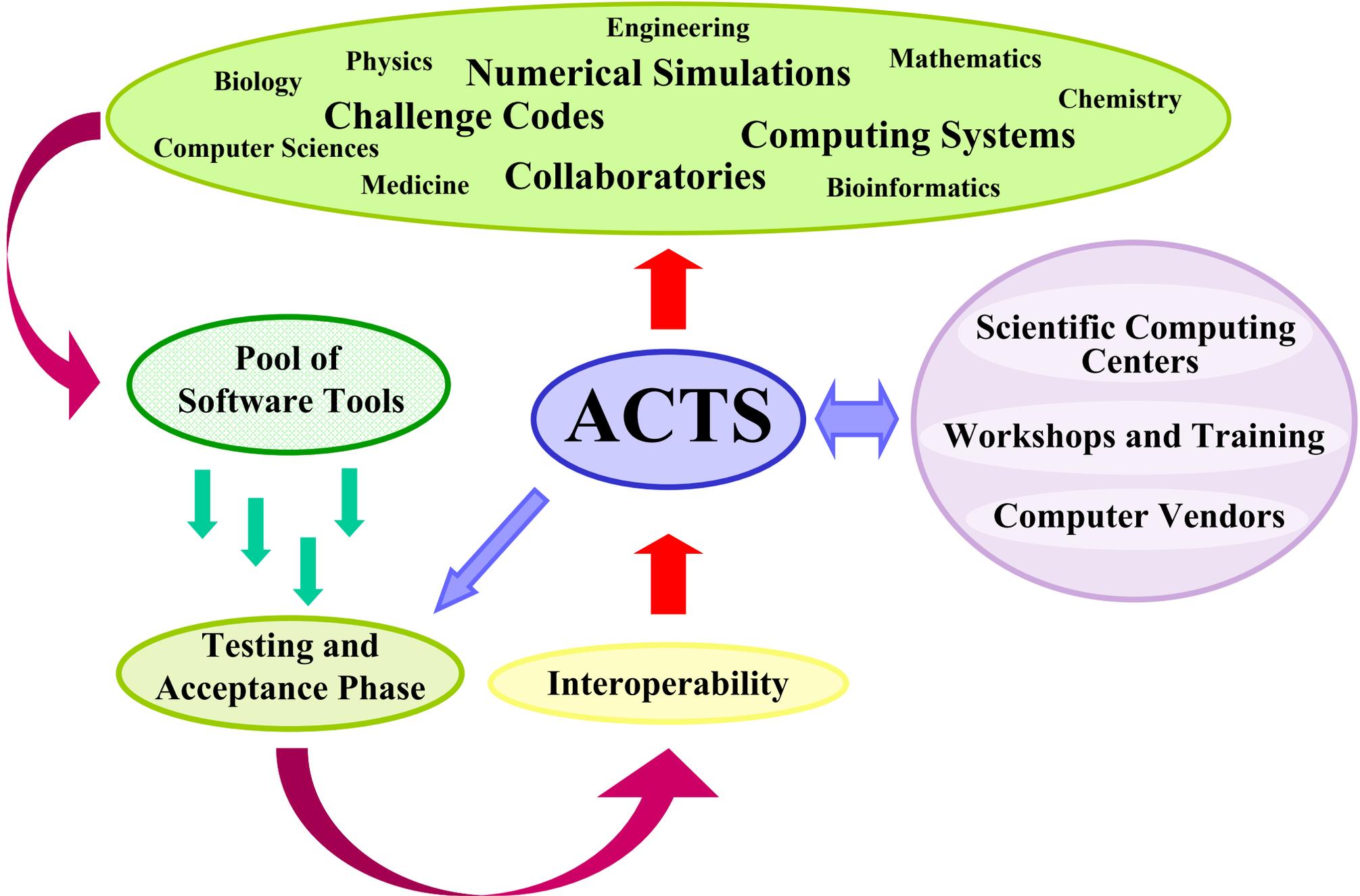
The international BOOMERanG collaboration announced results of the most detailed measurement of the cosmic microwave background radiation (CMB), which strongly indicated that the universe is flat (Apr. 27, 2000). Likelihood methods implemented in the MADCAP software package, using routines from *ScaLAPACK*, were used to examine the large dataset generated by BOOMERanG.

- High Performance Tools
 - portable
 - library calls
 - robust algorithms
 - help code optimization
- More code development in less time!
- More simulation in less computer time!



- *There is still a gap between tool developers and application developers which leads to duplication of efforts.*
- *The tools currently included in the ACTS Toolkit should be seen as dynamical configurable toolkits and should be grouped into toolkits upon user/application demand.*
- *Users demand long-term support of the tools.*
- *Applications and users play an important role in making the tools mature.*
- *Tools evolve or are superseded by other tools.*
- *There is a demand for tool interoperability and more uniformity in the documentation and user interfaces.*
- *There is a need for an intelligent and dynamic catalog/repository of high performance tools.*

User Community



<http://www.science.doe.gov/scidac>

- Scientific Discovery through Advanced Computing:
 - Creation of a new generation of *Scientific Challenge Codes* for terascale computers to tackle critical scientific problems.
 - Creation of *Mathematical and Computing Systems Software* to enable the Scientific Challenge Codes to take full advantage of the computing power advances.
 - Creation of a *Collaboratory Software Infrastructure* to enhance remote collaboration and access to facilities and data.
- Program Areas:
 - Advanced Scientific Computing
 - Basic Energy Sciences
 - Biology and Environment
 - Fusion Energy Sciences
 - High-Energy and Nuclear Physics
- SciDAC will be one important source of new tools and new users for the ACTS Collection.

- ACTS Toolkit Workshop: *Solving Problems in Science and Engineering*. LBNL, October 9-13, 2001.
- ACTS Workshop: High Performance Libraries for Science and Engineering. LACSI Symposium, Santa Fe, October 18, 2001.
- Tutorial on High-Performance Math Libraries. NPACI All-Hands Meeting, San Diego, March 6, 2002.
- Workshop on High Performance Numerical Libraries for Science and Engineering, Seventh Copper Mountain Conference on Iterative Methods, March 25, 2002.
- Scaling to New Heights Workshop, Pittsburgh Supercomputing Center, May 20-21, 2002.
- ACTS Workshop at the IMA 2002 Summer Program, University of Kentucky Center for Computational Sciences, July 18-19, 2002.

- Workshop 2000 Graduates:
 - Mark McKeown, from the University of Virginia (UVa), installed several of the ACTS tools on the UVa IBM SP2 and reported that several researchers at UVa use the tools.
 - Paulo Goldfeld, from the Courant Institute of Mathematical Sciences, started an active collaboration with the PETSc group, for the development of domain decomposition based preconditioners for mixed finite elements.
 - Joshua Breslau, from the Princeton Plasma Physics Laboratory, reported that with the expertise he acquired at the workshop he was able to easily upgrade some of the routines in the M3D code (multi-level 3D plasma physics) using PETSc.
- Workshop 2001 Graduates:
 - Mary Ann Leung, a DOE Computational Science Graduate Fellow, is spending her summer practicum at LBNL doing research on the use of ACTS tools in the algorithms and codes that she has been developing for material sciences calculations.
 - Ron Choy and Tong Wen, from MIT, are using ACTS tools in MATLAB*P (a parallel version of Matlab).
- Collaborations:
 - Dr. Jose Roman from the *Universidad Politecnica de Valencia*, Spain, visited LBNL in October 2001, and worked on SLEPc, which is a software library that extends the functionality of PETSc for the solution of large-scale sparse eigenvalue problems.
 - Prof. Eric Carlson from the Department of Chemical Engineering, University of Alabama, was granted a DOE EPSCoR proposal for the development of anisotropic diffusion equation solver using ACTS Tools.

- Special issue of the ACM Transactions on Mathematical Software (TOMS) containing a paper on the aims, scope, and successes of the ACTS Project, together with a collection of papers, each of which focusing on a specific tool.
- Birds of a feather at SC2002 (Baltimore):
 - Tool inclusion
 - Tool retirement
 - Peer-review of tools
 - Missing functionalities
- We would like to hear from you and your computational problems!

- Numerical Tools:
 - Hypre
 - OPT++
 - PETSc
 - ScaLAPACK
 - SuperLU
 - TAO
 - Trilinos
- Tools for code development:
 - Global Arrays
 - Overture
- Tools for code execution:
 - Chasm
 - CUMULVS
 - PAWS
 - TAU
- Grid:
 - GLOBUS
 - PyGLOBUS
- SciDAC:
 - *Center for Terascale Optimal PDE Simulations (TOPS)*
 - *Center for Component Technology for Terascale Simulation Software (CCTSS)*
 - *Terascale Simulation Tools and Technology Center (TSTT)*
 - *An Algorithmic and Software Framework for Applied Partial Differential Equations (APDEC)*
- Invited Talks:
 - *Facts and Wishful Thinking about the Future of Supercomputing*
 - User experiences
 - IBM tools