A Workshop on the ACTS Toolkit: Solving Problems in Science and Engineering

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What is the ACTS Toolkit?

http://acts.nersc.gov

- Advanced Computational Testing and Simulation
- Tools for development of parallel applications
  - originally conceived as autonomous tools
  - developed (primarily) at DOE labs
  - (currently) 20 tools
- ACTS is an “umbrella” project
  - leverage numerous independently funded projects
  - collect tools

ACTS Project Goals

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- Promote general solutions to complex programming needs
- Bring software packages together into a “toolkit”
- Provide consistent application interfaces
- Make the software interoperable
- Enable large scale applications
- Promote code reusability

How can ACTS work for you?

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- Some examples in computational sciences.
- Which tool? What approach? What do you get?
- A sample of scientific applications using ACTS Tools.
- Why do we need all these tools?
- Services provided at NERSC.
- Agenda for the Workshop.

Example: *data fitting*

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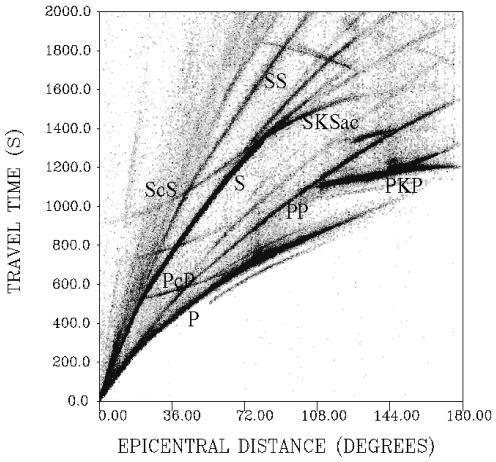
Data: *n* temperature measurements t_i at depths z_i in the Earth
Goal: define a model assuming a quadratic variation of temperature with depth

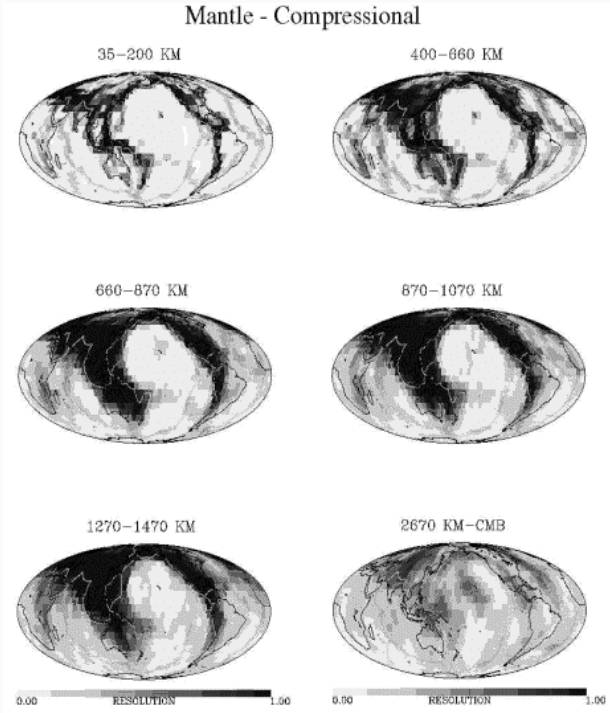
$$\begin{aligned} t_1 &= a + bz_1 + cz_1^2 \\ t_2 &= a + bz_2 + cz_2^2 \\ &\vdots \\ t_n &= a + bz_n + cz_n^2 \end{aligned} \quad \longrightarrow \quad \begin{Bmatrix} t_1 \\ t_2 \\ \vdots \\ t_n \end{Bmatrix} = \begin{bmatrix} 1 & z_1 & z_1^2 \\ 1 & z_2 & z_2^2 \\ & \vdots & \\ 1 & z_n & z_n^2 \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix}$$

***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 1x10^6 data points, and 2x10^5 parameters



Example: *Poisson's Equation in 1D*

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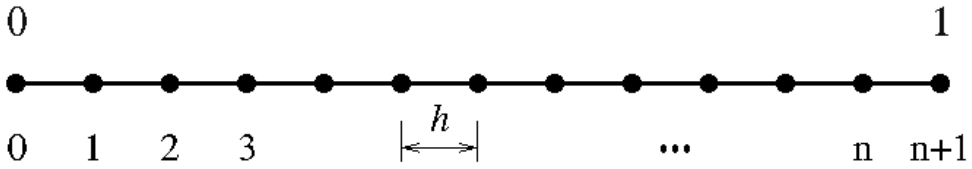
$$-\frac{d^2v(x)}{dx^2} = f(x),\ 0 < x < 1$$
$$v(0) = v(1) = 0\ \ (Dirichlet)$$



Centered Finite Difference Approximation:

$$\frac{dv(x)}{dx}\Big|_{x=(i-\frac{1}{2})h} \approx \frac{v_i - v_{i-1}}{h}$$
$$\frac{dv(x)}{dx}\Big|_{x=(i+\frac{1}{2})h} \approx \frac{v_{i+1} - v_i}{h}$$
$$\frac{d^2v(x)}{dx^2}\Big|_{x=x_i} \approx -\frac{2v_i - v_{i-1} - v_{i+1}}{h^2}$$

point i :

$$-v_{i-1} + 2v_i - v_{i+1} = h^2 f_i$$

$$\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix} \begin{Bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{Bmatrix} = h^2 \begin{Bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{Bmatrix}$$

Example: *complex PDE's*

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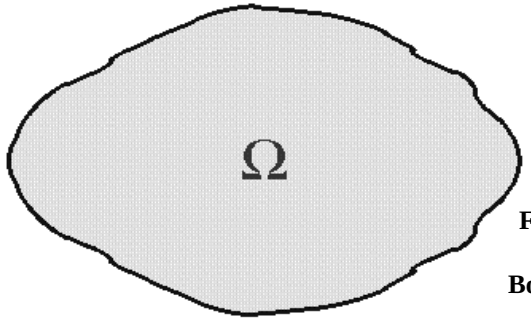
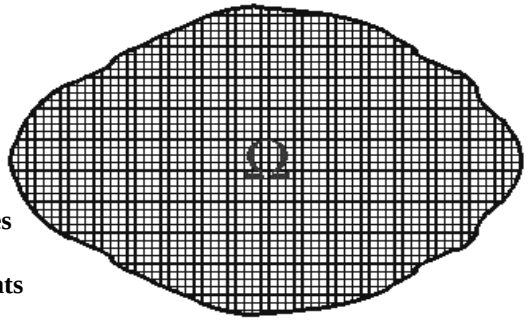
continuous problem

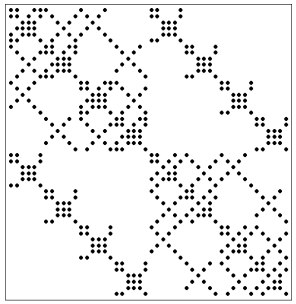


grid

Finite Differences
Finite Elements
Boundary Elements
Fourier
⋮

discrete problem





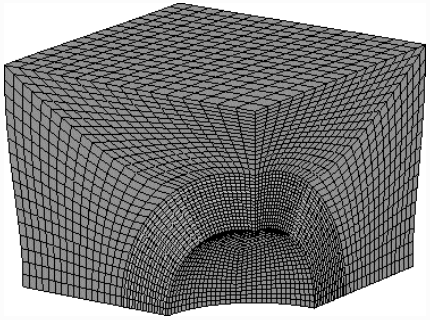
$= A$

(sparse matrix)

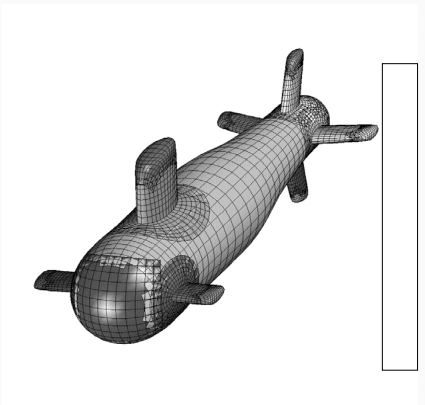
$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = f(t)$$

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

⋮



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.

Example: *Motions of Proteins*

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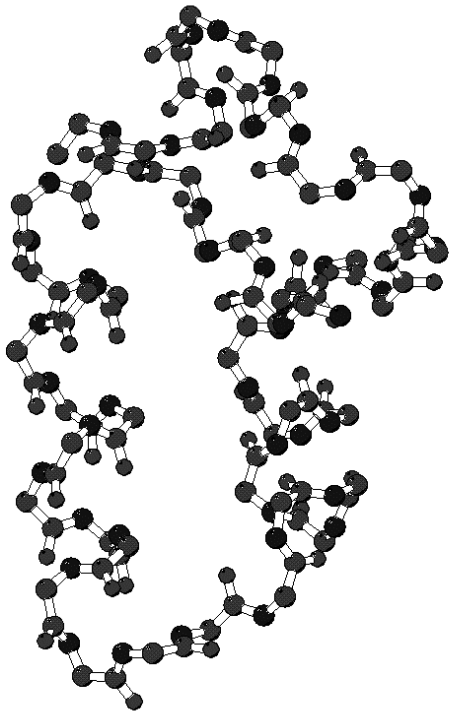


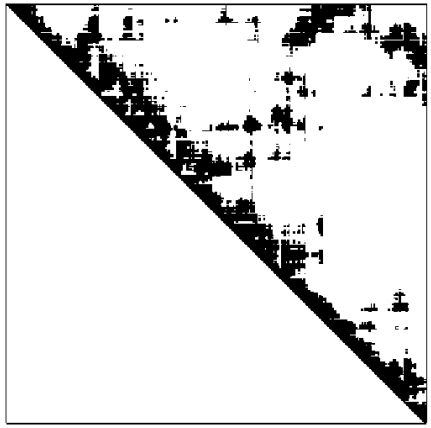
$$V = \frac{1}{2}\sum_{i=1}^{3n}\sum_{j=1}^{3n} k_{ij}(r_i - r_i^s)(r_j - r_j^s)$$

$$r_i(t) = r_i^s + \frac{1}{\sqrt{m_i}}\sum_{j=1}^{3n} a_{ij} q_j(t), \quad i = 1,2,\ldots 3n$$

$$q_j(t) = C_j \cos(\omega_j t + \phi_j)$$

$$\longrightarrow$$

$$A = M^{-\frac{1}{2}}(\nabla^2 E)M^{-\frac{1}{2}}$$



(sparse matrix)

What needs to be computed?

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$$Ax = b$$

(system of linear equations)

Direct Methods:

1. $A = LU$ (L lower triangular, U upper triangular)
2. $Ly = b$
3. $Ux = y$

SuperLU
ScaLAPACK

Iterative Methods:

$x_k = x_{k-1} + \alpha_k p_{k-1}$

only matrix - vector multiplies are needed

preconditoning is usually required

Trilinos
Hypre
PETSc

What needs to be computed?

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$$Az = \lambda z$$

(eigenvalue problem) — ScaLAPACK

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

(singular value decomposition) — ScaLAPACK

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

(systems of nonlinear equations) — PETSc TAO

PDEs — PETSc

ODEs — PVODE Trio

⋮

Other services may also be needed...

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- Computational steering
- Interactive visualization
- Distributed computation
- Data distribution and management
- Performance analysis
- Scripting Languages
- Interoperability

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Globus
CUMULVS
TAU
Global Arrays
PAWS
SILOON
Overture
Babel
CCA

Use of ACTS Tools

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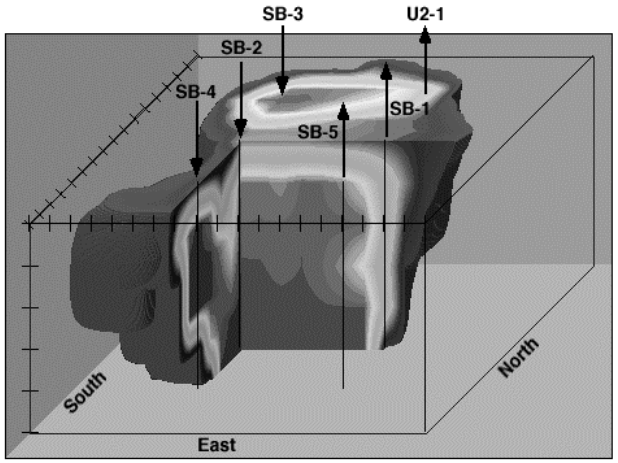
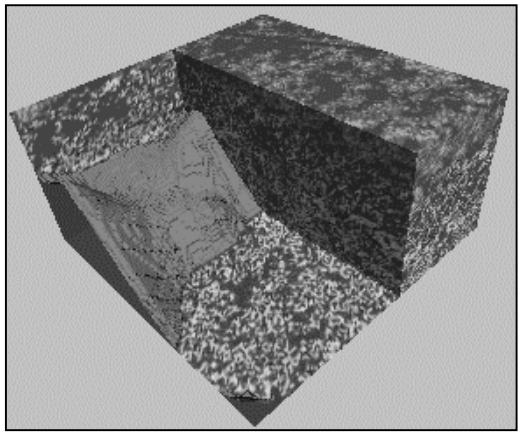
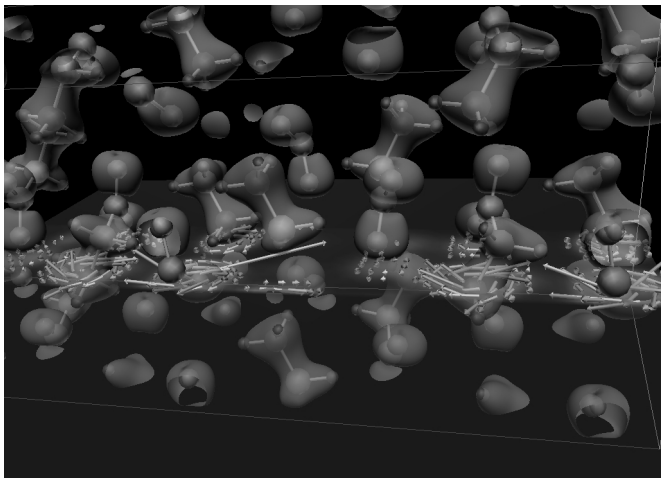


Multiphase flow, 4 million cell blocks, 32 million DOF, over 10.6 Gflops on an IBM SP (128 nodes), entire simulation runs in less than 30 minutes (Pope, Gropp, Morgan, Seperhrnoori, Smith and Wheeler).



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

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.



Use of ACTS Tools

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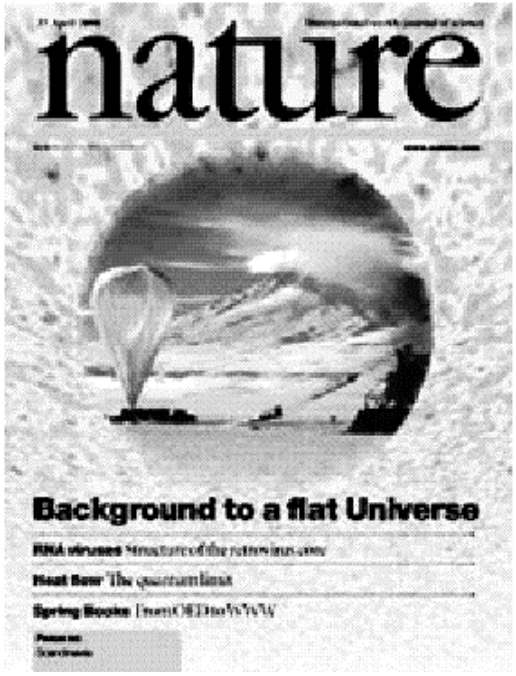
Collaborators at the LBNL, LLNL and the UC Davis obtained a complete solution of the ionization of a hydrogen atom by collision with an electron, the simplest nontrivial example of the long-standing unsolved problem of scattering in a quantum system of three charge particles. The images show representative 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.



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.

Why do we need these tools?

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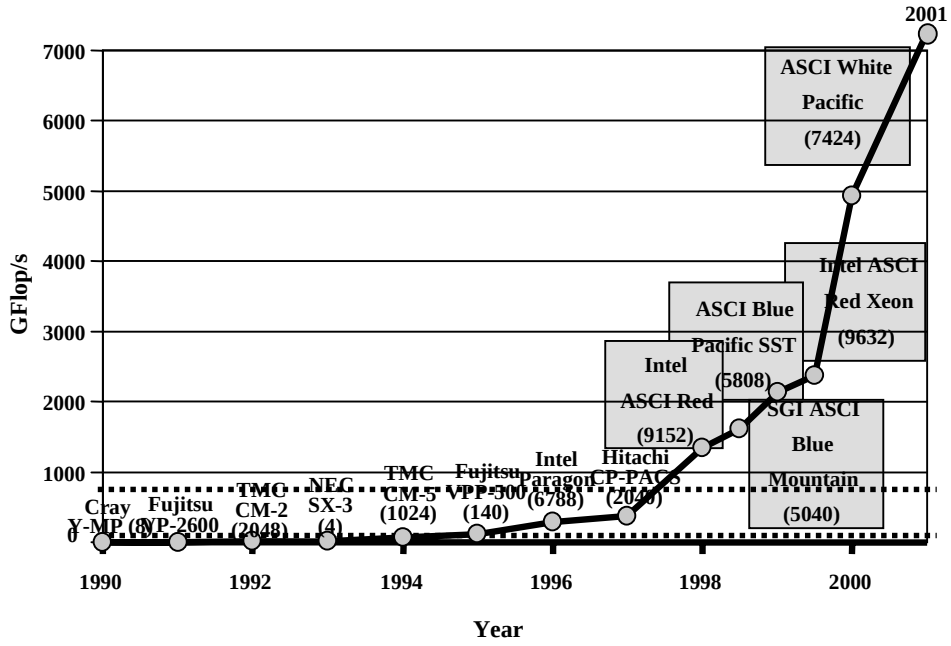

- High Performance Tools
  - portable
  - library calls
  - robust algorithms
  - help code optimization
- More code development in less time
- More simulation in less computer time

A computation that took
1 full year to complete
in 1980 could be done
in ~ 10 hours in 1992,
in ~ 16 minutes in 1997
and now can be done
in ~ 27 seconds in 2001!

ACTS@NERSC

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- Make ACTS tools available on NERSC platforms
- Provide technical support
- Perform independent evaluation of tools
- Maintain online ACTS information center
- Identify new users who can benefit from toolkit
- Work with users to integrate tools into applications
- Minimize risk to users

Workshop Agenda

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- Wednesday: numerical tools (ScaLAPACK, SuperLU) and interoperability (Babel, CCA); hands-on (ScaLAPACK, SuperLU)
- Thursday: numerical tools (Trilinos, Hypre, The PVODE Trio), tools for code development (Global Arrays, Overture), tools for code execution (CUMULVS); hands-on (CUMULVS).
- Friday: numerical tools (PETSc, TAO), tools for code execution (Globus); hands-on (PETSc, TAO).
- Saturday: tools for code execution (TAU, SILOON, PAWS); hands-on (TAU, SILOON, PAWS).
- ACTS is more than what we will be able to cover in the next three and half-days!

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