Overview of the U. S. DOE Scientific Discovery through Advanced Computing (SciDAC) Project

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NASA Langley Research Center

Institute for Scientific Computing Research
Lawrence Livermore National Laboratory
Terascale simulation has been “sold”

In these, and many other areas, simulation is an important complement to experiment.
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Experiments prohibited or impossible

Experiments dangerous

Experiments controversial

Scientific Simulation

Environment global climate contaminant transport

Applied Physics radiation transport supernovae

Engineering crash testing aerodynamics

Lasers & Energy combustion ICF

Biology drug design genomics

In these, and many other areas, simulation is an important complement to experiment.
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Experiments prohibited or impossible

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Scientific Simulation

Applied Physics
- radiation transport
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Lasers & Energy
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Biology
- drug design
- genomics

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However, simulation is far from proven! To meet expectations, we need to handle problems of multiple physical scales.
Enabling technologies groups to develop reusable software and partner with application groups

For 2001 start-up, 51 projects share $57M/year

- Approximately one-third for applications
- A third for “integrated software infrastructure centers”
- A third for grid infrastructure and collaboratories

Plus, two new 5 Tflop/s IBM SP machines available for SciDAC researchers
SciDAC project characteristics

- **Affirmation of importance of simulation**
  - for new scientific discovery, not just for “fitting” experiments

- **Recognition that leading-edge simulation is interdisciplinary**
  - no support for physicists and chemists to write their own software infrastructure; must collaborate with math & CS experts

- **Commitment to distributed hierarchical memory computers**
  - new code must target this architecture type

- **Requirement of lab-university collaborations**
  - complementary strengths in simulation
  - 13 laboratories and 50 universities in first round of projects
Major DOE labs

DOE Science Lab
- Lawrence Berkeley
- Pacific Northwest
- Argonne
- Brookhaven
- Old Dominion University
- Sandia
- Lawrence Livermore
- Los Alamos
- Oak Ridge

DOE Defense Lab
- Sandia Livermore
Large platforms provided for ASCI ...

ASCI program of the U.S. DOE has roadmap to go to 100 Tflop/s by 2006
www.llnl.gov/asci/platforms
...and now for SciDAC

**IBM Power3+ SMP**
- 16 procs per node
- 208 nodes
- 24 Gflop/s per node
- 5 Tflop/s

**IBM Power4 Regatta**
- 32 procs per node
- 24 nodes
- 166 Gflop/s per node
- 4 Tflop/s (10 in 2003)
NSF’s 13.6 Tflop/s TeraGrid coming on line

TeraGrid: NCSA, SDSC, Caltech, Argonne

NSF's 13.6 Tflop/s TeraGrid coming on line

TeraGrid: NCSA, SDSC, Caltech, Argonne

www.teragrid.org

Caltech

40 Gb/s (OC-192)

SDSC
4.1 TF
225 TB

Argonne

NCSA/PACI
8 TF
240 TB

c/o I. Foster

ITST Lecture Series #1
Idealized Kiviat diagram for architecture
Japan’s Earth Simulator

- 35.6 Tflop/s LINPACK
- Disks
- Cartridge Tape Library System
- Processor Node (PN) Cabinets
- Power Supply System
- Air Conditioning System
- Double Floor for IN Cables
- Network System
- Interconnection Network (IN) Cabinets
- Japan’s Earth Simulator
Cross-section of Earth Simulator Building

- Lightning protection system
- Air-conditioning return duct
- Double floor for IN cables and air-conditioning
- Power supply system
- Air-conditioning system
Earth Simulator Bird’s Eye

Operations and research

Power plant

Computer system
Boundary conditions from architecture

Algorithms must run on physically distributed memory units connected by message-passing network, each serving one or more processors with multiple levels of cache

“horizontal” aspects

network latency, BW, diameter

“vertical” aspects

memory latency, BW; L/S (cache/reg) BW
Following the platforms …

... Algorithms must be
  - highly concurrent and straightforward to load balance
  - not communication bound
  - cache friendly (temporal and spatial locality of reference)
  - highly scalable (in the sense of convergence)

Goal for algorithmic scalability: fill up memory of arbitrarily large machines while preserving nearly constant* running times with respect to proportionally smaller problem on one processor

*logarithmically growing
## Gordon Bell Prize performance

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Gordon Bell Prize outpaces Moore’s Law

Four orders of magnitude in 13 years
Official SciDAC Goals

“Create a new generation of scientific simulation codes that take full advantage of the extraordinary computing capabilities of terascale computers.”

“Create the mathematical and systems software to enable the scientific simulation codes to effectively and efficiently use terascale computers.”

“Create a collaboratory software environment to enable geographically separated scientists to effectively work together as a team and to facilitate remote access to both facilities and data.”
Four science programs involved ...

“14 projects will advance the science of climate simulation and prediction. These projects involve novel methods and computationally efficient approaches for simulating components of the climate system and work on an integrated climate model.”

“10 projects will address quantum chemistry and fluid dynamics, for modeling energy-related chemical transformations such as combustion, catalysis, and photochemical energy conversion. The goal of these projects is efficient computational algorithms to predict complex molecular structures and reaction rates with unprecedented accuracy.”
Four science programs involved …

“4 projects in high energy and nuclear physics will explore the fundamental processes of nature. The projects include the search for the explosion mechanism of core-collapse supernovae, development of a new generation of accelerator simulation codes, and simulations of quantum chromodynamics.”

“5 projects are focused on developing and improving the physics models needed for integrated simulations of plasma systems to advance fusion energy science. These projects will focus on such fundamental phenomena as electromagnetic wave-plasma interactions, plasma turbulence, and macroscopic stability of magnetically confined plasmas.”
SciDAC 1st Year Portfolio: $57M

SciDAC- Program Offices
$ in M

$7
$2
$8
$3
$37

for Math, Information and Computer Sciences

MICS
BER
BES
HENP
FES
Data Grids and Collaboratories

- National data grids
  - Particle physics grid
  - Earth system grid
  - Plasma physics for magnetic fusion
  - DOE Science Grid

- Middleware
  - Security and policy for group collaboration
  - Middleware technology for science portals

- Network research
  - Bandwidth estimation, measurement methodologies and application
  - Optimizing performance of distributed applications
  - Edge-based traffic processing
  - Enabling technology for wide-area data intensive applications
What is the/a “Grid”?

- The Grid refers to an infrastructure that enables the integrated, collaborative use of high-end computers, networks, databases, and scientific instruments owned and managed by multiple organizations.

- Grid applications often involve large amounts of data and/or computing and often require secure resource sharing across organizational boundaries, and are thus not easily handled by today’s Internet and Web infrastructures.
Grid example: smart instruments

- **Advanced Photon Source**
- **DOE X-ray grand challenge**
- **Wide-area dissemination**
- **Real-time collection**
- **Archival storage**
- **Desktop & VR clients with shared controls**
- **Tomographic reconstruction**
First Grid textbook

- “The Grid: Blueprint for a New Computing Infrastructure”
- Edited by Ian Foster & Carl Kesselman
- July 1998, 701 pages
- “This is a source book for the history of the future.”
  Vint Cerf, Senior Vice President, Internet Architecture and Engineering, MCI
Computer Science ISICs

- **Scalable Systems Software**
  Provide software tools for management and utilization of terascale resources.

- **High-end Computer System Performance: Science and Engineering**
  Develop a science of performance prediction based on concepts of program signatures, machine signatures, detailed profiling, and performance simulation and apply to complex DOE applications. Develop tools that assist users to engineer better performance.

- **Scientific Data Management**
  Provide a framework for efficient management and data mining of large, heterogeneous, distributed data sets.

- **Component Technology for Terascale Software**
  Develop software component technology for high-performance parallel scientific codes, promoting reuse and interoperability of complex software, and assist application groups to incorporate component technology into their high-value codes.
Applied Math ISICs

☞ Terascale Simulation Tools and Technologies

Develop framework for use of multiple mesh and discretization strategies within a single PDE simulation. Focus on high-quality hybrid mesh generation for representing complex and evolving domains, high-order discretization techniques, and adaptive strategies for automatically optimizing a mesh to follow moving fronts or to capture important solution features.

☞ Algorithmic and Software Framework for Partial Differential Equations

Develop framework for PDE simulation based on locally structured grid methods, including adaptive meshes for problems with multiple length scales; embedded boundary and overset grid methods for complex geometries; efficient and accurate methods for particle and hybrid particle/mesh simulations.

☞ Terascale Optimal PDE Simulations

Develop an integrated toolkit of near optimal complexity solvers for nonlinear PDE simulations. Focus on multilevel methods for nonlinear PDEs, PDE-based eigenanalysis, and optimization of PDE-constrained systems. Packages sharing same distributed data structures include: adaptive time integrators for stiff systems, nonlinear implicit solvers, optimization, linear solvers, and eigenanalysis.
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Exciting time for enabling technologies

SciDAC application groups have been chartered to build new and improved **COMMUNITY CODES**. Such codes, such as NWCHEM, consume hundreds of person-years of development, run at hundreds of installations, are given large fractions of community compute resources for decades, and acquire an “authority” that can enable or limit what is done and accepted as science in their respective communities. Except at the beginning, it is difficult to promote major algorithmic ideas in such codes, since change is expensive and sometimes resisted.

ISIC groups have a chance, due to the interdependence **built into the SciDAC program structure**, to simultaneously influence many of these codes, by delivering software incorporating optimal algorithms that may be reused across many applications. Improvements driven by one application will be available to all. While they are building community codes, this is our chance to build a **CODE COMMUNITY**!
SciDAC themes

- Chance to do community codes “right”
- Meant to set “new paradigm” for other DOE programs
- Cultural barriers to interdisciplinary research acknowledged up front
- Accountabilities constructed in order to force the “scientific culture” issue
What “Integration” means to SciDAC
## Sample Application/ISIC Interactions

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<tr>
<td>BES</td>
<td>Advanced Methods for Electronic Structure</td>
<td>Yes</td>
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<td>BES</td>
<td>Advancing Multi-Referance Methods in Electronic Structure Theory</td>
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<td>BES</td>
<td>Accurate Properties for Open-Shell States of Large Molecules</td>
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<td>BES</td>
<td>Advanced Software for the Calculation of Thermochemistry, Kinetics and Dynamics</td>
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<td>ASCR</td>
<td>DOE Science Grid: Enabling and Deploying the SciDAC Collaboratory Software Environment</td>
<td>Yes</td>
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<td>ASCR</td>
<td>A National Collaboratory to Advance the Science of High-Temperature Plasma Physics for Magnetic Fusion</td>
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<td>ASCR</td>
<td>Particle Physics Data Grid Collaborative Pilot</td>
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<td>ASCR</td>
<td>Earth System Grid II: Turning Climate Datasets into Community Resources</td>
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<td>ASCR</td>
<td>A High-Performance Data Grid Toolkit: Enabling Technology for Wide Area Data-Intensive Applications</td>
<td>Yes</td>
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<td>ASCR</td>
<td>Scalable Systems Software Center (SSS)</td>
<td>Yes</td>
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<td>ASCR</td>
<td>High-End Computer Systems Performance: Science and Engineering (PERC)</td>
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<td>ASCR</td>
<td>Center for Component Technology for Terascale Simulation Software (CCA)</td>
<td>Yes</td>
<td>Yes</td>
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<tr>
<td>ASCR</td>
<td>Scientific Data Management Center (SDM)</td>
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<tr>
<td>ASCR</td>
<td>Terascale Optimal PDE Simulations (TOPS)</td>
<td>Yes</td>
<td>Yes</td>
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<tr>
<td>ASCR</td>
<td>Terascale Simulation Tools &amp; Technologies Center (TSTT)</td>
<td>Yes</td>
<td>Yes</td>
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<td>ASCR</td>
<td>Algorithmic and Software Framework for Applied Partial Differential Equations (APDE)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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What’s new in SciDAC library software?

- Philosophy of library usage
  - complex algorithms with lots of callbacks to user code (e.g., to physics routines by implicit solvers)
  - extensibility
  - polyalgorithmic adaptivity

- Resources for development, maintenance, and support
  - not just for “dissertation scope” ideas

- Experience on terascale scale computers
Traditional approach to software interoperability

- Direct interfacing between different packages/libraries/apps
  - Public interfaces are unique

- Many-to-Many couplings require Many \(^2\) interfaces
  - Often a heroic effort to understand the details of both codes
  - Not a scalable solution

Diagram:

- Data / mesh software: Overture, GRACE, SUMAA3d, DAs
- Linear solvers: Hypre, Trilinos, ISIS+, PETSc
CCA approach: common interface specification

- Reduces the Many-to-Many problem to a Many-to-One problem
  - Allows interchangeability and experimentation
  - Difficulties
    - Interface agreement
    - Functionality limitations
    - Maintaining performance
CCA concept: SCMD (SPMD) components

MPI application using CCA for interaction between components A and B within the same address space

Direct Connection supplied by framework at compile/runtime

Adaptive mesh component written by user1

Solver component written by user2

Proc1  Proc2  Proc3  etc...
Interacting with ISICs

Applications

- APDEC
- TSTT
- TOPS
- SDM
- PERC
- CCA
- SS

Indicates “dependence on”
Interacting with ISICs

Applications

APDEC → TOPS → PERC, CCA → SS

TSTT → TOPS

SDM → TOPS

Indicates “dependence on”
Introducing “Terascale Optimal PDE Simulations” (TOPS) ISIC
Nine institutions, $17M, five years, 24 co-PIs
34 apps groups (BER, BES, FES, HENP)

7 ISIC groups (4 CS, 3 Math)

10 grid, data collaboratory groups

Adaptive gridding, discretization

Solvers

Systems software, component architecture, performance engineering, data management

Ax = b
Ax = ? Bx
f(x, t, p) < 0
F(x, p) < 0

min_u (x, u) s.t.
F(x, u) < 0

Software integration

Performance optimization
Who we are...

... the PETSc and TAO people

... the hypre and PVODE people

... the SuperLU and PARPACK people

... as well as the builders of other widely used packages ...
Plus some university collaborators

Demmel et al.  Manteuffel et al.  Dongarra et al.

Carnegie Mellon

Widlund et al.  Ghattas et al.  Keyes et al.

Our DOE lab collaborations predate SciDAC by many years.
You may know our “Templates”

www.netlib.org

... but what we are doing now goes “in between” and far beyond!

www.siam.org
Scope for TOPS

- **Design and implementation of “solvers”**
  - Time integrators (w/ sens. anal.)
    - $f(x, x, t, p) \neq 0$
  - Nonlinear solvers (w/ sens. anal.)
    - $F(x, p) \neq 0$
  - Constrained optimizers
    - $\min_u (x, u) \text{ s.t. } F(x, u) \neq 0, u \neq 0$
  - Linear solvers
    - $Ax \neq b$
  - Eigensolvers
    - $Ax \neq ?Bx$

- **Software integration**
- **Performance optimization**
Motivation for TOPS

- Many DOE mission-critical systems are modeled by PDEs
- Finite-dimensional models for infinite-dimensional PDEs must be large for accuracy
  - “Qualitative insight” is not enough
  - Simulations must resolve policy controversies, in some cases
- Algorithms are as important as hardware in supporting simulation
  - Easily demonstrated for PDEs in the period 1945–2000
  - Continuous problems provide exploitable hierarchy of approximation models, creating hope for “optimal” algorithms
- Software lags both hardware and algorithms

- Not just algorithms, but vertically integrated software suites
- Portable, scalable, extensible, tunable implementations
- Motivated by representative apps, intended for many others
- Starring hyspre and PETSc, among other existing packages
- Driven by three applications SciDAC groups
  - LBNL-led “21st Century Accelerator” designs
  - ORNL-led core collapse supernovae simulations
  - PPPL-led magnetic fusion energy simulations
- Coordinated with other ISIC SciDAC groups
Salient Application Properties

- **Multirate**
  - requiring fully or semi-implicit in time solvers

- **Multiscale**
  - requiring finest mesh spacing much smaller than domain diameter

- **Multicomponent**
  - requiring physics-informed preconditioners, transfer operators, and smoothers

- **Not linear**
- **Not selfadjoint**
- **Not structured**
Keyword: “Optimal”

- Convergence rate nearly independent of discretization parameters
  - Multilevel schemes for rapid linear convergence of linear problems
  - Newton-like schemes for quadratic convergence of nonlinear problems

- Convergence rate as independent as possible of physical parameters
  - Continuation schemes
  - Physics-based preconditioning

- Problem Size (increasing with number of processors)
  - Time to Solution

The solver is a key part, but not the only part, of the simulation that needs to be scalable.
Why Optimal?

- The more powerful the computer, the *greater* the importance of optimality

**Example:**
- Suppose $Alg1$ solves a problem in time $CN^2$, where $N$ is the input size
- Suppose $Alg2$ solves the same problem in time $CN$
- Suppose that the machine on which $Alg1$ and $Alg2$ run has 10,000 processors, on which they have been parallelized to run

- In constant time (compared to serial), $Alg1$ can run a problem 100X larger, whereas $Alg2$ can run a problem 10,000X larger
Why Optimal?, cont.

- Alternatively, filling the machine’s memory, \textit{Alg1} requires 100X time, whereas \textit{Alg2} runs in constant time.

- Is 10,000 processors a reasonable expectation?
  - Yes, we have it today (ASCI White).

- Could computational scientists really use 10,000X?
  - Of course; we are approximating the continuum.
  - A grid for weather prediction allows points every 1km versus every 100km on the earth’s surface.
  - In 2D 10,000X disappears fast; in 3D even faster.

- However, these machines are expensive (ASCI White is $100M, plus ongoing operating costs), and optimal algorithms are the only algorithms that we can afford to run on them.
It’s 2002; do you know what your solver is up to?

- Has your solver not been updated in the past five years?
- Is your solver running at 1-10% of machine peak?
- Do you spend more time in your solver than in your physics?
- Is your discretization or model fidelity limited by the solver?
- Is your time stepping limited by stability?
- Are you running loops around your analysis code?
- Do you care how sensitive to parameters your results are?

If the answer to any of these questions is “yes”, you are a potential customer!
What we believe

Many of us came to work on solvers through interests in applications

What we believe about …

- applications
- users
- solvers
- legacy codes
- software

… will impact how comfortable you are collaborating with us
What we believe about apps

_solution of a system of PDEs is rarely a goal in itself_

- PDEs are solved to derive various outputs from specified inputs
- Actual goal is characterization of a response surface or a design or control strategy
- Together with analysis, sensitivities and stability are often desired

- Software tools for PDE solution should also support related follow-on desires

-no general purpose PDE solver can anticipate all needs_

- Why we have national laboratories, not numerical libraries for PDEs today
- A PDE solver improves with user interaction
- Pace of algorithmic development is very rapid

- Extensibility is important
What we believe about users

- Solvers are used by people of varying numerical backgrounds
  - Some expect MATLAB-like defaults
  - Others want to control everything, e.g., even varying the type of smoother and number of smoothings on different levels of a multigrid algorithm

- Users’ demand for resolution is virtually insatiable
  - Relieving resolution requirements with modeling (e.g., turbulence closures, homogenization) only defers the demand for resolution to the next level
  - Validating such models requires high resolution

- Multilayered software design is important

- Processor scalability and algorithmic scalability (optimality) are critical
What we believe about legacy code

- Porting to a scalable framework does not mean starting from scratch
  - High-value meshing and physics routines in original languages can be substantially preserved
  - Partitioning, reordering and mapping onto distributed data structures (that we may provide) adds code but little runtime

- Legacy solvers may be limiting resolution, accuracy, and generality of modeling overall
  - Replacing the solver may “solve” several other issues
  - However, pieces of the legacy solver may have value as part of a preconditioner

- Distributions should include code samples exemplifying “separation of concerns”
- Solver toolkits should include “shells” for callbacks to high value legacy routines
What we believe about solvers

- Solvers are employed as part of a larger code
  - Solver library is not only library to be linked
  - Solvers may be called in multiple, nested places
  - Solvers typically make callbacks
  - Solvers should be swappable

- Solver threads must not interfere with other component threads, including other active instances of themselves

- Solvers are employed in many ways over the life cycle of an applications code
  - During development and upgrading, robustness (of the solver) and verbose diagnostics are important
  - During production, solvers are streamlined for performance

- Tunability is important
What we believe about software

- A continuous operator may appear in a discrete code in many different instances
  - Optimal algorithms tend to be hierarchical and nested iterative
  - Processor-scalable algorithms tend to be domain-decomposed and concurrent iterative
  - Majority of progress towards desired highly resolved, high fidelity result occurs through cost-effective low resolution, low fidelity parallel efficient stages

- Hardware changes many times over the life cycle of a software package
  - Processors, memory, and networks evolve annually
  - Machines are replaced every 3-5 years at major DOE centers
  - Codes persist for decades

- Portability is critical

- Operator abstractions and recurrence are important
Why is TOPS needed?

What exists already?

- Adaptive time integrators for stiff systems: variable-step BDF methods
- Nonlinear implicit solvers: Newton-like methods, FAS multilevel methods
- Optimizers (with constraints): quasi-Newton RSQP methods
- Linear solvers: subspace projection methods (multigrid, Schwarz, classical smoothers), Krylov methods (CG, GMRES), sparse direct methods
- Eigensolvers: matrix reduction techniques followed by tridiagonal eigensolvers, Arnoldi solvers

What is wrong?

- Many widely used libraries are “behind the times” algorithmically
- Logically innermost (solver) kernels are often the most computationally complex — should be designed from the inside out by experts and present the right “handles” to users
- Today’s components do not “talk to” each other very well
- Mixing and matching procedures too often requires mapping data between different storage structures (taxes memory and memory bandwidth)
Nonlinear Solvers

What’s ready?
- **KINSOL** (LLNL) and **PETSc** (ANL)
- Preconditioned Newton-Krylov (NK) methods with MPI-based objects
- Asymptotically nearly quadratically convergent and mesh independent
- Matrix-free implementations (FD and AD access to Jacobian elements)
- Thousands of direct downloads (PETSc) and active worldwide “friendly user” base
- Interfaced with hypre preconditioners (KINSOL)
- Sensitivity analysis extensions (KINSOL)
- 1999 Bell Prize for unstructured implicit CFD computation at 0.227 Tflop/s on a legacy F77 NASA code

What’s next?
- Semi-automated continuation schemes (e.g., pseudo-transience)
- Additive-Schwarz Preconditioned Inexact Newton (ASPIN)
- Full Approximation Scheme (FAS) multigrid
- Polyalgorithmic combinations of ASPIN, FAS, and NK-MG, together with new linear solvers/preconditioners
- Automated Jacobian calculations with parallel colorings
- New grid transfer and nonlinear coarse grid operators
- Guidance of trade-offs for cheap/expensive residual function calls
- Further forward and adjoint sensitivities
Optimizers

What’s ready?

- TAO (ANL) and VELTISTO (CMU)
- Bound-constrained and equality-constrained optimization
- Achieve optimum in number of PDE solves independent of number of control variables
- TAO released 2000, VELTISTO 2001
- Both built on top of PETSc
- Applied to problems with thousands of controls and millions of constraints on hundreds of processors
- Used for design, control, parameter identification
- Used in nonlinear elasticity, Navier-Stokes, acoustics
- State-of-art Lagrange-Newton-Krylov-Schur algorithmics

What’s next?

- Extensions to inequality constraints (beyond simple bound constraints)
- Extensions to time-dependent PDEs, especially for inverse problems
- Multilevel globalization strategies
- Toleration strategies for approximate Jacobians and Hessians
- “Hardening” of promising control strategies to deal with negative curvature of Hessian
- Pipelining of PDE solutions into sensitivity analysis
Linear Solvers

What’s ready?
- **PETSc** (ANL), **hypre** (LLNL), **SuperLU** (UCB), **Oblio** (ODU)
- Krylov, multilevel, sparse direct
- Numerous preconditioners, incl. BNN, SPAI, PILU/PICC
- Mesh-independent convergence for ever expanding set of problems
- **hypre** used in several ASCI codes and milestones to date
- **SuperLU** in ScaLAPACK
- State-of-art algebraic multigrid (**hypre**) and supernodal (**SuperLU**) efforts
- Algorithmic replacements *alone* yield up to two orders of magnitude in DOE apps, before parallelization

What’s next?
- Hooks for physics-based operator-split preconditionings
- AMGe, focusing on incorporation of neighbor information and strong cross-variable coupling
- Spectral AMGe for problems with geometrically oscillatory but algebraically smooth components
- FOSLS-AMGe for saddle-point problems
- Hierarchical basis ILU
- Incomplete factorization adaptations of **SuperLU**
- Convergence-enhancing orders for ILU
- Stability-enhancing orderings for sparse direct methods for indefinite problems
Eigensolvers

What’s ready?

- LAPACK and ScaLAPACK symmetric eigensolvers (UCB, UTenn, LBNL)
- PARPACK for sparse and nonsymmetric problems
- Reductions to symmetric tridiagonal or Hessenberg form, followed by new “Holy Grail” algorithm
- Holy Grail optimal (!): $O(kn)$ work for $k n$-dimensional eigenvectors

What’s next?

- Direct and iterative linear solution methods for shift-invert Lanczos for selected eigenpairs in large symmetric eigenproblems
- Jacobi-Davidson projection methods for selected eigenpairs
- Multilevel methods for eigenproblems arising from PDE applications
- Hybrid multilevel/Jacobi-Davidson methods
Each color module represents an algorithmic research idea on its way to becoming part of a supported community software tool. At any moment (vertical time slice), TOPS has work underway at multiple levels. While some codes are in applications already, they are being improved in functionality and performance as part of the TOPS research agenda.
Background of PETSc Library

- Developed by at Argonne to support research, prototyping, and production parallel solutions of operator equations in message-passing environments; now joined by four additional staff under SciDAC
- Distributed data structures as fundamental objects - index sets, vectors/gridfunctions, and matrices/arrays
- Iterative linear and nonlinear solvers, combinable modularly and recursively, and extensibly
- Portable, and callable from C, C++, Fortran
- Uniform high-level API, with multi-layered entry
- Aggressively optimized: copies minimized, communication aggregated and overlapped, caches and registers reused, memory chunks preallocated, inspector-executor model for repetitive tasks (e.g., gather/scatter)

See http://www.mcs.anl.gov/petsc
User Code/PETSc Library Interactions

Main Routine

Timestepping Solvers (TS)

Nonlinear Solvers (SNES)

Linear Solvers (SLES)

PETSc

PC

KSP

Application Initialization

Function Evaluation

Jacobian Evaluation

Post-Processing

User code

PETSc code
User Code/PETSc Library Interactions

Main Routine

Timestepping Solvers (TS)

Nonlinear Solvers (SNES)

Linear Solvers (SLES)

PC  KSP

Application Initialization

Function Evaluation

Jacobian Evaluation

Post-Processing

User code
PETSc code
ADIC code
Background of Hypre Library
(to be combined with PETSc under SciDAC)

- Developed by Livermore to support research, prototyping, and production parallel solutions of operator equations in message-passing environments; now joined by seven additional staff under ASCI and SciDAC
- Object-oriented design similar to PETSc
- Concentrates on linear problems only
- Richer in preconditioners than PETSc, with focus on algebraic multigrid
- Includes other preconditioners, including sparse approximate inverse (Parasails) and parallel ILU (Euclid)

Hypre’s “Conceptual Interfaces”

**Linear System Interfaces**

- Structured
- Composite
- Block-structured
- Unstructured

**Linear Solvers**

- GMG, ...
- FAC, ...
- Hybrid, ...
- AMGe, ...
- ILU, ...

**Data Layout**

- Structured
- Composite
- Block-structured
- Unstructured
- CSR

Slide c/o R. Falgout, LLNL
Goals/Success Metrics

TOPS users —

- Understand range of algorithmic options and their tradeoffs (e.g., memory versus time)
- Can try all reasonable options easily without recoding or extensive recompilation
- Know how their solvers are performing
- Spend more time in their physics than in their solvers
- Are intelligently driving solver research, and publishing joint papers with TOPS researchers
- Can simulate *truly new physics*, as solver limits are steadily pushed back
Expectations TOPS has of Users

☞ Be willing to experiment with novel algorithmic choices – optimality is rarely achieved beyond model problems without interplay between physics and algorithmics!

☞ Adopt flexible, extensible programming styles in which algorithmic and data structures are not hardwired

☞ Be willing to let us play with the real code you care about, but be willing, as well to abstract out relevant compact tests

☞ Be willing to make concrete requests, to understand that requests must be prioritized, and to work with us in addressing the high priority requests

☞ If possible, profile, profile, profile before seeking help
A Computational Facility for Reacting Flow Science

This project aims to advance the state of the art in understanding and predicting chemical reaction processes and their interactions with fluid flow. This will be done using a two-pronged approach. First, a flexible software toolkit for reacting flow computations will be developed, where distinct functionalities, developed by experts, are implemented as components within the Common Component Architecture. Second, advanced analysis/computation components will be developed that enable enhanced physical understanding of reacting flows. The assembled software will be applied to 2D/3D reacting flow problems and validated with respect to reacting flow databases at the Combustion Research Facility.

Habib Najm
SNL
Geodesic Climate Model

A Geodesic Climate Model with Quasi-Lagrangian Vertical Coordinates

Colorado State University will lead a multi-institutional collaboration of universities and government laboratories in an integrated program of climate science, applied mathematics and computational science to develop the climate model of the future. This project will build upon capabilities climate modeling, advanced mathematical research, and high-end computer architectures to provide useful projections of climate variability and change at regional to global scales. An existing atmospheric dynamical core based on parallel multigrid on a geodesic sphere will be augmented with an ocean model and enhanced algorithms.

David Randall
Colorado State University
Magnetic Reconnection

Magnetic Reconnection: Applications to Sawtooth Oscillations, Error Field Induced Islands and the Dynamo Effect

The research goals of this project include producing a unique high performance code and using this code to study magnetic reconnection in astrophysical plasmas, in smaller scale laboratory experiments, and in fusion devices. The modular code that will be developed will be a fully three-dimensional, compressible Hall MHD code with options to run in slab, cylindrical and toroidal geometry and flexible enough to allow change in algorithms as needed. The code will use adaptive grid refinement, will run on massively parallel computers, and will be portable and scalable. The research goals include studies that will provide increased understanding of sawtooth oscillations in tokamaks, magnetotail substorms, error-fields in tokamaks, reverse field pinch dynamos, astrophysical dynamos, and laboratory reconnection experiments.

Amitava Bhattacharjee
University of Iowa
Extended MHD

Center for Extended Magnetohydrodynamic Modeling

This research project will develop computer codes that will enable a realistic assessment of the mechanisms leading to disruptive and other stability limits in the present and next generation of fusion devices. With an improvement in the efficiency of codes and with the extension of the leading 3D nonlinear magneto-fluid models of hot, magnetized fusion plasmas, this research will pioneer new plasma simulations of unprecedented realism and resolution. These simulations will provide new insights into low frequency, long-wavelength non-linear dynamics in hot magnetized plasmas, some of the most critical and complex phenomena in plasma and fusion science. The underlying models will be validated through cross-code and experimental comparisons.

Steve Jardin
PPPL
Lattice Gauge Center

National Infrastructure for Lattice Gauge Computing

The project will focus on simulations of quantum chromodynamics (QCD), the sector of the Standard Model of elementary particle physics that describes the strong forces between particles. The entire US community of theorists, both nuclear physicists and high-energy physicists, who work on Lattice Gauge theory, have joined together in this proposal. There is no doubt that in order to achieve the sort of scientific breakthroughs they are aiming at, highly cost-effective terascale computing resources will be needed. This project aims to fully understand the performance and costs for both a special-purpose Lattice Gauge Theory super-computer and for clusters of commodity computers, with special-purpose interconnects. It will also lay the foundations necessary to build community-wide codes that can take maximum advantage of future computing hardware. These calculations, when carried out on terascale machines, will provide important theoretical insights and support for the large experimental efforts in high energy and nuclear physics.

Robert Sugar, University of California, Santa Barbara
Accelerated Simulation Environment

Advanced Computing for 21st Century Accelerator Science and Technology

The project will work on simulating particle accelerators, some of the largest and most complex scientific instruments. A new generation of accelerator simulation codes will help us to use existing accelerators more efficiently and will strongly impact the design, technology and cost of future accelerators.

Robert Ryne, Lawrence Berkeley Laboratory and Kwok Ko, Stanford Linear Accelerator Center
Terascale Supernova Initiative

Shedding New Light on Exploding Stars:

The project will use modeling of integrated complex systems to search for the explosion mechanism of core-collapse supernovae – one of the most important and challenging problems in nuclear astrophysics. The project involves a very broad multi-disciplinary team of scientists, computer scientists and mathematicians.

Anthony Mezzacappa, Oak Ridge National Laboratory
TOPS may be for you!

For more information ...

dkeyes@odu.edu

http://www.math.odu.edu/~keyes/scidac
Related URLs

✦ Personal homepage: papers, talks, etc.
   http://www.math.odu.edu/~keyes

✦ SciDAC initiative
   http://www.science.doe.gov/scidac

✦ TOPS project
   http://www.math.odu.edu/~keyes/scidac

✦ PETSc project
   http://www.mcs.anl.gov/petsc

✦ Hypre project
   http://www.llnl.gov/CASC/hypre

✦ ASCI platforms
   http://www.llnl.gov/asci/platforms

✦ Earth Simulator project
   http://www.es.jamstec.go.jp