DOE 2000 Numerics Capability

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Targets

- Large Scale (100,000,000 dof) simulations
  - computational fluid dynamics
  - combustion
  - structures
  - materials
  - usually PDE based
- Large scale (1000 cv) optimization
  - often involving simulation
  - maybe stochastic

Organization of Presentation

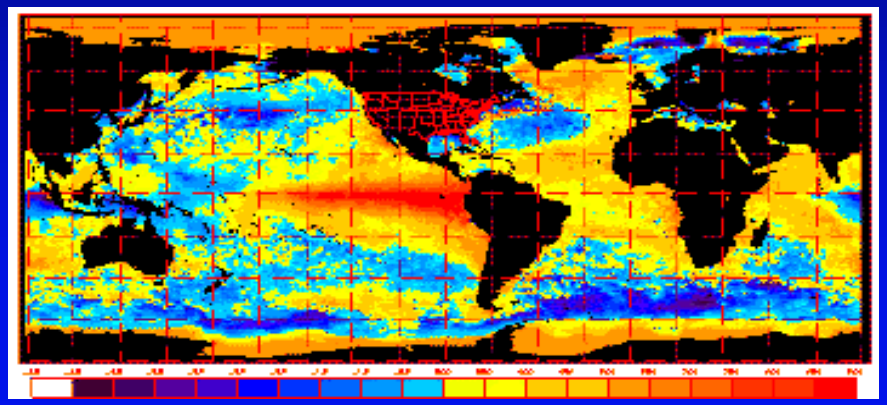
- Sample computations (to give an idea of scale)
- Background on computational infrastructure
- Summary of current toolkits
- Efforts on toolkit interoperability

Oil Reservoir Simulation Multiphase Flow

- Three-dimensional EOS model with 3 components (8 DOF per cell)
- Structured Cartesian grid
- Over 4 million cell blocks, 32 million DOF
- Fully implicit, time-dependent
- Over 10.6 gigaflops sustained performance on 128 nodes of an IBM SP
- Entire simulation runs in less then 30 minutes

Ocean Circulation Model

- Uses second-order finite differences with an explicit leapfrog time stepping scheme on a logically rectangular grid.

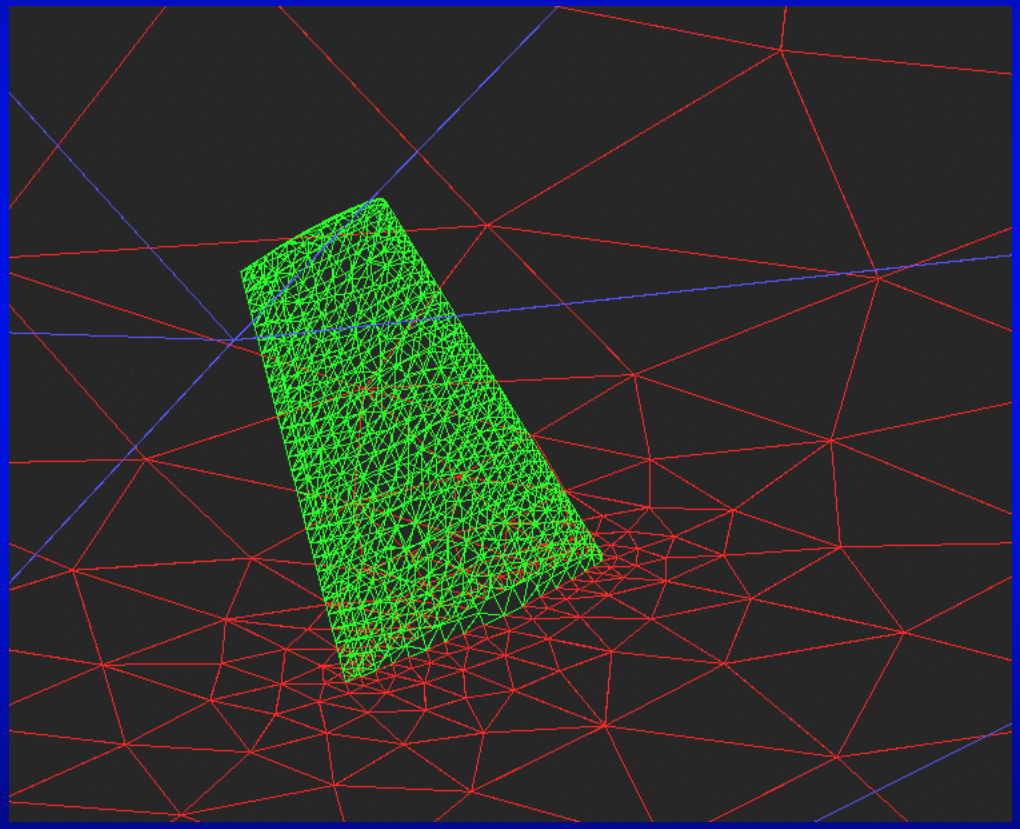


  - A. Wallcraft, H. Hurlburt, R. Rhodes, & J. Shriver, NRL - Stennis
- 540% speedup over the previous parallel software (64*145.6 Mflop/s) = 9.3 Gflop/s
- 2 hours is now 25 minutes

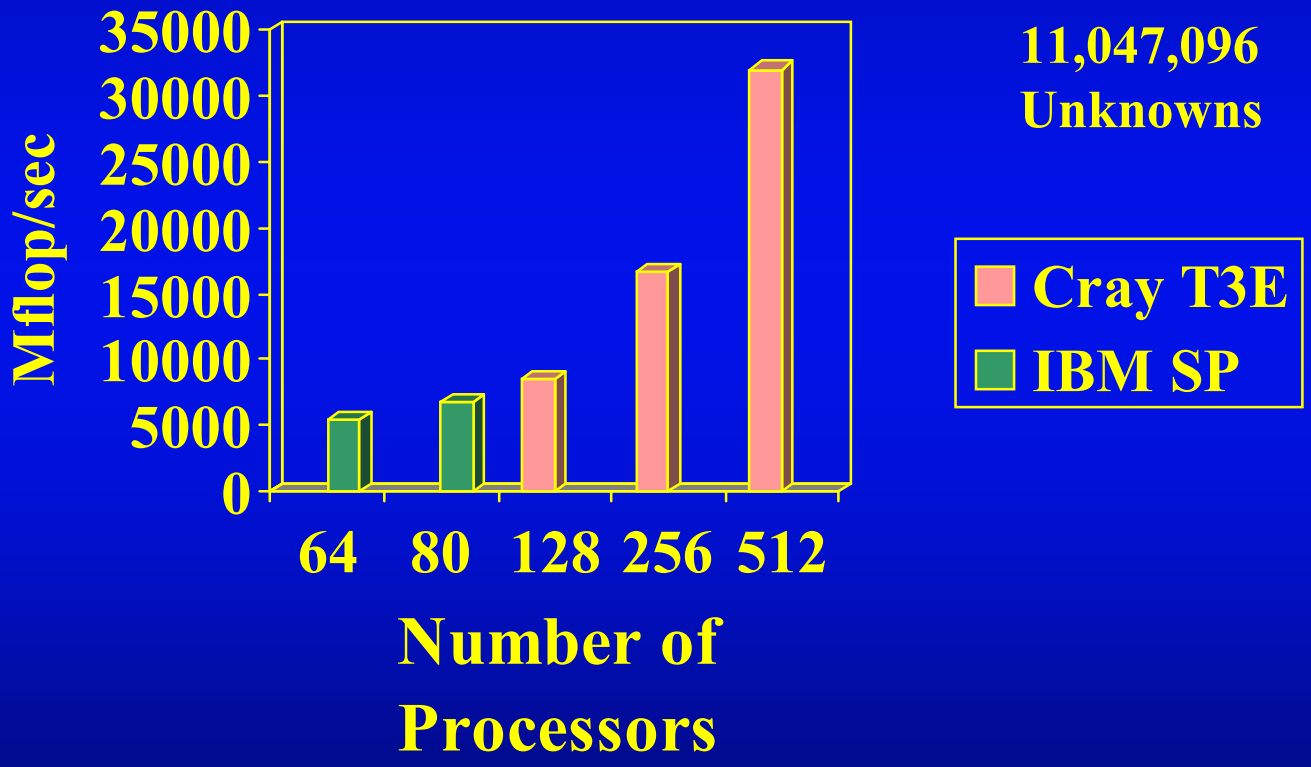
CFD on an Unstructured Grid

- Three-dimensional incompressible Euler
- Tetrahedral grid
- Up to 11.0 million degrees of freedom
- Based on a legacy NASA code
- Now runs several hundred times faster than legacy code

Unstructured Computational Grid



Floating-Point Performance



DOE Hardware Infrastruture

- IBM SP
  - Currently up to 512 nodes with 1-4 way SMP nodes
  - MPI machine
  - Processor peak ~ 640 MFlops
- SGI Origin
  - Currently up to 128 processors in a box
  - cc-NUMA - cache coherent - non-uniform memory access
  - Boxes connected via message passing (MPI)
  - Processor Peak ~ 500 MFlops
- Clusters (including ASCI Red, Linux, and DEC alphas)
  - 7000+ processors
  - MPI based

DOE Numerics Software Infrastruture

- MPI basic model for parallelism
- Toolkits (libraries)
  - in F77/F90, C, C++
  - sometimes object oriented or at least object based
  - hide much of the MPI details from application codes
  - attempt to support use from multiple languages
- Applications
  - F77/F90, C, C++
  - some use of scripting languages (Python)

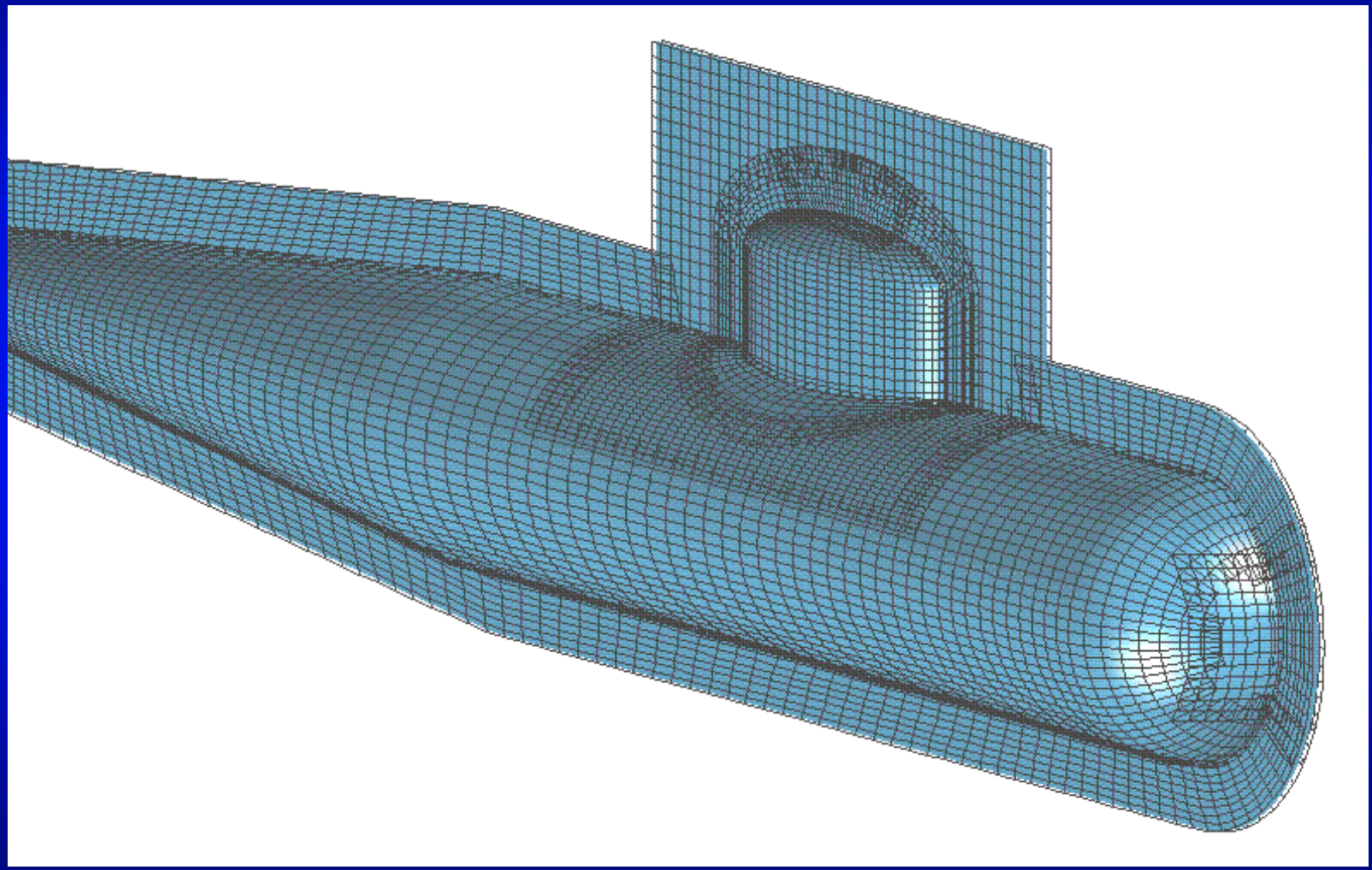
Toolkit Categories

- PDE/Grid management systems
- ODE integrators
- Nonlinear solvers
- Eigenvalue computations
- Linear solvers
- Nonlinear optimization

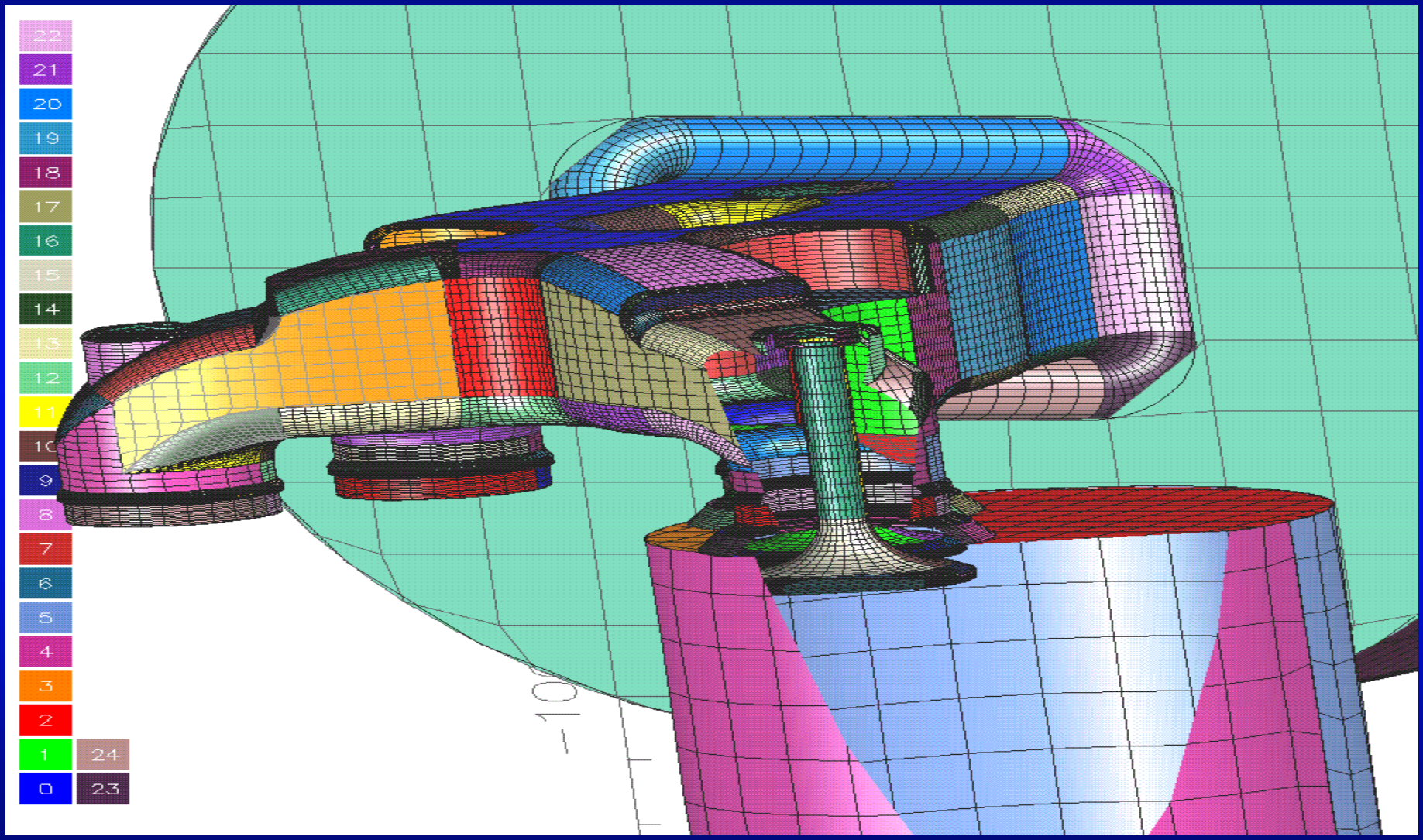
PDE/Grid management systems

- Overture
  - overlapping composite grids
  - complex geometry
- POOMA (Parallel Object-oriented Methods and Applications)
  - Data parallel style support for
    - finite difference
    - particle methods

Sample Overture Grid



Sample Overture Grid



ODE Integrators

- PVODE (Parallel variable order ODE integrators)
  - can use linear solvers from other ACTS toolkits
  - BDF (backward differentiation formula) multi-step methods for stiff problems
  - Adams multi-step method for non-stiff
  - also differential-algebraic systems

Nonlinear Solvers

- PETSc (Portable Extensible Toolkit for Scientific computation)
- Kinsol (part of PVODE, may also be used independently)

  - Newton-based solvers
  - Globalization strategies include
    - line search
    - trust region
    - pseudo-transient continuation (false time-stepping)
  - Will support several toolkits' linear solvers

Linear Solvers

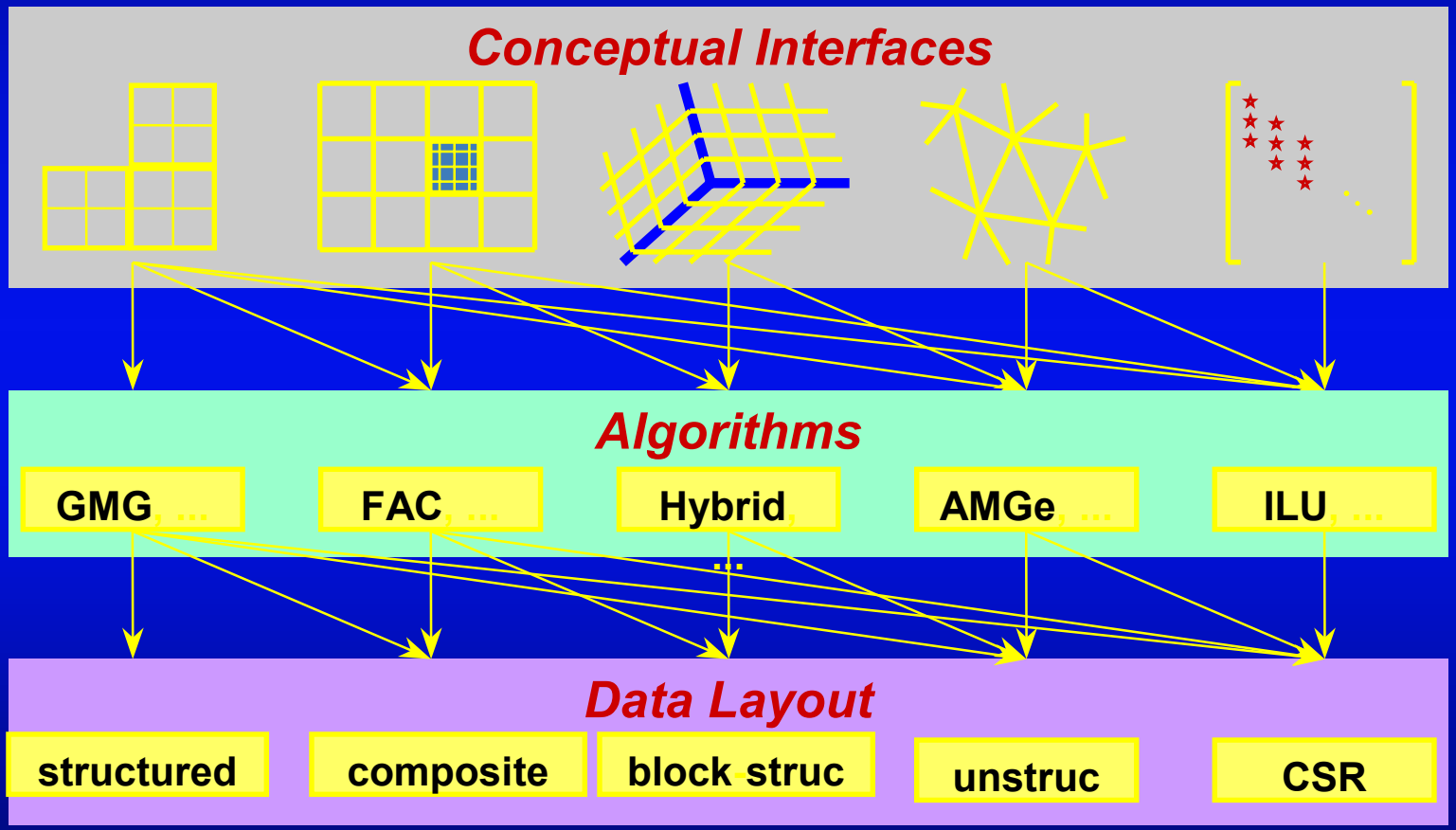
- Aztec
  - General purpose iterative solver
- Hypre
  - Family of application-centric (physics based) preconditioners
- PETSc
  - Extensible family of general purpose iterative solvers
- QMRPack
  - Full implementation of QMR
- ScaLAPACK
  - Direct solvers

Aztec

- General purpose parallel iterative solver
- Supports point and block storage of sparse matrices
- Includes 5 Krylov solvers
- Includes polynomial and overlapping additive Schwarz preconditioning
- Has scaled successfully to 1000s of processors (ASCI Red) on some applications

Hypre

- Family of application-centric (physics or grid based) preconditioners



PETSc

- Over 10 Krylov subspace methods including
  - GMRES, TFQMR, CG, Bi-CG-stab
- A suite of preconditioners including
  - additive overlapping Schwarz
  - access to parallel ILU(0) and ICC(0) via BlockSolve95
  - 5 matrix storage formats provided
- Many additional tools, such as vector scatter operations and mapping operations to simplify the coding of parallel PDE applications
- Modular and object oriented

QMRPack

- Implements several variants of the quasi-minimal residual (QMR) algorithm for the solution of general,non-Hermitian linear systems
- Only implementation that includes the full suite of look-ahead techniques
- Includes an eigensolver
- Now interfacing with other ACTS toolkits

ScaLAPACK

- SuperLU
  - Direct solution of large, sparse nonsymmetric systems of linear equations.
  - Runs on shared memory, MPI version expected soon
  - Attained 8.3 Gflops on a 52,000 unknown linear system arising from device simulation. 512 processors on a Cray T3E. 014% to 2.4% matrix density.
- MPI and PVM based direct dense solvers
  - Based on BLACS (basic linear algebra communication subroutines), BLAS and LAPACK
  - Well known, trusted community standard

Eigenvalue Computations

- ScaLAPACK
  - Dense matrix eigensolvers
  - Based on BLACS (basic linear algebra communication subroutines), BLAS and LAPACK
  - Well known, trusted community standard
  - Sustained 605 Gflops on ASCI Red in DOE materials simulations.

Nonlinear Optimization

- Opt++
  - Allows for rapid prototyping of new optimization methods
  - Abstract base classes for nonlinear optimization problem:
    - NLP0: no analytic derivatives
    - NLP1: analytic first derivatives (gradient)
    - NLP2: analytic first and second derivatives (gradient, Hessian)
  - Gradient methods for nonlinear least-squares problems
  - available in the NEWTON-LIKE optimization class:
    - finite-difference Newton
    - quasi-Newton
    - Gauss-Newton
  - Derived nonlinear problem classes:
    - FDNLF1: generate numerical-difference gradients
    - NLF2: first and second derivatives supplied

DOE "Standards" Collaborators

- CCA - Common Component Architecture group: arising out of DOE2000 activities to develop "standard" ways of managing numerical components so that ones developed by different groups may be mixed-and-matched

- ESI - Equation Solver Interface Forum: group arising out of the DOE labs to develop common interfaces for scalable linear solvers

DOE 2000 Numerics Capability

We provide a variety of powerful toolkits to assist in the development of scalable simulation codes

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