



A Look at More Complex Component-Based Applications

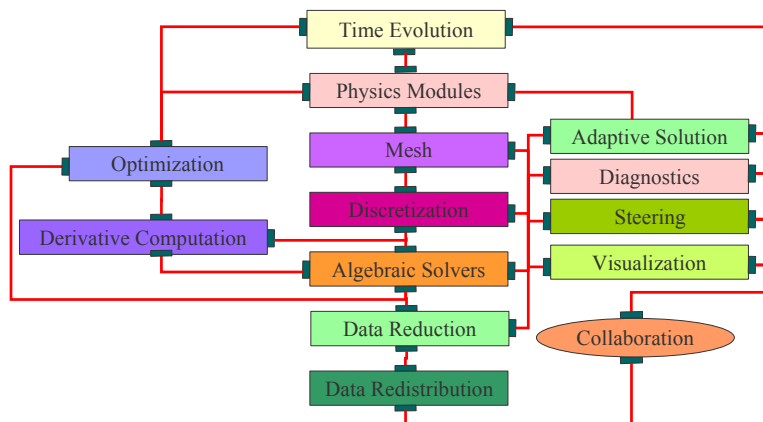
CCA Forum Tutorial Working Group

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Modern Scientific Software Development

- Terascale computing will enable high-fidelity calculations based on multiple coupled physical processes and multiple physical scales
 - Adaptive algorithms and high-order discretization strategies
 - Composite or hybrid solution strategies
 - Sophisticated numerical tools



Overview

- Using components in high performance simulation codes
 - Examples of increasing complexity
 - Performance
 - Single processor
 - Scalability
- Developing components for high performance simulation codes
 - Strategies for thinking about your own application
 - Developing interoperable and interchangeable components

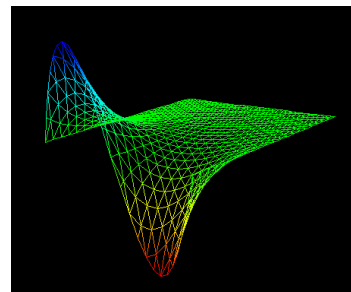
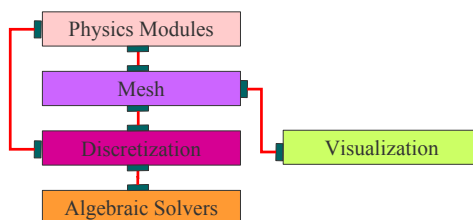
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Our Starting Point

$$\nabla^2 \varphi(x, y) = 0 \in [0, 1] \times [0, 1]$$

$$\varphi(0, y) = 0 \quad \varphi(1, y) = \sin(2\pi y)$$

$$\delta\varphi/\delta y(x, 0) = \delta\varphi/\delta y(x, 1) = 0$$



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Numerical Solution of Example 1

- Physics: Poisson's equation
- Grid: Unstructured triangular mesh
- Discretization: Finite element method
- Algebraic Solvers: PETSc (Portable Extensible Toolkit for Scientific Computation)
- Visualization: VTK tool
- Original Language: C

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Creating Components: Step 1

- Separate the application code into well-defined pieces that encapsulate functionalities
 - Decouple code along numerical functionality
 - Mesh, discretization, solver, visualization
 - Physics is kept separate
 - Determine what questions each component can ask of and answer for other components (this determines the ports)
 - Mesh provides geometry and topology (needed by discretization and visualization)
 - Mesh allows user defined data to be attached to its entities (needed by physics and discretization)
 - Mesh *does not* provide access to its data structures
 - If this is not part of the original code design, this is by far the hardest, most time-consuming aspect of componentization

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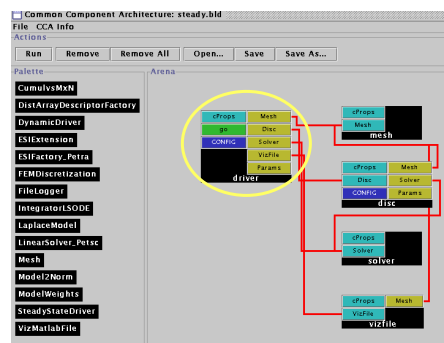
Creating the Components: Step 2

- Writing C++ Components
 - Create an abstract base class for each port
 - Create C++ objects that inherit from the abstract base port class and the CCA component class
 - Wrap the existing code as a C++ object
 - Implement the setServices method
- This process was significantly less time consuming (with an expert present) than the decoupling process
 - Lessons learned
 - Definitely look at an existing, working example for the targeted framework
 - Experts are very handy people to have around ;-)

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The Componentized Example

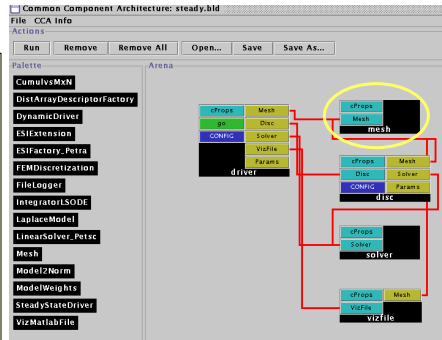
- The Driver Component
 - Responsible for the overall application flow
 - Initializes the mesh, discretization, solver and visualization components
 - Sets the physics parameters and boundary condition information



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The Componentized Example

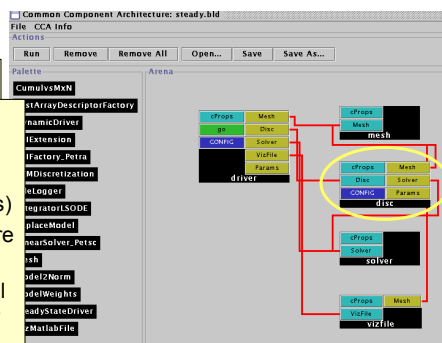
- The Driver Component
 - The Mesh Component
 - Provides geometry, topology, and boundary information
 - Provides the ability to attach user defined data as tags to mesh entities
 - Is used by the driver, discretization and visualization components



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The Componentized Example

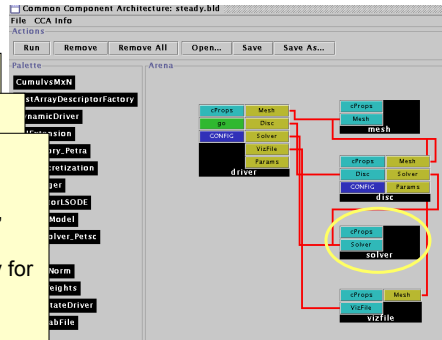
- The Driver Component
 - The Mesh Component
 - The Discretization Component
 - Provides a finite element discretization of basic operators (gradient, Laplacian, scalar terms)
 - Driver determines which terms are included and their coefficients
 - Provides mechanisms for general Dirichlet and Neumann boundary condition matrix manipulations
 - Computes element matrices and assembles them into the global stiffness matrix via set methods on the solver
 - Gathers and scatters vectors to the mesh (in this case ϕ)



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The Componentized Example

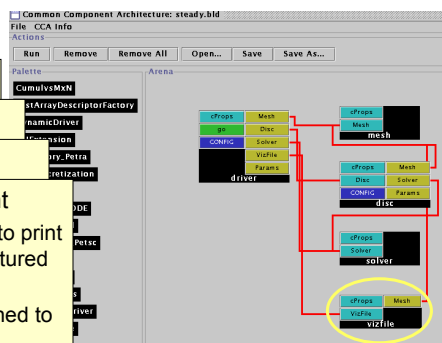
- The Driver Component
- The Mesh Component
- The Discretization Component
- The Solver Component
 - Provides access to vector and matrix operations (e.g., create, destroy, get, set)
 - Provides a "solve" functionality for a linear operator



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The Componentized Example

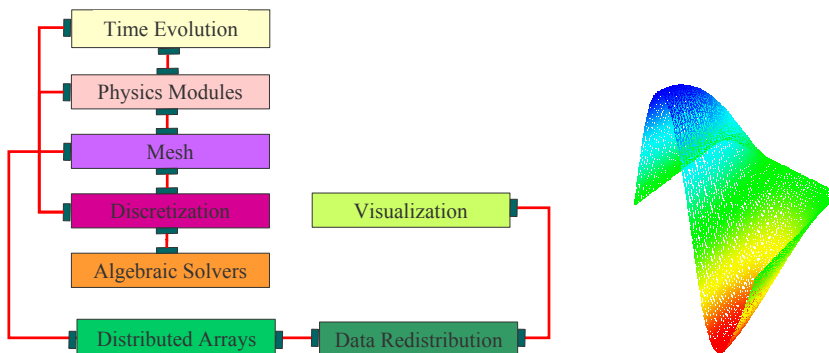
- The Driver Component
- The Mesh Component
- The Discretization Component
- The Solver Component
- The Visualization Component
 - Uses the mesh component to print a vtk file of ϕ on the unstructured triangular mesh
 - Assumes user data is attached to mesh vertex entities



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The next step... time dependence

$$\begin{aligned}\delta\phi/\delta t &= \nabla^2\phi \quad (x,y,t) \in [0,1] \times [0,1] \\ \phi(0,y,t) &= 0 \quad \phi(1,y,t) = .5\sin(2\pi y)\cos(t/2) \\ \delta\phi/\delta y(x,0) &= \delta\phi/\delta y(x,1) = 0 \\ \phi(x,y,0) &= \sin(.5\pi x) \sin(2\pi y)\end{aligned}$$



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Some things change...

- Requires a time integration component
 - Based on the LSODE library (LLNL)
 - Component implementation developed by Ben Allan (SNL)
- Uses a new visualization component
 - Based on AVS
 - Requires an MxN data redistribution component
 - Developed by Jim Kohl (ORNL)
- The MxN redistribution component requires a Distributed Array Descriptor component
 - Similar to HPF arrays
 - Developed by David Bernholdt (ORNL)
- The driver component changes to accommodate the new physics

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- The mesh component doesn't change
- The discretization component doesn't change
- The solver component doesn't change
 - What we use from the solver component changes
 - Only vectors are needed

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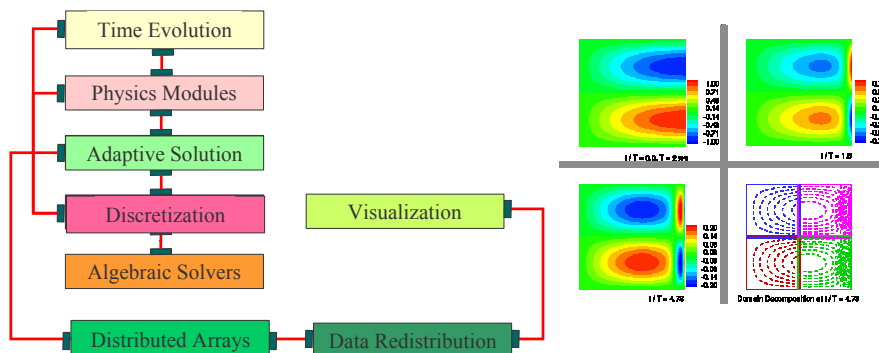
What did this exercise teach us?

- It was easy to incorporate the functionalities of components developed at other labs and institutions given a well-defined interface and header file.
 - In fact, some components (one uses and one provides) were developed simultaneously across the country from each other after the definition of a header file.
 - Amazingly enough, they usually “just worked” when linked together (and debugged individually).
- In this case, the complexity of the component-based approach was higher than the original code complexity.
 - Partially due to the simplicity of this example
 - Partially due to the limitations of the some of the current implementations of components

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One more layer of complexity... AMR

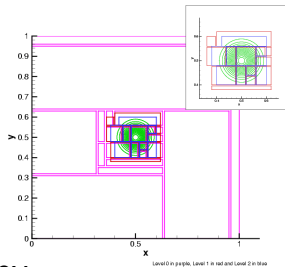
The same physics but use a block structured adaptive mesh



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Adaptive Mesh Refinement

- Used to accurately capture a wide spectrum of length scales
- Many different techniques
 - We use structured axis-aligned patches
 - Provided by the GrACE library
- Start with a uniform coarse mesh
 - Identify regions needing refinement
 - Collate into rectangular patches
 - Impose finer mesh in patches
 - Recurse and obtain a mesh hierarchy



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Some things change...

- The mesh component changes
 - Block structured AMR based on GRACE
- The discretization component changes
 - Finite difference on patches
 - BC handled differently
- The driver component changes

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- The integration component stays the same
- The solver component stays the same
- The data redistribution component stays the same
- The distributed array component stays the same
- The visualization component stays the same

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[illegible]

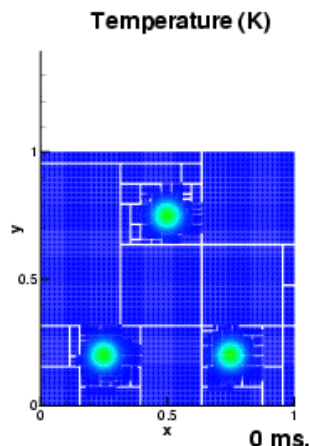
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Beyond the heat equation...

- Flame Approximation
 - H₂-Air mixture; ignition via 3 hot-spots
 - 9-species, 19 reactions, stiff chemistry
- Governing equation

$$\frac{\partial Y_i}{\partial t} = \nabla \cdot \alpha \nabla Y_i + \dot{w}_i$$

- Domain
 - 1cm X 1cm domain
 - 100x100 coarse mesh
 - finest mesh = 12.5 micron.
- Timescales
 - O(10ns) to O(10 microseconds)



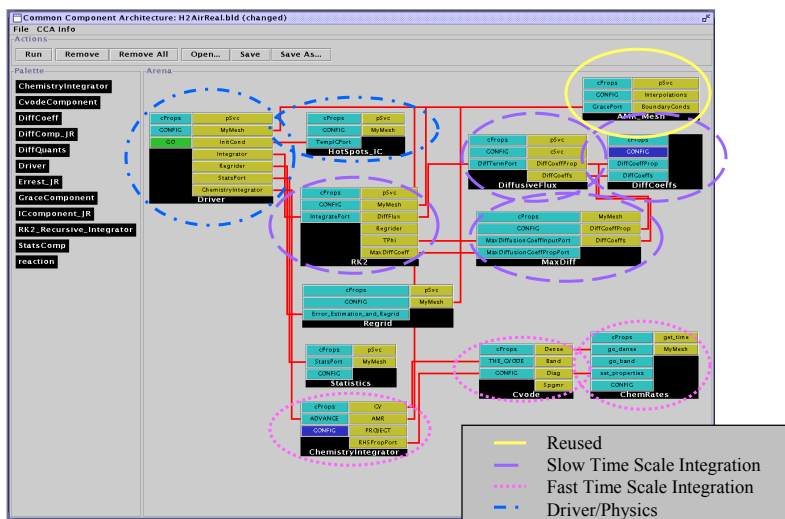
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Numerical Solution

- Adaptive Mesh Refinement: GrACE
- Stiff integrator: CVODE (LLNL)
- Diffusive integrator: 2nd Order Runge Kutta
- Chemical Rates: legacy f77 code (SNL)
- Diffusion Coefficients: legacy f77 code (SNL)
- New code less than 10%

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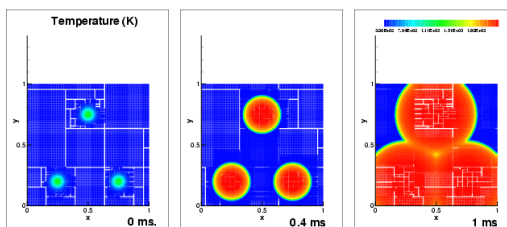
The CCA Wiring Diagram



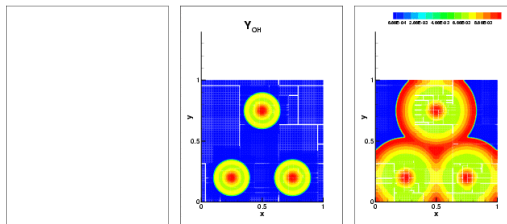
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Evolution of the Solution

Temperature



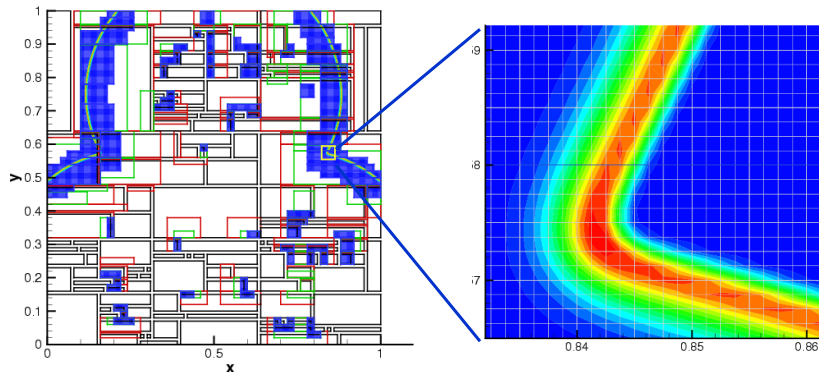
OH Profile



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The need for AMR

- H_2O_2 chemical subspecies profile
 - Only 100 microns thick (about 10 fine level cells)
 - Not resolvable on coarsest mesh

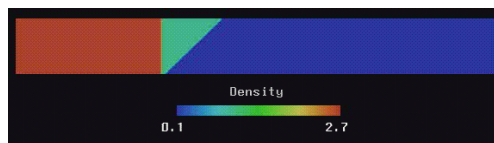


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Shock-Hydrodynamics

- Governing equation

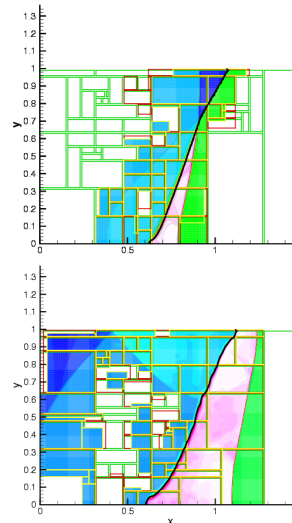
$$U_t = F_x(U) + G_y(U) \quad U = \{\rho, \rho u, \rho v, \rho E, \rho \zeta\}$$
- Domain
 - Square cross section shock-tube
- Experiment
 - Two gases are separated by a clean interface
 - Shock moves from left to right and interacts with the interface
 - Deposits vorticity
 - Reflects
 - Refracts



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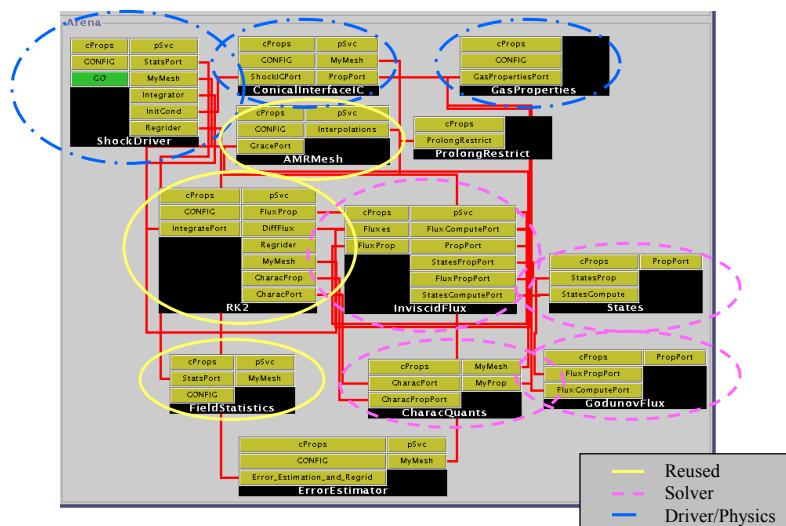
Interesting features

- Shock & interface are sharp discontinuities which need refinement
- Shock deposits vorticity – a governing quantity for turbulence, mixing, ...
- If there is insufficient refinement
 - under predict vorticity
 - slower mixing/turbulence.



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The CCA Wiring Diagram

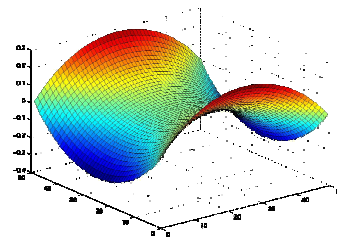


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Unconstrained Minimization Problem

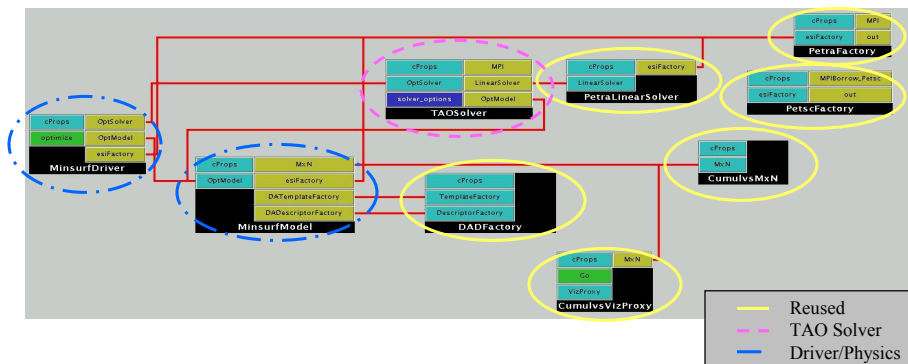
- Given a rectangular 2-dimensional domain and boundary values along the edges of the domain
- Find the surface with minimal area that satisfies the boundary conditions, i.e., compute

$$\min f(x), \text{ where } f: \mathbb{R}^n \rightarrow \mathbb{R}$$
- Solve using optimization components based on TAO (ANL)



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Unconstrained Minimization Using a Structured Mesh

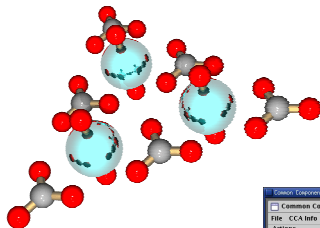


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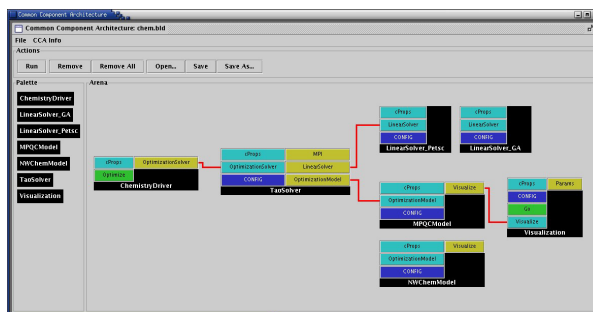
Molecular Geometry Optimization

Wiring diagram using Ccaffeine framework and:

- Electronic structure components based on NWChem (PNNL) and MPQC (SNL)
- Optimization components based on TAO (ANL)
- Linear algebra components based on Global Arrays (PNNL) and PETSc (ANL)

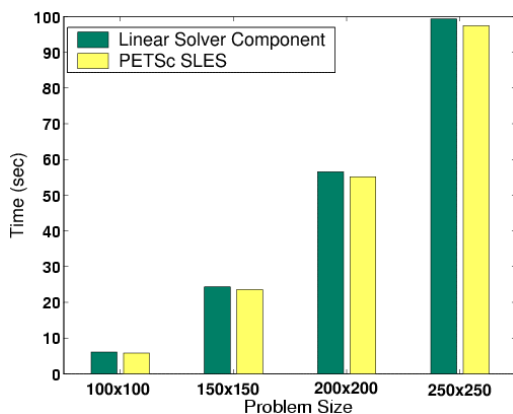


Relativistic quantum chemistry calculation of $(\text{UO}_2)_3(\text{CO}_3)_6$ using NWChem. Image courtesy of Wibe deJong, PNNL.



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Component Overhead



Aggregate time for linear solver component in unconstrained minimization problem.

- Negligible overhead for component implementation and abstract interfaces when using appropriate levels of abstraction
- Linear solver component currently supports any methods available via the ESI interfaces to PETSc and Trilinos; plan to support additional interfaces the future, e.g., those under development within the TOPS center
- Here: Use the conjugate gradient method with no-fill incomplete factorization preconditioning

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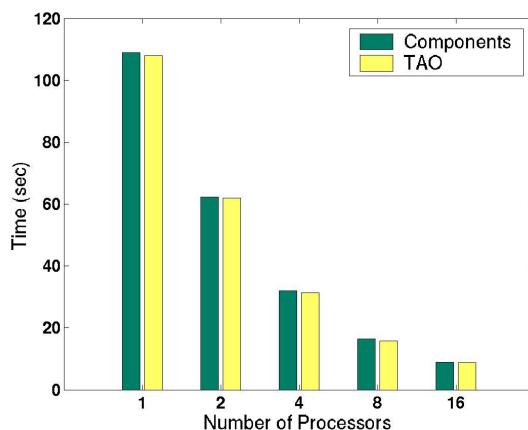
Overhead from Component Invocation

- Invoke a component with different arguments
 - Array
 - Complex
 - Double Complex
- Compare with f77 method invocation
- Environment
 - 500 MHz Pentium III
 - Linux 2.4.18
 - GCC 2.95.4-15
- Components took 3X longer
- Ensure granularity is appropriate!
- Paper by Bernholdt, Elwasif, Kohl and Epperly

Function arg type	f77	Component
Array	80 ns	224ns
Complex	75ns	209ns
Double complex	86ns	241ns

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Scalability on a Linux Cluster



Total execution time for the minimum surface minimization problem using a fixed-sized 250x250 mesh.

- Newton method with line search
- Solve linear systems with the conjugate gradient method and block Jacobi preconditioning (with no-fill incomplete factorization as each block's solver, and 1 block per process)
- Negligible component overhead; good scalability

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List of Component Re-Use

- Various services in Ccaffeine
- Integrator
 - *IntegratorLSODE* (2)
 - *RK2* (2)
- Linear solvers
 - *LinearSolver_Petra* (4)
 - *LinearSolver_PETSc* (4)
- AMR
 - *AMRmesh* (3)
- Data description
 - *DADFactory* (3)
- Data redistribution
 - *CumulvsMxN* (3)
- Visualization
 - *CumulvsVizProxy* (3)

Component interfaces
to numerical libraries

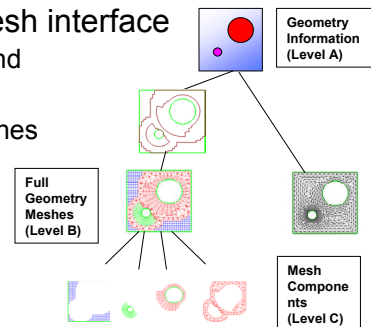
Component interfaces
to parallel data
management and
visualization tools

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The Next Level



- Common Interface Specification
 - Provides plug-and-play interchangeability
 - Requires domain specific experts
 - Typically a difficult, time-consuming task
 - A success story: MPI
- A case study... the TSTT/CCA mesh interface
 - TSTT = Terascale Simulation Tools and Technologies (www.tstt-scidac.org)
 - A DOE SciDAC ISIC focusing on meshes and discretization
 - Goal is to enable
 - hybrid solution strategies
 - high order discretization
 - Adaptive techniques

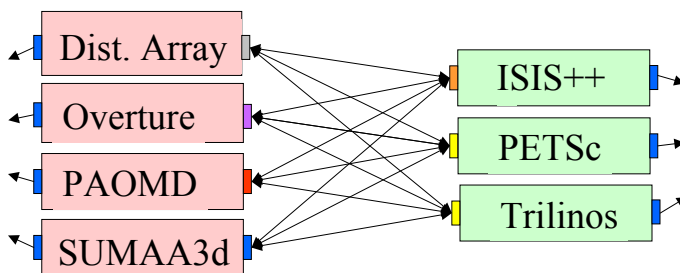


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Current Situation

Current Situation

- Public interfaces for numerical libraries are unique
- *Many-to-Many* couplings require *Many²* interfaces
 - Often a heroic effort to understand the inner workings of both codes
 - Not a scalable solution

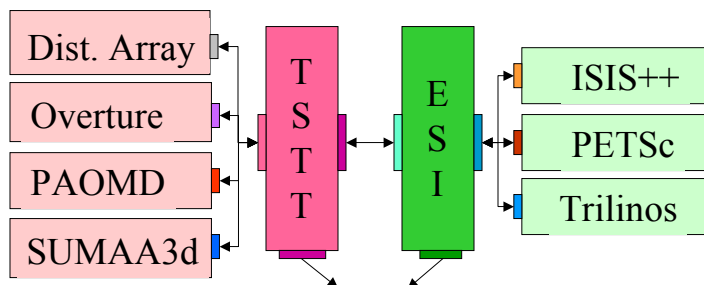


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Common Interface Specification

Reduces the *Many-to-Many* problem to a *Many-to-One* problem

- Allows interchangeability and experimentation
- Challenges
 - Interface agreement
 - Functionality limitations
 - Maintaining performance



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TSTT Philosophy

- Create a small set of interfaces that existing packages can support
 - AOMD, CUBIT, Overture, GrACE, ...
 - Enable both interchangeability and interoperability
- Balance performance and flexibility
- Work with a large tool provider and application community to ensure applicability
 - Tool providers: TSTT and CCA SciDAC centers
 - Application community: SciDAC and other DOE applications

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Basic Interface

- Enumerated types
 - Entity Type: VERTEX, EDGE, FACE, REGION
 - Entity Topology: POINT, LINE, POLYGON, TRIANGLE, QUADRILATERAL, POLYHEDRON, TETRAHEDRON, HEXAHEDRON, PRISM, PYRAMID, SEPTAHEDRON
- Opaque Types
 - Mesh, Entity, Workset, Tag
- Required interfaces
 - Entity queries (geometry, adjacencies), Entity iterators, Array-based query, Workset iterators, Mesh/Entity Tags, Mesh Services

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Issues that have arisen

- Nomenclature is harder than we first thought
- Cannot achieve the 100 percent solution, so...
 - What level of functionality should be supported?
 - Minimal interfaces only?
 - Interfaces for convenience and performance?
 - What about support of existing packages?
 - Are there atomic operations that all support?
 - What additional functionalities from existing packages should be required?
 - What about additional functionalities such as locking?
- Language interoperability is a problem
 - Most TSTT tools are in C++, most target applications are in Fortran
 - How can we avoid the “least common denominator” solution?
 - Exploring the SIDL/Babel language interoperability tool

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Summary

- Complex applications that use components are possible
 - Shock hydrodynamics
 - Chemistry applications
 - Optimization problems
- Component reuse is significant
 - Adaptive Meshes
 - Linear Solvers (PETSc, Trilinos)
 - Distributed Arrays and MxN Redistribution
 - Time Integrators
 - Visualization
- Examples shown here leverage and extend parallel software and interfaces developed at different institutions
 - Including CUMULVS, ESI, GrACE, LODE, MPICH, PAWS, PETSc, PVM, TAO, Trilinos, TSTT.
- Performance is not significantly affected by component use
- Definition of domain-specific common interfaces is key

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Componentizing your own application

- The key step: think about the decomposition strategy
 - By physics module?
 - Along numerical solver functionality?
 - Are there tools that already exist for certain pieces? (solvers, integrators, meshes?)
 - Are there common interfaces that already exist for certain pieces?
 - Be mindful of the level of granularity
- Decouple the application into pieces
 - Can be a painful, time-consuming process
- Incorporate CCA-compliance
- Compose your new component application
- Enjoy!

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Next: Status and Plans

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