CCA
Common Component Architecture

A Look at More Complex Component-Based Applications

CCA Forum Tutorial Working Group
http://www.cca-forum.org/tutorials/
tutorial-wg@cca-forum.org

CCA
Common Component Architecture

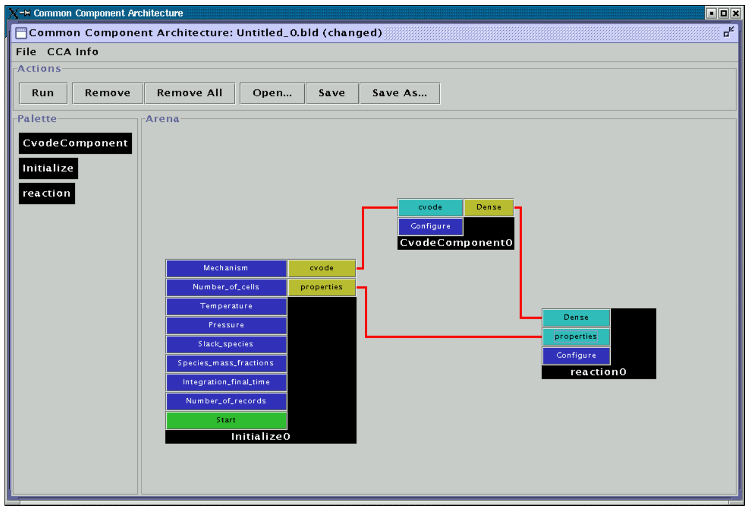
Compaq

Component model for high performance computing

- Components
  - C++ objects with a functionality
  - Ports : Provides and uses
  - Compiled into shared libraries
- Framework
  - Loads and instantiates components
  - Connects uses and provides ports
  - Driven by a script or GUI

2

A CCA code



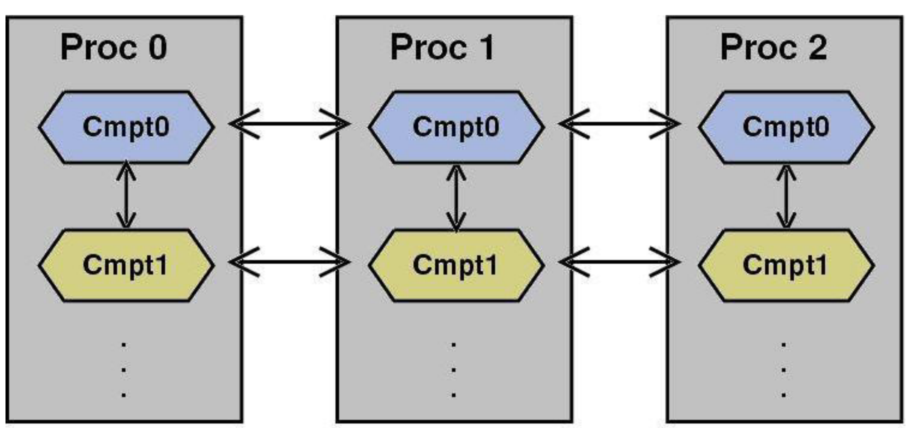
CCA model for high performance computing

- Requirements
  - High single cpu performance
  - Need parallelism, NOT distributed computing
  - SPMD quite sufficient, RMI not needed.
  - No parallel computing prescription/model
    - No one-size-fits-all
- Translates to :
  - Light-weight framework
  - Onus on the component writer.

Component model for high performance computing

- Solution :
  - Identical frameworks with identical components and connection on P processors.
  - Comp. A on proc Q can call methods on Comp. B also on proc Q.
  - Comp. A s of all P procs communicate via MPI.
  - No RMI – Comp. A on proc Q DOES NOT interact with Comp. B on proc N.
  - No parallel comp. Model – the component does what's right.
  - 2 such frameworks – Sandia, Utah.

Pictorial example



Summary

- A lightweight component model for high performance computing.
- A restriction on parallel communication
  - Comm. Only between a cohort of components.
- No RMI – no dist. computing.
- Components with a physics / chemistry / numerical algo functionalities.
- Standardized interfaces – Ports.
- That's the theory – does it work ?

Problem categories

- Decomposition of simulation codes
  - How ? Along physics ? Numerics ?
  - Math model provides a hint ?
  - What granularity ?
  - Interfaces
- Libraries
  - Interfaces
- Nested containers
  - I.e. framework enhancements ?

Decomposition of simulation codes

- 2 different physics simulations
- Component reuse
- Parallel, scalable, good single CPU performance
- A formalism for decomposing a big code into
  - Subsystem
  - Components.
  - Common underlying mathematical structure
- Dirty secrets / restrictions / flexibility.

Guidelines regarding apps

- Hydrodynamics
- P.D.E

$$\Phi_t = F(\Phi, \nabla\Phi, \nabla^2\Phi, \ldots) + G(\Phi)$$

- Spatial derivatives
  - Finite differences, finite volumes
- Timescales
- Length scales

Solution strategy

- Timescales
  - Explicit integration of slow ones
  - Implicit integration of fast ones
- Strang-splitting

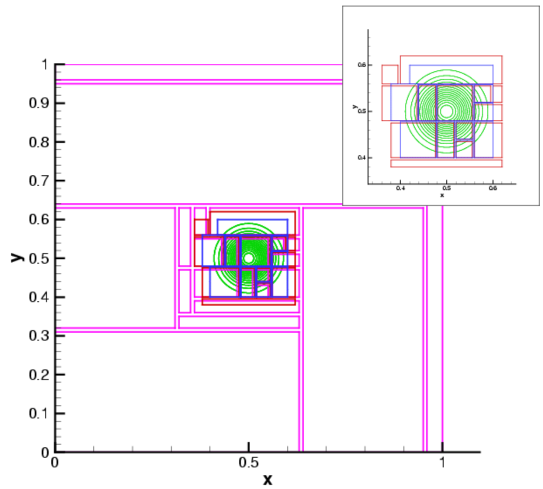
$$\Phi_t = F(\Phi, \nabla\Phi, \nabla^2\Phi \ldots.) + G(\Phi)$$

$$\begin{array}{llll}
1. & \Phi_t = G(\Phi), & t^n \to t^n + \Delta t/2 & \{\Phi^n, \tilde{\Phi}\} \\
2. & \Phi_t = F(\Phi, \nabla\Phi, \nabla^2\Phi \ldots.), & t^n \to t^n + \Delta t, & \{\tilde{\Phi}, \hat{\Phi}\} \\
3. & \Phi_t = G(\Phi), & t^n + \Delta t/2 \to t^n + \Delta t, & \{\hat{\Phi}, \Phi^{n+1}\}
\end{array}$$

Solution strategy (cont'd)

- Wide spectrum of length scales
  - Adaptive mesh refinement
  - Structured axis-aligned patches
  - GrACE.
- Start with a uniform coarse mesh
  - Identify regions needing refinement, collate into rectangular patches
  - Impose finer mesh in patches
  - Recurse; mesh hierarchy.

A mesh hierarchy



Level 0 in purple, Level 1 in red and Level 2 in blue

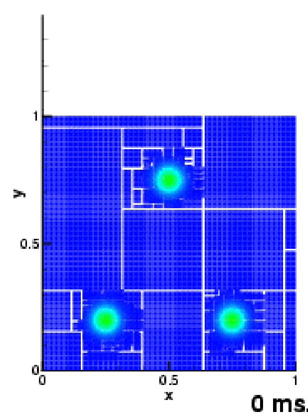
App 1. A reaction-diffusion system.

- A coarse approx. to a flame.
- H_2-Air mixture; ignition via 3 hot-spots
- 9-species, 19 reactions, stiff chemistry

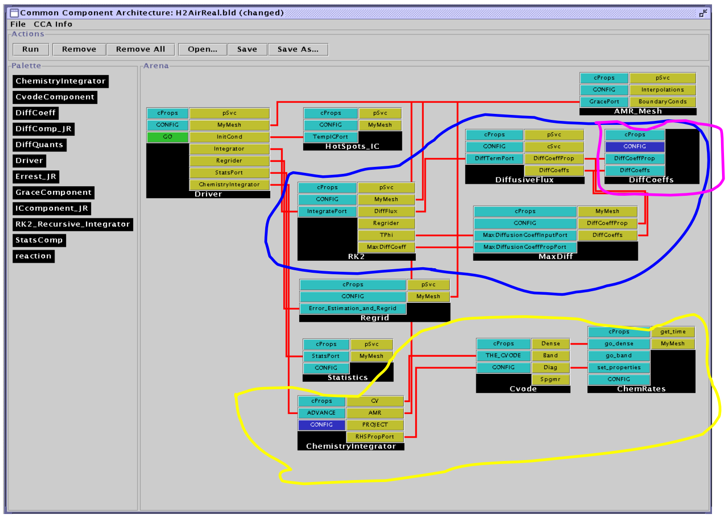
$$\frac{\partial Y_i}{\partial t} = \nabla.\alpha\nabla Y_i + \dot{w}_i$$

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

Temperature (K)



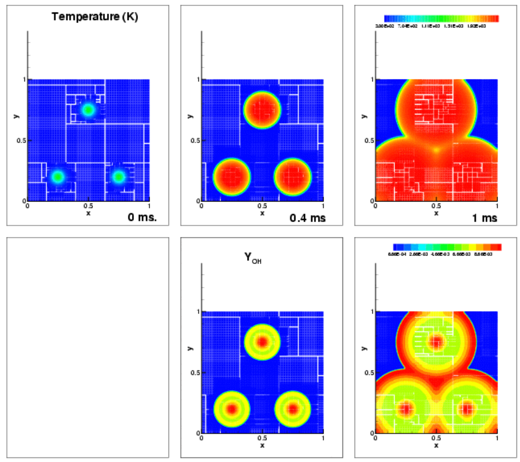
App. 1 - the code



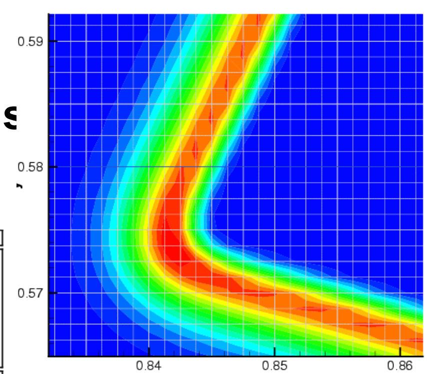
So, how much is new code ?

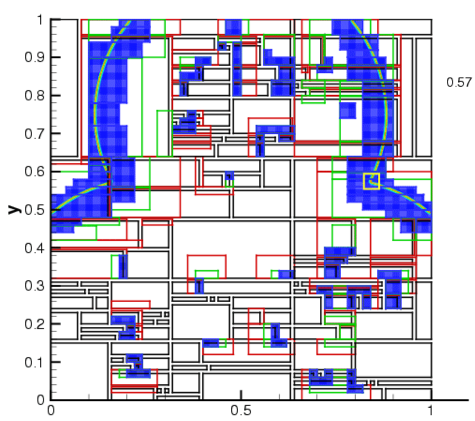
- The mesh – GrACE
- Stiff-integrator – CVODE, LLNL
- ChemicalRates – old Sandia F77 subroutines
- Diff. Coeffs – based on DRFM – old Sandia F77 library
- The rest
  - We coded – me and the gang.

Evolution



Details





- H_2O_2 mass fraction profiles.

CCA
Common Component Architecture

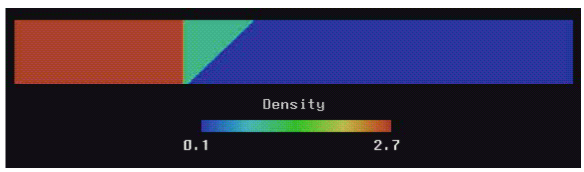
Compaq

App. 2 shock-hydrodynamics

- Shock hydrodynamics

$$U_t = F_x(U) + G_y(U) \quad U = \{\rho, \rho u, \rho v, \rho E, \rho\zeta\}$$

- Finite volume method (Godunov)



19

CCA
Common Component Architecture

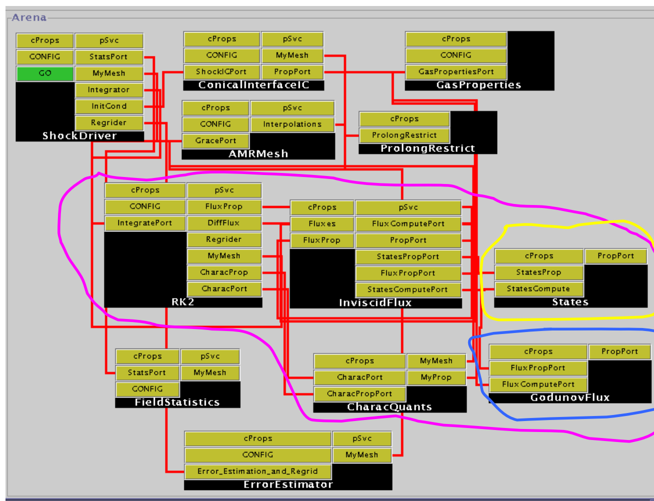
Compaq

Interesting features

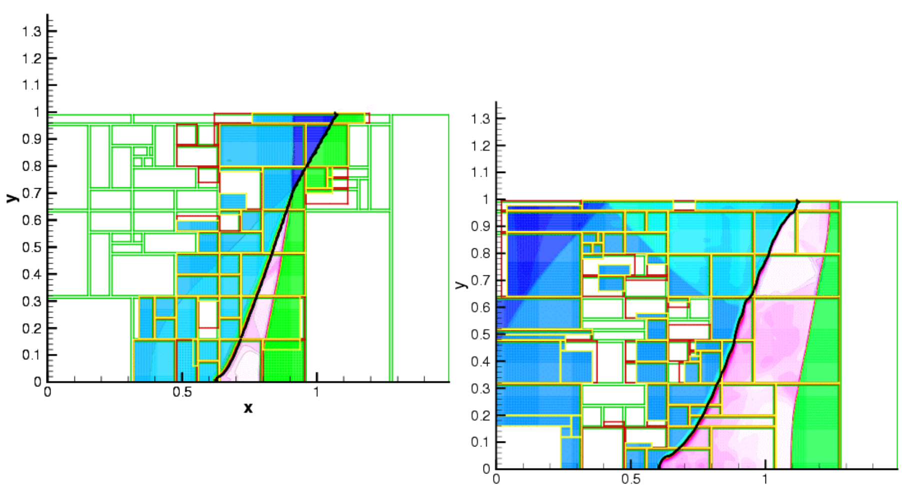
- Shock & interface are sharp discontinuities
- Need refinement
- Shock deposits vorticity – a governing quantity for turbulence, mixing, …
- Insufficient refinement – under predict vorticity, slower mixing/turbulence.

20

App 2. The code



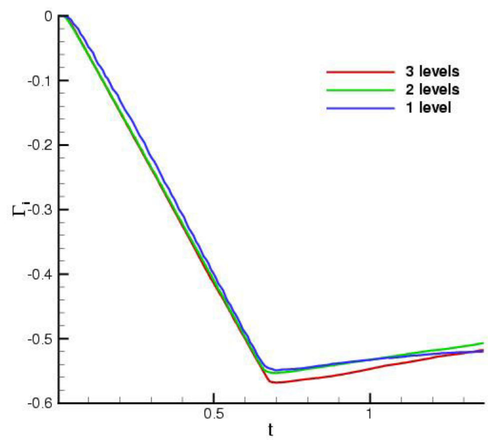
Evolution



CCA
Common Component Architecture

Compaq

Convergence



23

CCA
Common Component Architecture

Compaq

Are components slow ?

- C++ compilers << Fortran compilers
- Virtual pointer lookup overhead when accessing a derived class via a pointer to base class
- $Y' = F$; $[I - \Delta t/2\ J]\ \Delta Y = H(Y^n) + G(Y_m)$; used Cvode to solve this system
- J & G evaluation requires a call to a component (Chemistry mockup)
- Δt changed to make convergence harder – more J & G evaluation
- Results compared to plain C and cvode library

24

Components versus library

Δt	G evaluations	Component time (sec)	Library time (sec)
0.1	66	1.18	1.23
1.0	150	2.34	2.38
100	405	6.27	6.14
1000	501	7.66	7.67

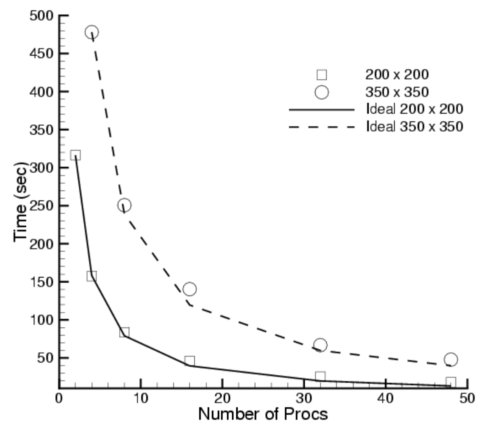
Really so ?

- Difference in *calling* overhead
- Test :
  - F77 versus componens
    - 500 MHz Pentium III
    - Linux 2.4.18
    - Gcc 2.95.4-15

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

Scalability

- Shock-hydro code
- No refinement
- 200 x 200 & 350 x 350 meshes
- Cplant cluster
  - 400 MHz EV5 Alphas
  - 1 Gb/s Myrinet
- Worst perf : 73 % scaling eff. For 200x200 on 48 procs



Summary

- Components, code
- Very different physics/numerics by replacing physics components
- Single cpu performance not harmed by componentization
- Scalability – no effect
- Flexible, parallel, etc. etc. …
- Success story …?
  - Not so fast …

Pros and cons

- Cons :
  - A set of components solve a PDE subject to a *particular* numerical scheme
  - Numerics decides the main subsystems of the component assembly
    - Variation on the main theme is easy
    - Too large a change and you have to recreate a big percentage of components
- Pros :
  - Physics components appear at the bottom of the hierarchy
  - Changing physics models is easy.
  - Note : Adding new physics, if requiring a brand-new numerical algorithm is NOT trivial.
- So what's a better design to accommodate this ?

What else is up ?

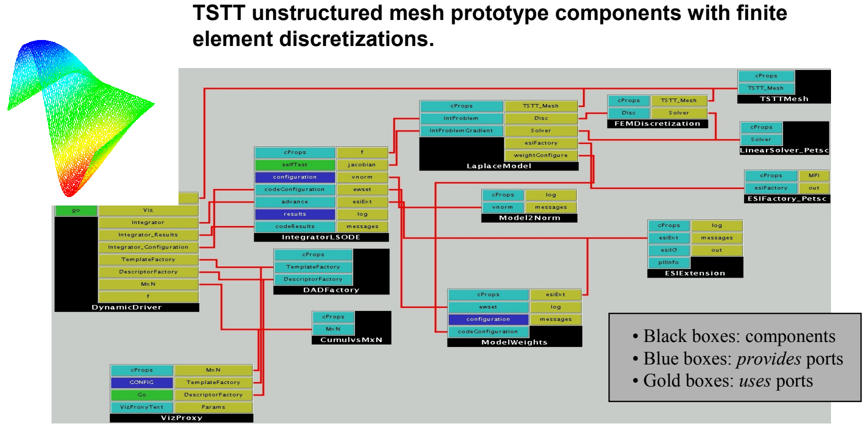
- "libraries" !
  - But as components, standard interfaces
    - "Linear solver component" (interface!)
      - PetSc, Trilinos etc, etc
- Meshes :
  - Standard interfaces for discretizing domains (unstructured meshes)
  - Math operators on such meshes
  - Data objects to hold fields on such meshes
- Strange things …
  - Data de- and re-composition, visualization …

Libraries ….

- Linear algebra
  – PETSc, Trilinos, etc → components
- Optimization
  – TAO
- ODE & DAE Integrators
  – LSODE, Cvode
- Profiling & optimization (cache artists ?!?)
  – TAU
- Data redist + Viz
  – CUMULVS, using AVS, no less !

Time-Dependent PDE on an Unstructured Mesh

TSTT unstructured mesh prototype components with finite element discretizations.



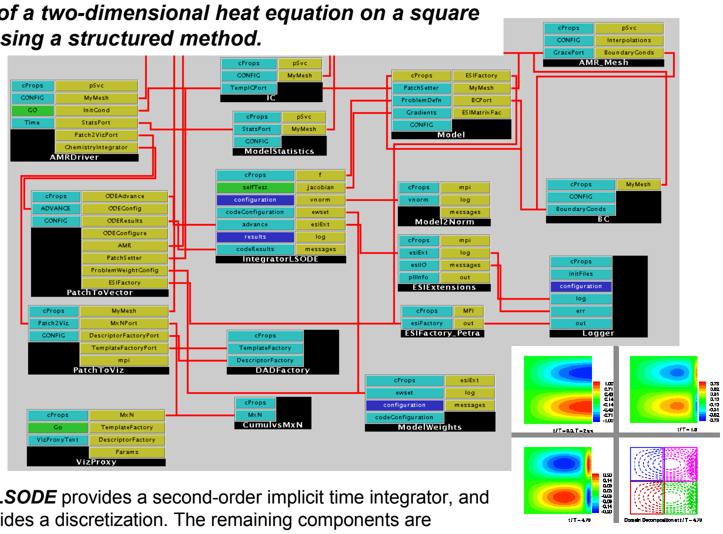
IntegratorLSODE provides a second-order implicit time integrator, and ***FEMDiscretization*** provides a discretization.

This application uses the ***DADFactory*** component to describe the parallel data layout so that the ***CumulsMxN*** data redistribution component can then collate the data from a multi-processor run to a single processor for runtime visualization.

Compaq

Heat Equation on an Adaptive Structured Mesh

Solution of a two-dimensional heat equation on a square domain using a structured method.



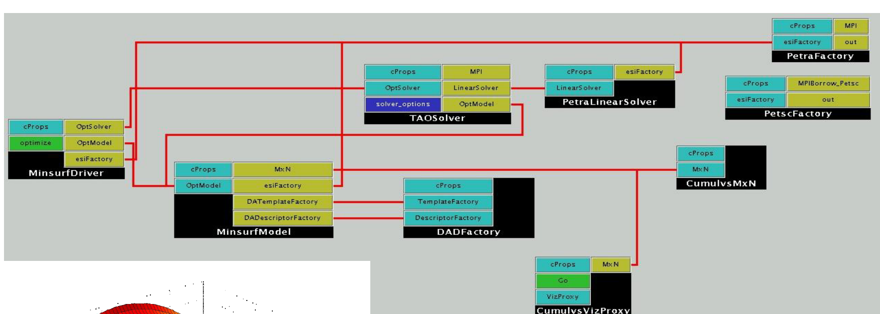
IntegratorLSODE provides a second-order implicit time integrator, and ***Model*** provides a discretization. The remaining components are essentially utilities that construct the global ODE system or adaptors that convert the patch-based data structures of the mesh to the globally distributed array structure used for runtime visualization.

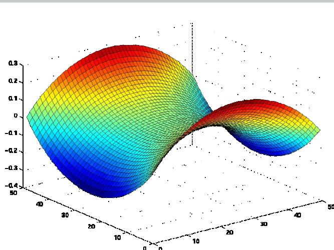
33

Compaq

Unconstrained Minimization Using a Structured Mesh

Determine minimal surface area given boundary conditions using the TAOSolver optimization component. I.e., solve ***min f(x), where $f: R^n \rightarrow R$.***





TAOSolver uses linear solver components that incorporate abstract interfaces under development by the DOE-wide Equation Solver Interface (ESI) working group. Underlying implementations are provided via the new ESI interfaces to parallel linear solvers within the PETSc (ANL) and Trilinos (SNL) libraries.

34

Conclusions

- Progress ..
  - Libraries <-> components : well ahead
  - Decomposing applications
    - Slower, but harder job
  - Language interoperability
    - Framework done
    - Adoption by people on
- Knotty points
  - Interfaces and scientists …