


Welcome to the Common Component Architecture Tutorial

HPC 2005
5 April 2005

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

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Agenda & Table of Contents

Time	Title	Slide No.	Presenter
1:30-1:35pm	Welcome	1	David Bernholdt, ORNL
1:35-2:15pm	A Pictorial Introduction to Components in Scientific Computing	6	David Bernholdt, ORNL
	An Introduction to Components & the CCA	26	David Bernholdt, ORNL
2:15-2:30pm	Distributed Computing with the CCA	67	David Bernholdt, ORNL
2:30-3:00pm	CCA Applications	84	Jaideep Ray, SNL
3:00-3:30pm	Language Interoperable CCA Components with Babel	130	Wael Elwasif, ORNL
3:30-5:30pm	Hands-On (and break as needed)	Hands-On Guide	Rob Armstrong, SNL & the Team

Note: Due to time constraints, this presentation is condensed relative to the notes provided. We would be happy to expand on specific questions or material on an individual basis during the Hands-On portion.

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The Common Component Architecture (CCA) Forum

- Combination of standards body and user group for the CCA
- Define Specifications for **High-Performance** Scientific Components & Frameworks
- Promote and Facilitate Development of Domain-Specific **Common Interfaces**
- Goal: **Interoperability** between components developed by different expert teams across different institutions
- Quarterly Meetings, Open membership...

Mailing List: cca-forum@cca-forum.org
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Acknowledgements: Tutorial Working Group

- **People:** Rob Armstrong, David Bernholdt, Randy Bramley, Wael Elwasif, Lori Freitag Diachin, Madhusudhan Govindaraju, Ragib Hasan, Dan Katz, Jim Kohl, Gary Kurfert, Lois Curfman McInnes, Boyana Norris, Craig Rasmussen, Jaideep Ray, Sameer Shende, Torsten Wilde, Shujia Zhou
- **Institutions:** ANL, Binghamton U, Indiana U, JPL, LANL, LLNL, NASA/Goddard, ORNL, SNL, U Illinois, U Oregon
- **Computer facilities** provided by the Computer Science Department and University Information Technology Services of Indiana University, supported in part by NSF grants CDA-9601632 and EIA-0202048.

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Acknowledgements: The CCA

- **ANL** –Steve Benson, Jay Larson, Ray Loy, Lois Curfman McInnes, Boyana Norris, Everest Ong, Jason Sarich...
 - **Binghamton University** - Madhu Govindaraju, Michael Lewis, ...
 - **Indiana University** - Randall Bramley, Dennis Gannon, ...
 - **JPL** – Dan Katz, ...
 - **LANL** - Craig Rasmussen, Matt Sotille, ...
 - **LLNL** – Lori Freitag Diachin, Tom Epperly, Scott Kohn, Gary Kumpfert, ...
 - **NASA/Goddard** – Shujia Zhou
 - **ORNL** - David Bernholdt, Wael Elwasif, Jim Kohl, Torsten Wilde, ...
 - **PNNL** - Jarek Nieplocha, Theresa Windus, ...
 - **SNL** - Rob Armstrong, Ben Allan, Lori Freitag Diachin, Curt Janssen, Jaideep Ray, ...
 - **University of Oregon** – Allen Malony, Sameer Shende, ...
 - **University of Utah** - Steve Parker, ...
- and many more... without whom we wouldn't have much to talk about!

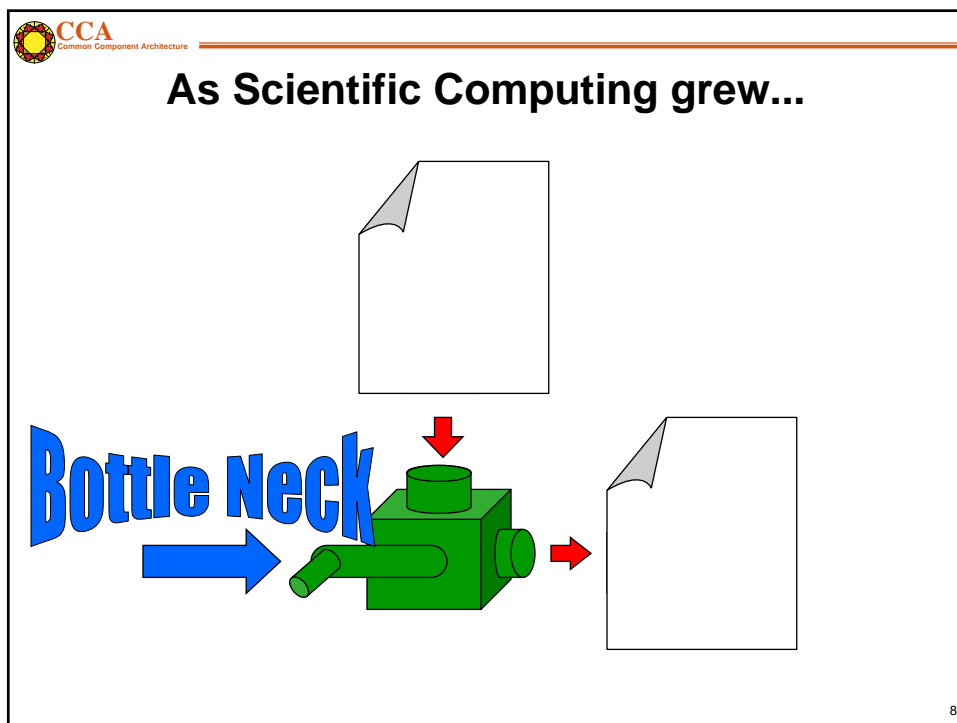
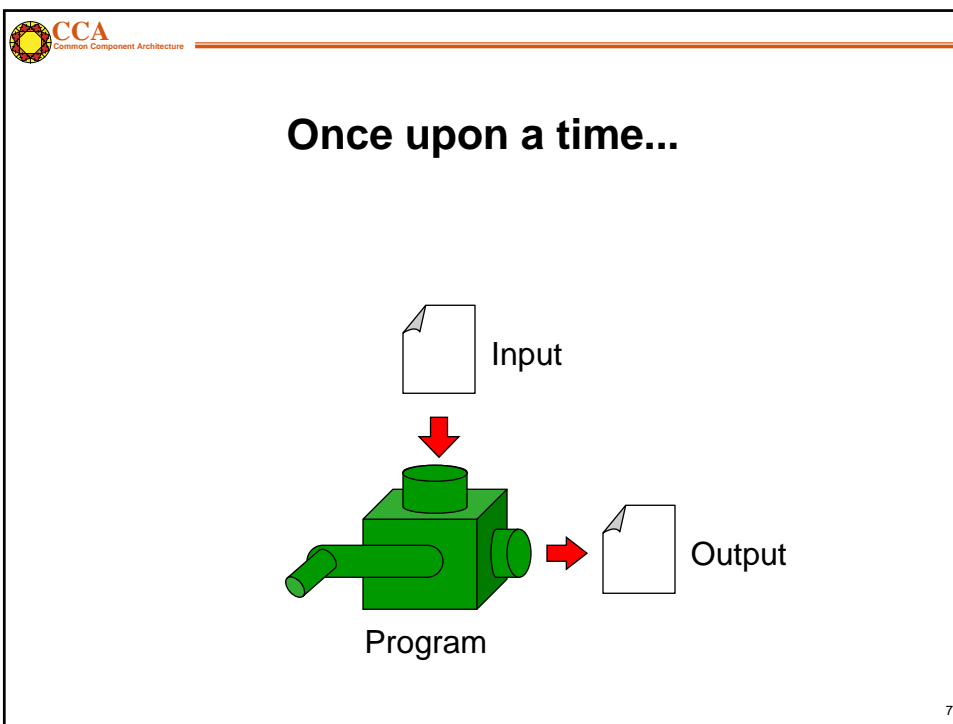
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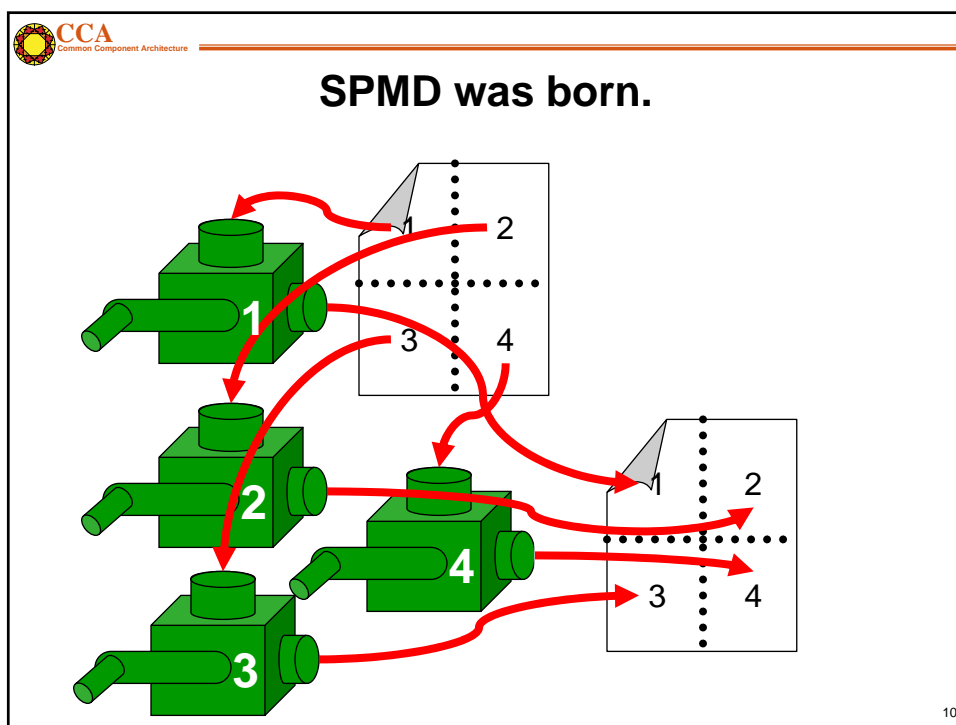
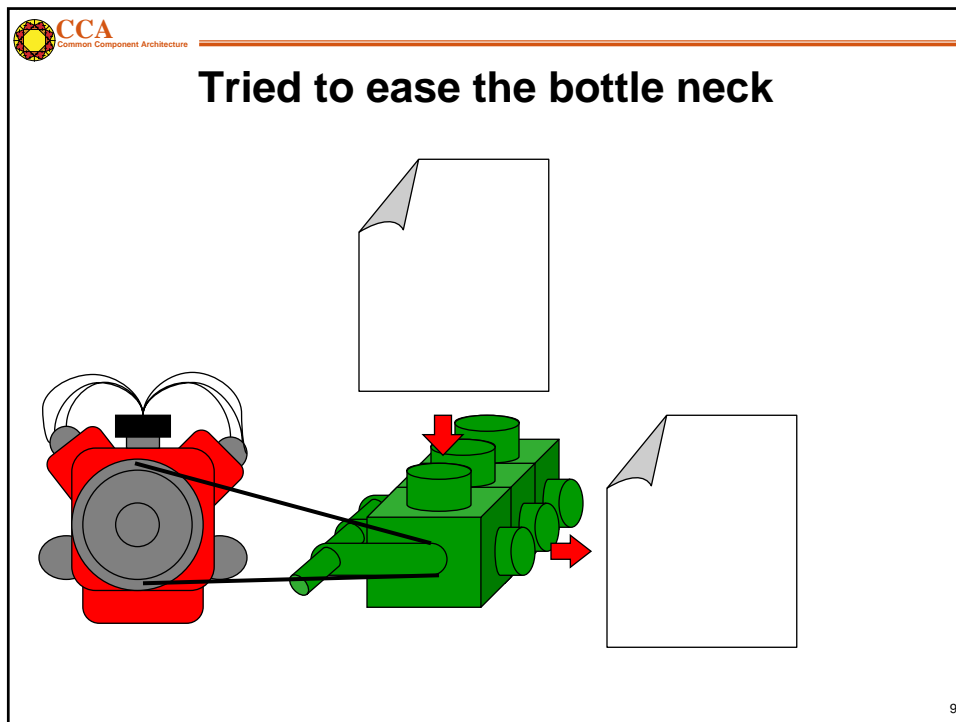


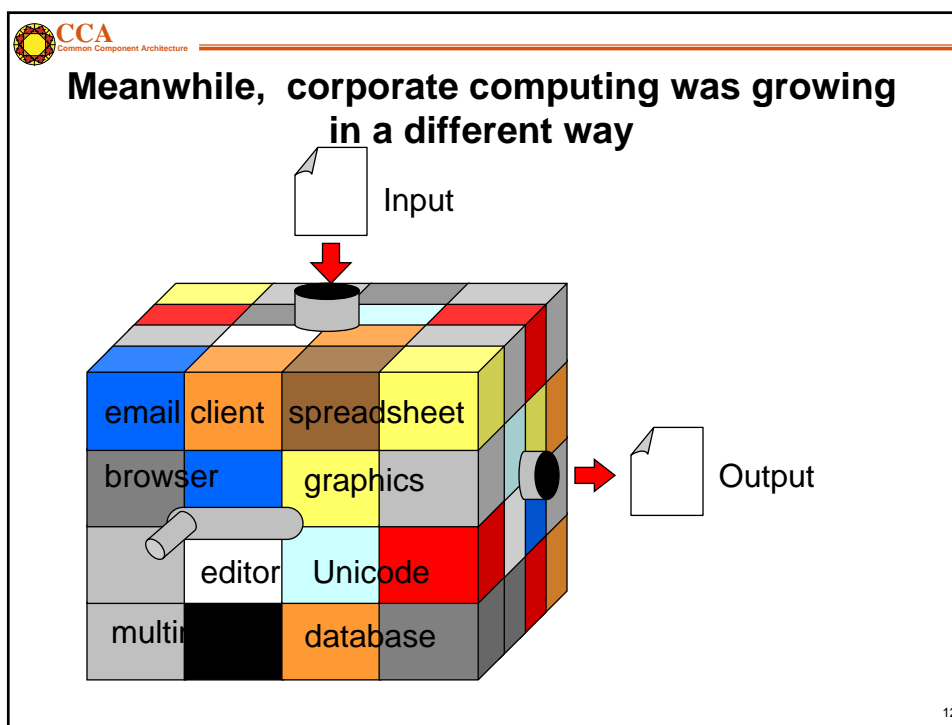
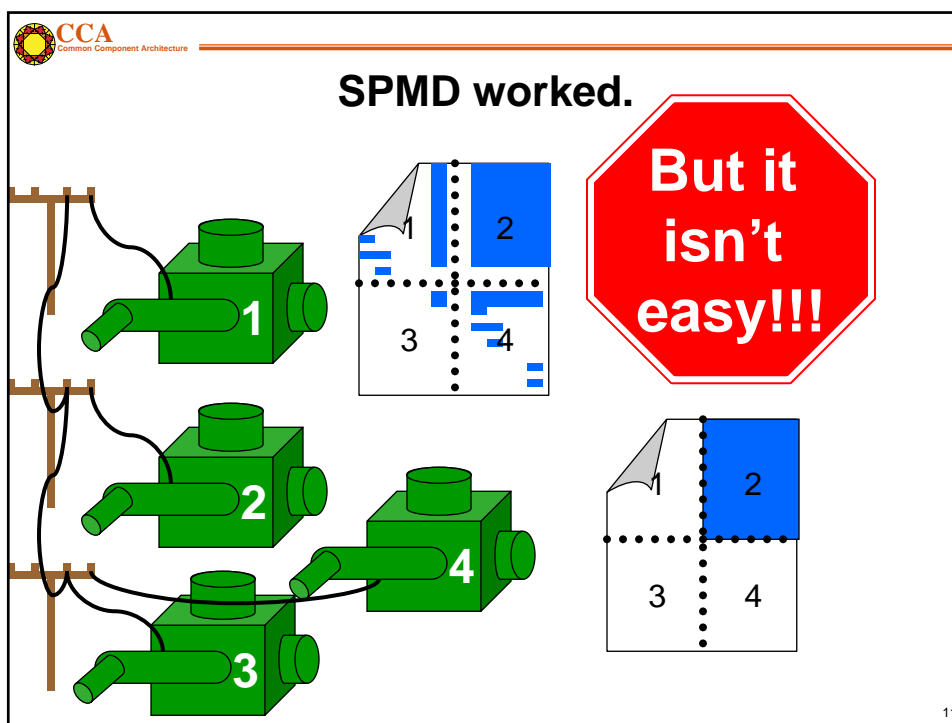
A Pictorial Introduction to Components in Scientific Computing

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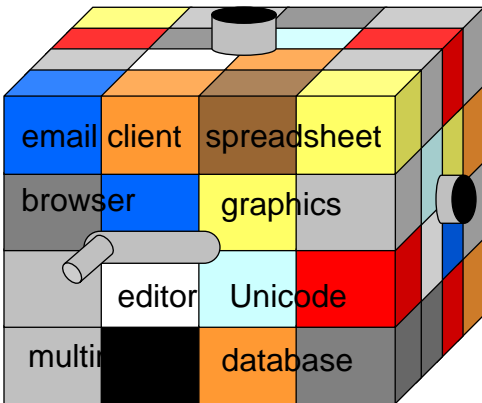






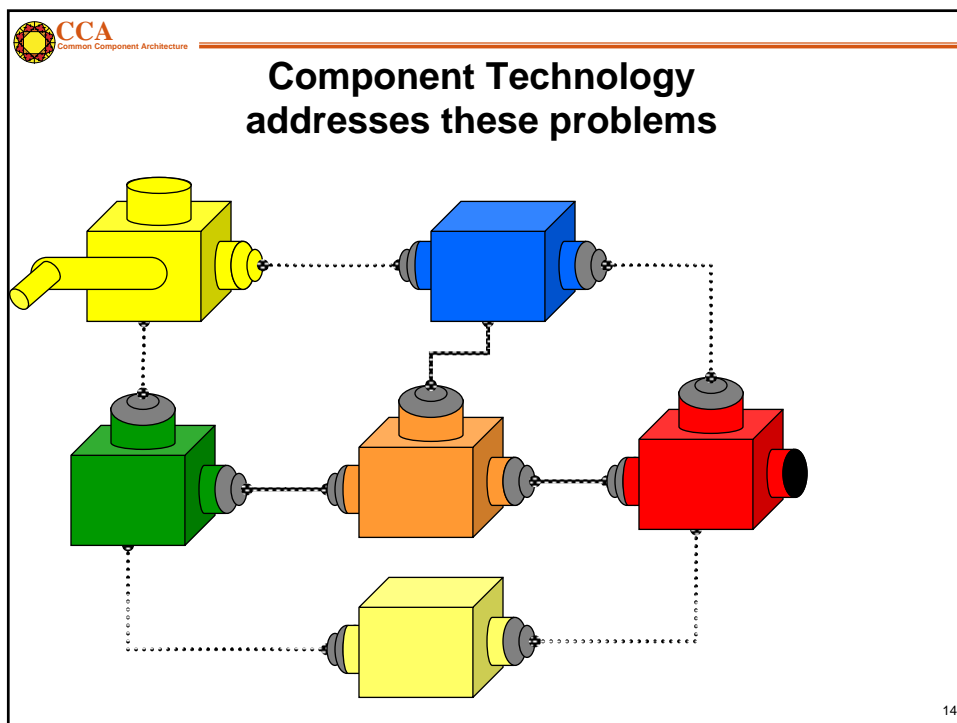
CCA
Common Component Architecture

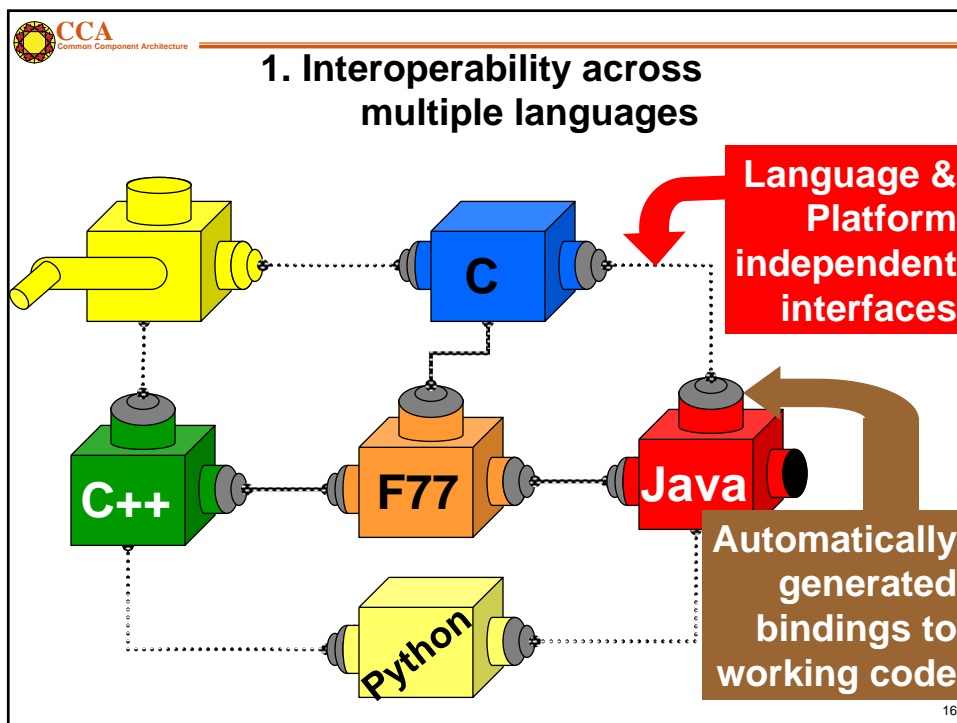
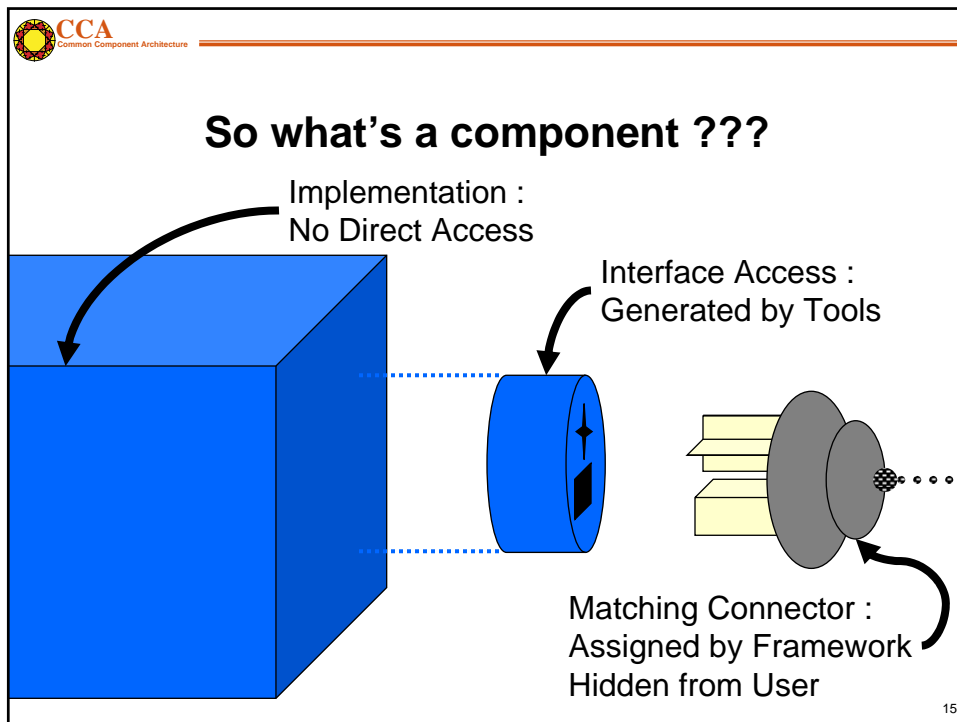
**This created a whole new set of problems
→ complexity**

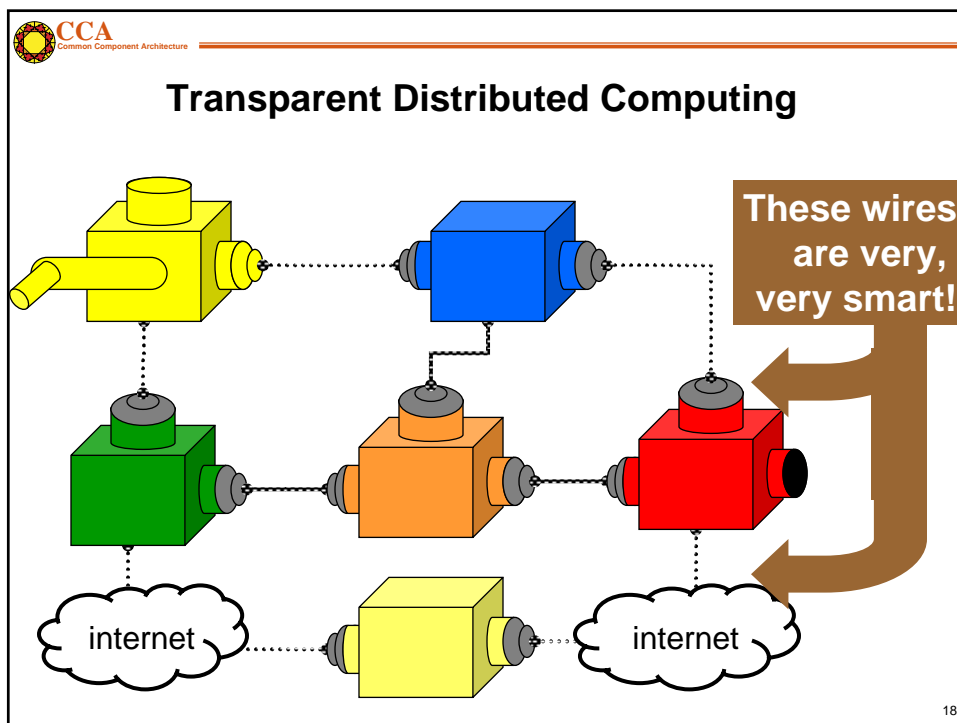
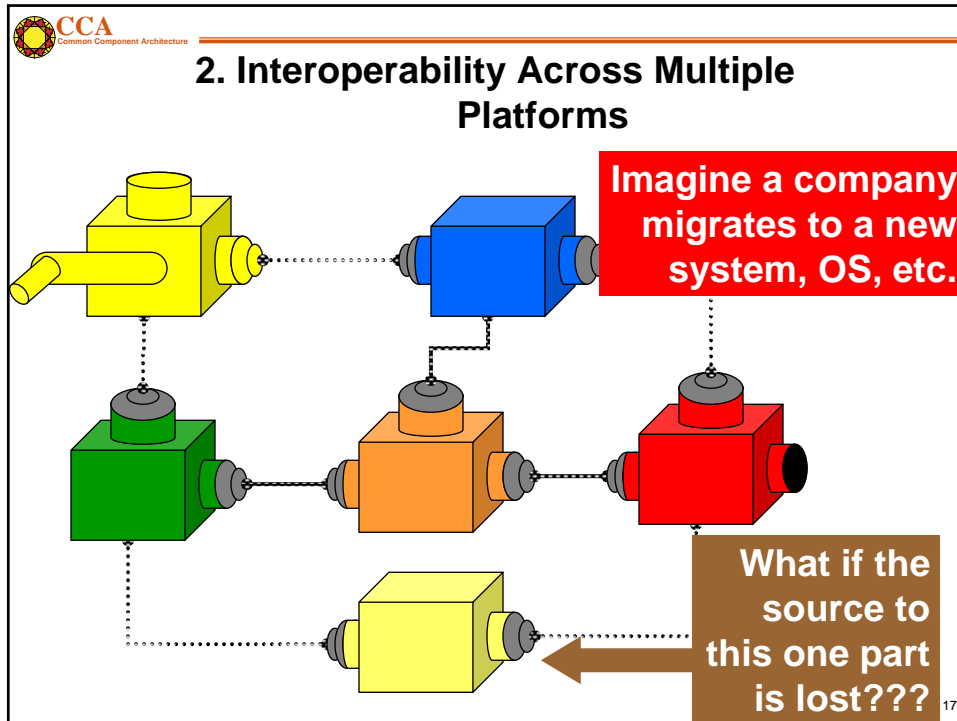


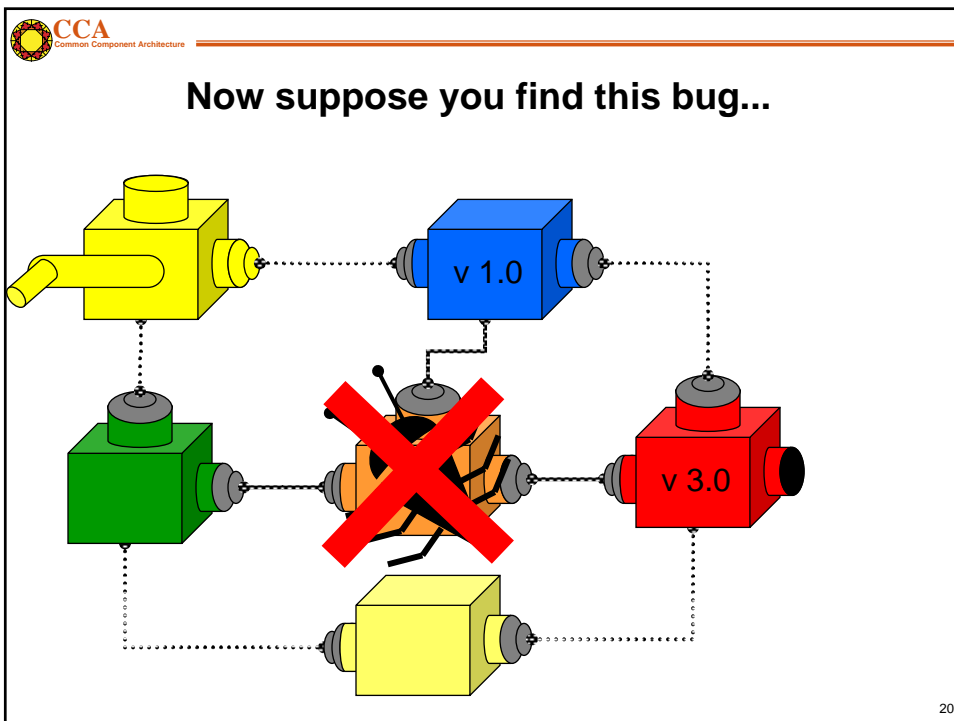
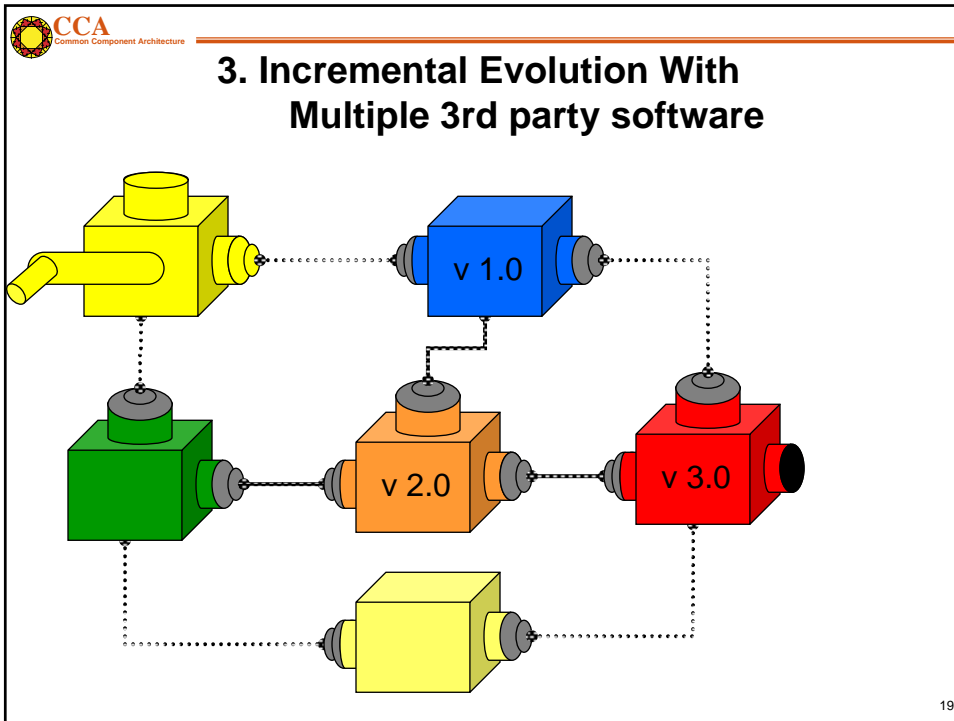
- Interoperability across multiple languages
- Interoperability across multiple platforms
- Incremental evolution of large legacy systems (esp. w/ multiple 3rd party software)

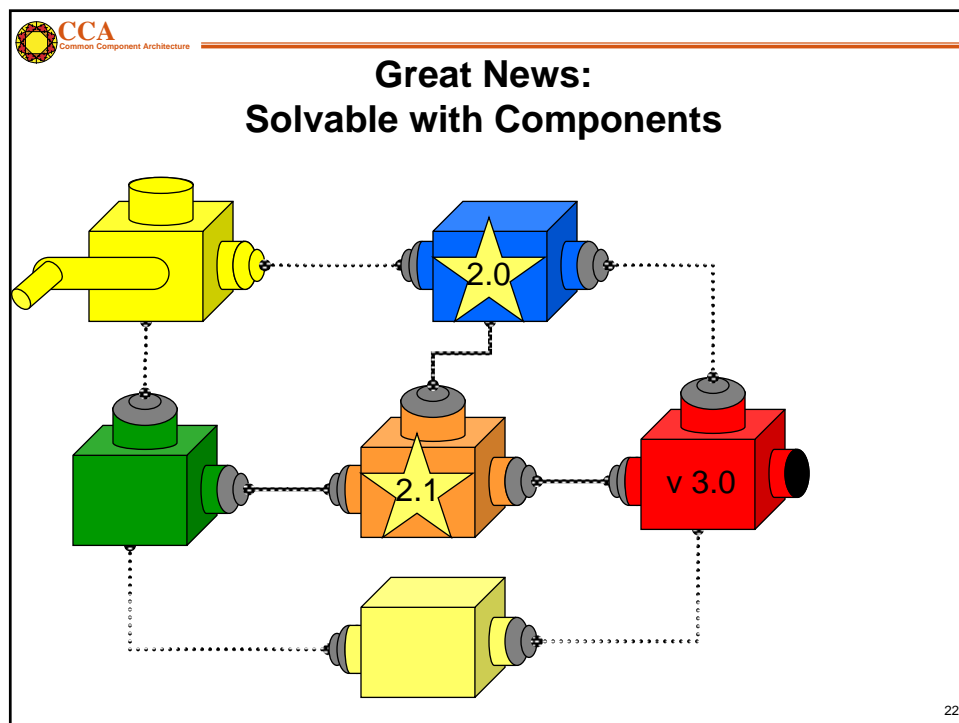
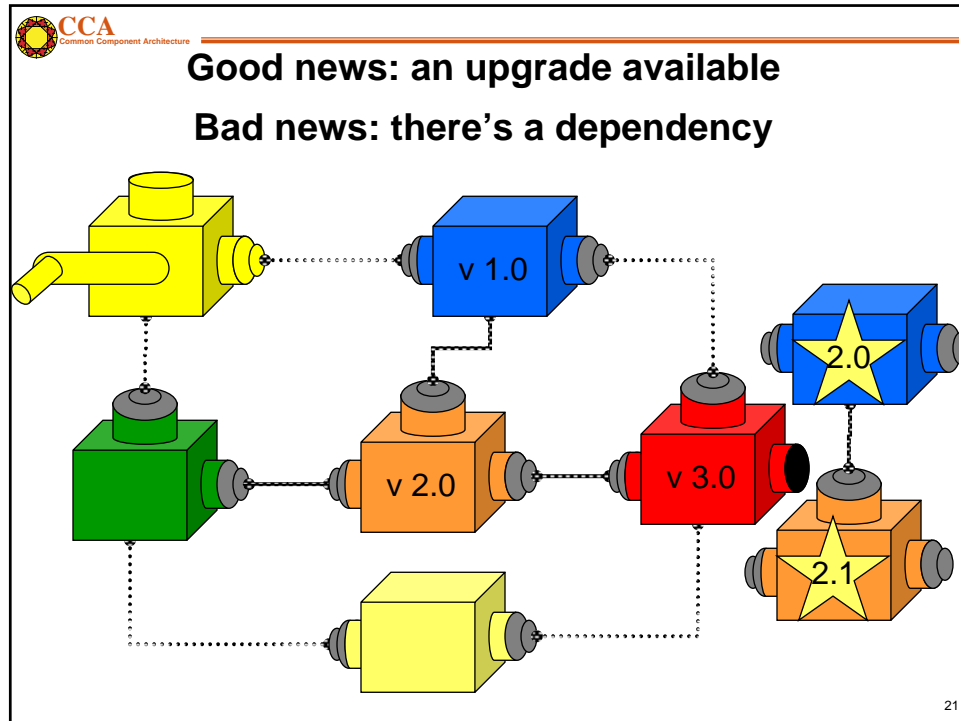
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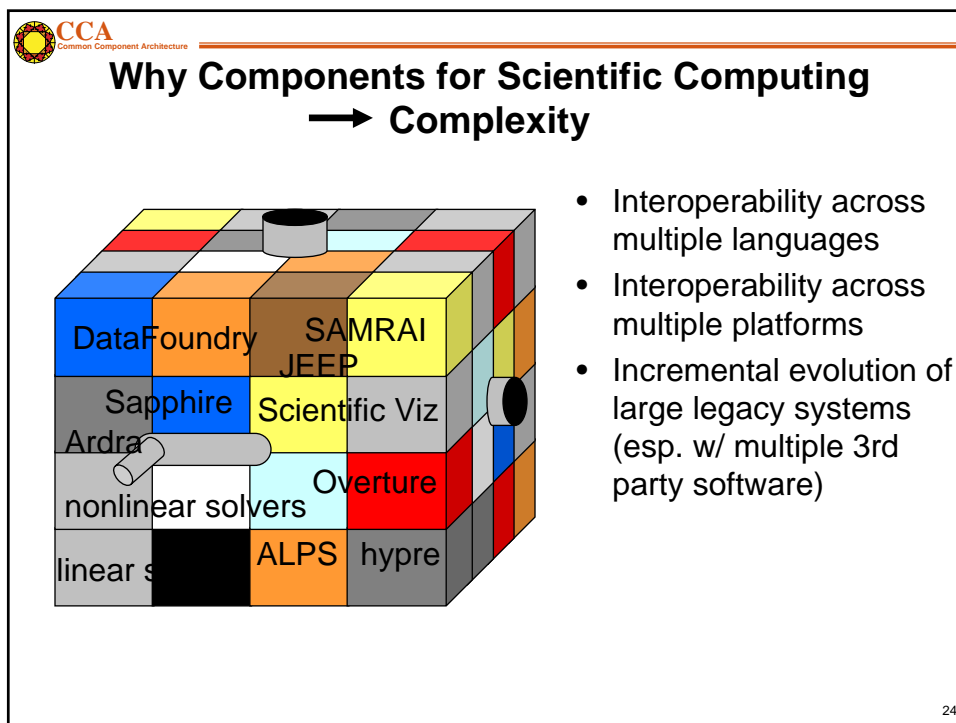
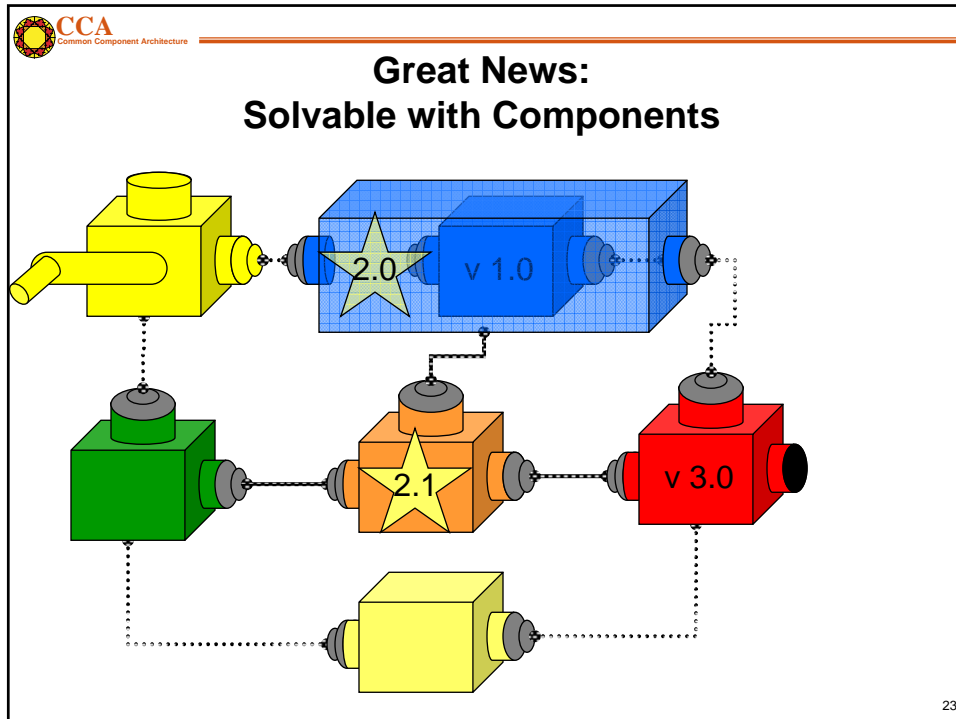


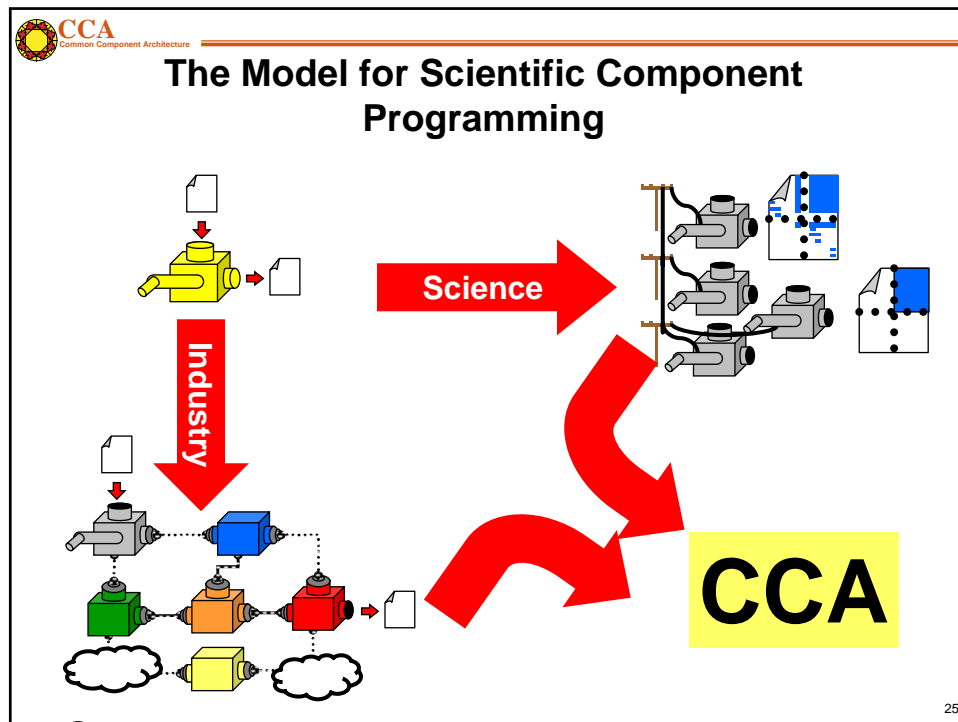












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An Introduction to Components and the Common Component Architecture

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Common Component Architecture

Goals of This Module

- Introduce basic **concepts and vocabulary** of component-based software engineering and the CCA
- Highlight the special **demands of high-performance scientific computing** on component environments

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Common Component Architecture

Component-Based Software Engineering

- CBSE methodology is an emerging approach to software development
 - Both in research and in practical application
 - Especially popular in business and internet areas
- Addresses software **complexity** issues
- Increases software **productivity**

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Motivation: For Library Developers

- People want to use your software, but need wrappers in languages you don't support
 - Many component models provide language interoperability
- Discussions about standardizing interfaces are often sidetracked into implementation issues
 - Components separate interfaces from implementation
- You want users to stick to your published interface and prevent them from stumbling (prying) into the implementation details
 - Most component models actively enforce the separation

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Motivation: For Application Developers and Users

- You have difficulty managing multiple third-party libraries in your code
- You (want to) use more than two languages in your application
- Your code is long-lived and different pieces evolve at different rates
- You want to be able to swap competing implementations of the same idea and test without modifying any of your code
- You want to compose your application with some other(s) that weren't originally designed to be combined

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What are Components?

- No universally accepted definition in computer science research ...yet
- A unit of software development/deployment/reuse
 - i.e. has **interesting functionality**
 - Ideally, functionality someone else might be able to **(re)use**
 - Can be **developed independently** of other components
- Interacts with the outside world only through well-defined interfaces
 - **Implementation is opaque** to the outside world
- Can be composed with other components
 - “Plug and play” model to build applications
 - **Composition based on interfaces**

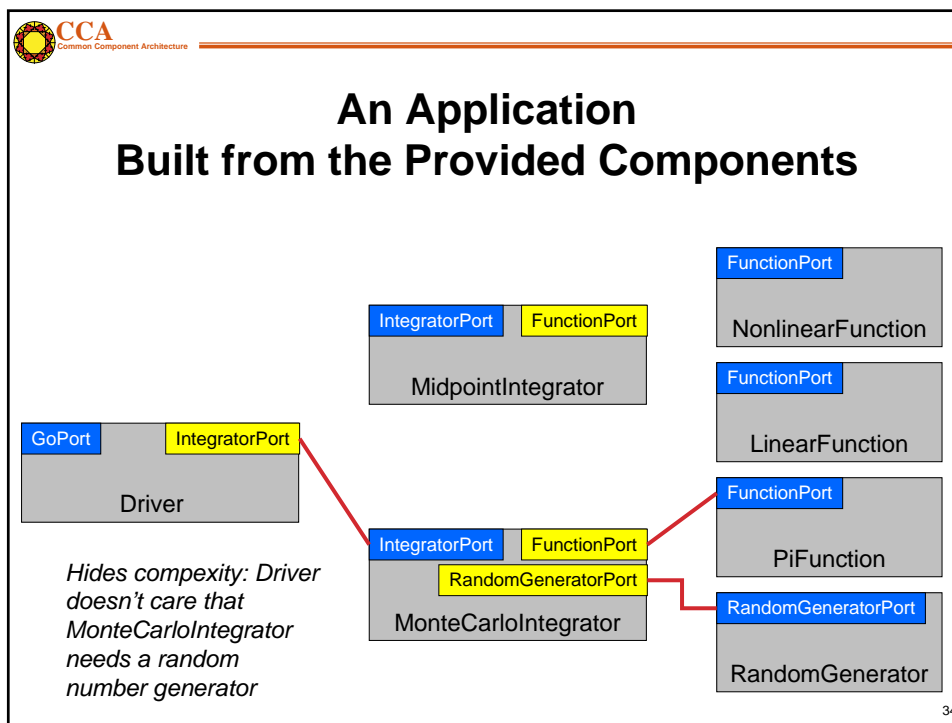
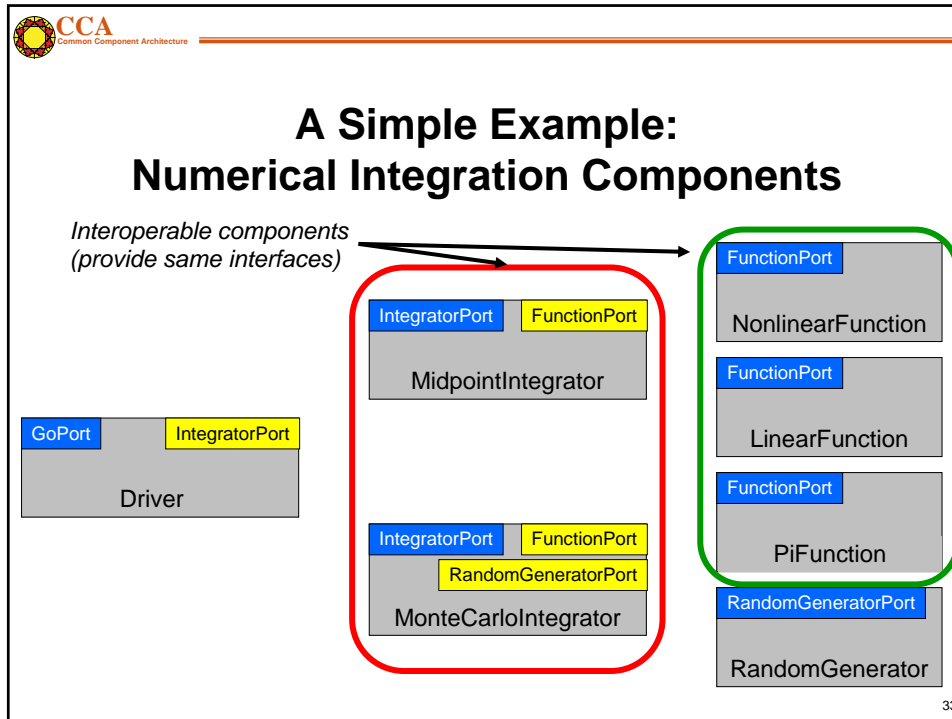
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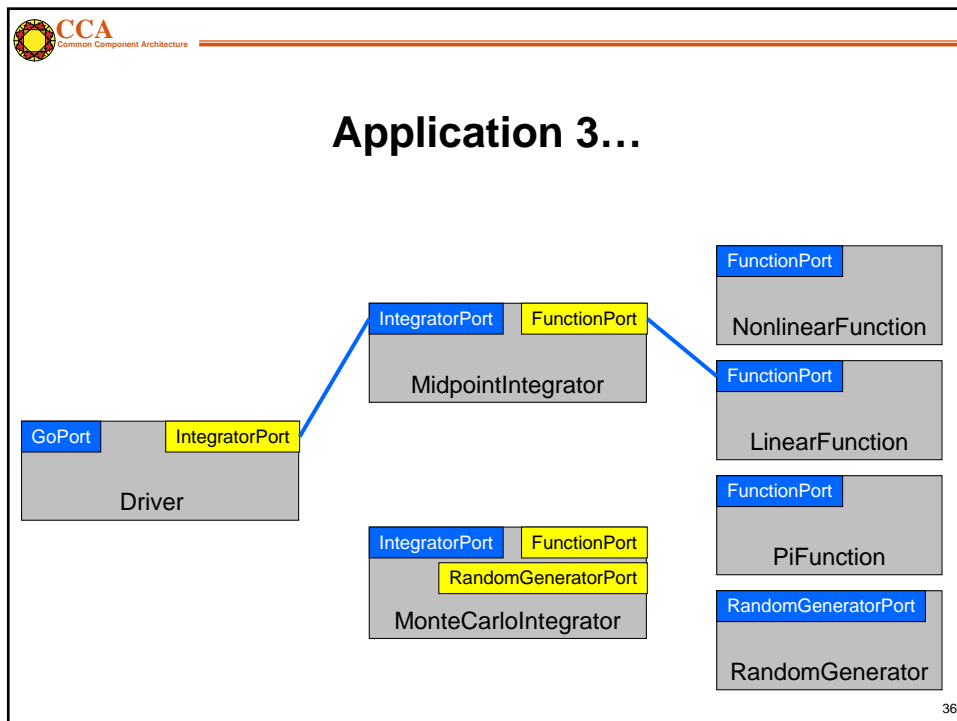
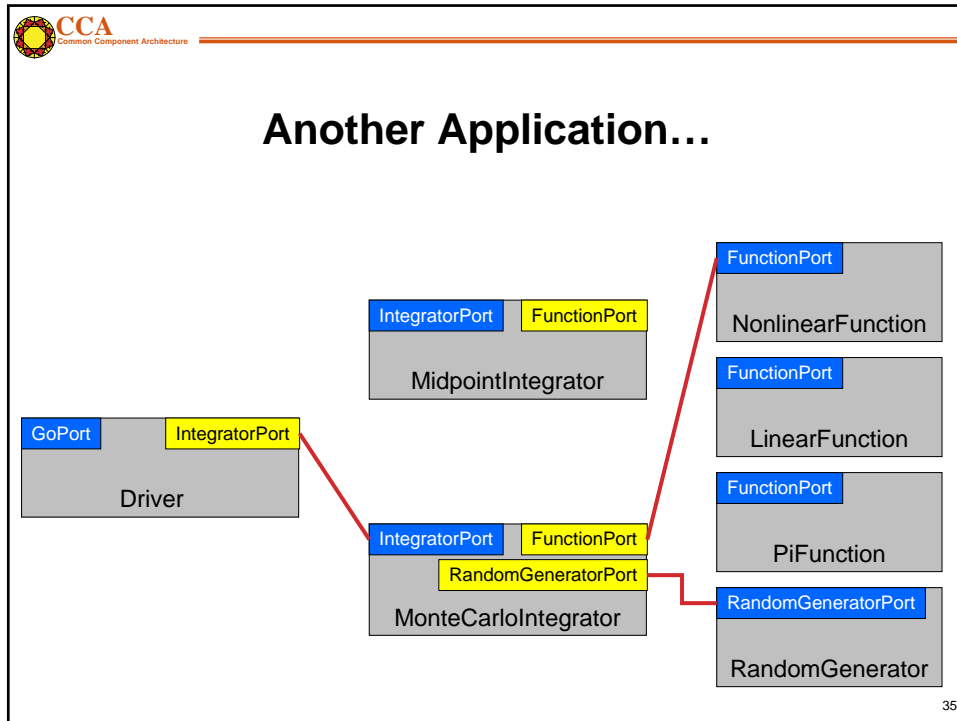


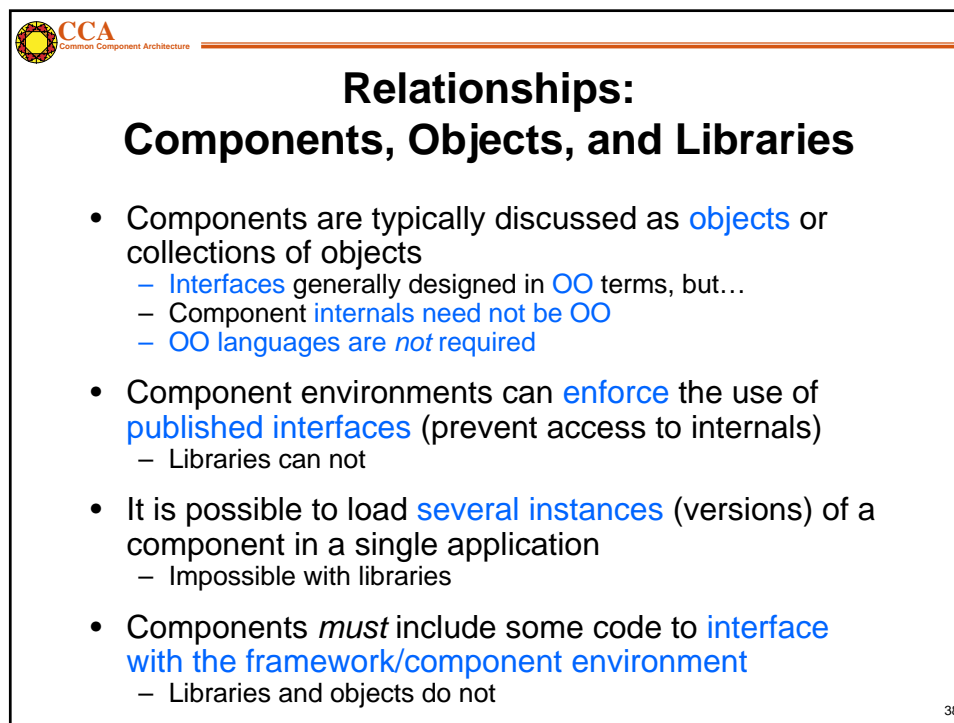
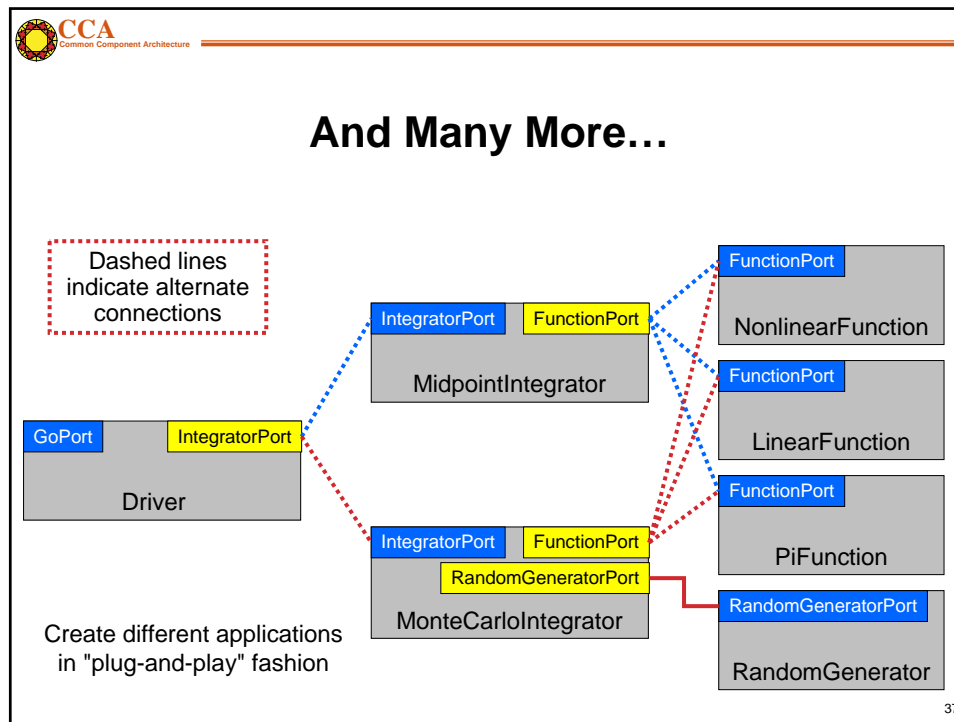
What is a Component Architecture?

- A set of **standards** that allows:
 - Multiple groups to write units of software (**components**)...
 - And have confidence that their components will **work with other components** written in the same architecture
- These standards **define**...
 - The rights and responsibilities of a **component**
 - How components express their **interfaces**
 - The environment in which are composed to form an application and executed (**framework**)
 - The rights and responsibilities of the framework

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Domain-Specific Frameworks vs Generic Component Architectures

Domain-Specific

- Often known as “frameworks”
- Provide a significant software infrastructure to support applications in a **given domain**
 - Often attempts to generalize an existing large application
- Often hard to adapt to use outside the original domain
 - Tend to assume a **particular structure/workflow** for application
- Relatively **common**
 - E.g. Cactus, ESMF, PRISM
 - Hypre, Overture, PETSc, POOMA

Generic

- Provide the infrastructure to **hook components** together
 - Domain-specific infrastructure can be built as components
- Usable in **many domains**
 - Few assumptions about application
 - **More opportunities for reuse**
- Better supports **model coupling** across traditional domain boundaries
- Relatively **rare** at present
 - e.g. CCA

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Interfaces, Interoperability, and Reuse

- Interfaces define how components interact...
- Therefore interfaces are key to **interoperability** and **reuse** of components
- In many cases, “any old interface” will do, but...
- Achieving reuse across multiple applications requires agreement on the same interface for all of them
- “**Common**” or “**community**” interfaces facilitate reuse and interoperability
 - Typically domain specific
 - Formality of “standards” process varies
 - Significant initial investment for long-term payback
- Biggerstaff’s Rule of Threes
 - Must look at at least **three systems** to understand what is common (reusable)
 - Reusable software requires **three times the effort** of usable software
 - Payback only after **third release**

More about community interface development efforts in “Applications” module

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Special Needs of Scientific HPC

- Support for legacy software
 - How much **change** required for component environment?
- Performance is important
 - What **overheads** are imposed by the component environment?
- Both parallel and distributed computing are important
 - What approaches does the component model support?
 - What **constraints** are imposed?
 - What are the **performance costs**?
- Support for **languages, data types, and platforms**
 - Fortran?
 - Complex numbers? Arrays? (as first-class objects)
 - Is it available on my parallel computer?

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Commodity Component Models

- CORBA Component Model (CCM), COM, Enterprise JavaBeans
 - Arise from business/internet software world
- Componentization **requirements** can be **high**
- Can impose significant **performance overheads**
- No recognition of **tightly-coupled parallelism**
- May be **platform specific**
- May have **language constraints**
- May not support common scientific **data types**

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Common Component Architecture

What is the CCA?

- CCA is a *specification of a component environment* designed for *high performance scientific computing*
 - Specification is decided by the *CCA Forum*
 - CCA Forum membership open to all
 - “*CCA-compliant*” just means conforming to the specification
 - Doesn't require using any of our code!
- A *tool* to enhance the productivity of scientific programmers
 - Make the hard things easier, make some intractable things tractable
 - Support & promote reuse & interoperability
 - *Not a magic bullet*

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Common Component Architecture

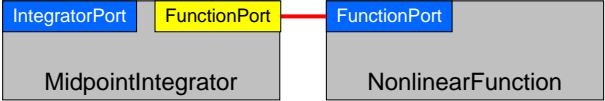
CCA Philosophy and Objectives

- *Local and remote components*
 - Support local, HPC parallel, and distributed computing
- *High Performance*
 - Design should support high-performance mechanisms wherever possible (i.e. minimize copies, extra communications, extra synchronization)
 - Support SPMD and MPMD parallelism
 - Allow user to choose parallel programming models
- *Heterogeneity*
 - Multiple architectures, languages, run-time systems used simultaneously in an application
- *Integration*
 - Components should be easy to make and easy to use
- *Openness and simplicity*
 - CCA spec should be open & usable with open software

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CCA Concepts: Components

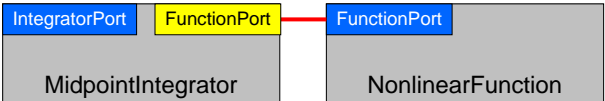


- Components provide/use one or more **ports**
 - A component with no ports isn't very interesting
- Components include some **code which interacts with a CCA framework**

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CCA Concepts: Ports



- Components interact through well-defined **interfaces**, or **ports**
 - In OO languages, a port is a **class** or **interface**
 - In Fortran, a port is a bunch of subroutines or a **module**
- Components may **provide** ports – **implement** the class or subroutines of the port (**"Provides" Port**)
- Components may **use** ports – **call** methods or subroutines in the port (**"Uses" Port**)
- Links between ports denote a procedural (caller/callee) relationship, **not dataflow!**
 - e.g., FunctionPort could contain: *evaluate*(*in* Arg, *out* Result)

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CCA Concepts: Frameworks

- The framework provides the means to “hold” components and **compose** them into applications
- Frameworks allow **connection of ports** without exposing component implementation details
- Frameworks provide a small set of **standard services** to components
- *Currently:* specific frameworks support specific computing models (parallel, distributed, etc.)
- *Future:* full flexibility through integration or interoperation

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Writing Components

- Components...
 - Inherit from **gov.cca.Component**
 - Implement **setServices** method to register ports this component will **provide** and **use**
 - Implement the ports they provide
 - Use ports on other components
 - **getPort/releasePort** from framework **Services** object
- Interfaces (ports) extend **gov.cca.Port**

Full details in the hands-on!

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Adapting Existing Code into Components

Example in
the hands-on!

Suitably structured code (programs, libraries) should be relatively easy to adapt to the CCA. Here's how:

1. Decide **level of componentization**
 - Can evolve with time (start with coarse components, later refine into smaller ones)
2. Define **interfaces** and write wrappers between them and existing code
3. Add **framework interaction code** for each component
 - `setServices`
4. Modify component internals to **use other components** as appropriate
 - `getPort`, `releasePort` and method invocations

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Writing Frameworks

- ***There is no reason for most people to write frameworks – just use the existing ones!***
- Frameworks must provide certain ports...
 - **ConnectionEventService**
 - Informs the component of connections
 - **AbstractFramework**
 - Allows the component to *behave as a framework*
 - **BuilderService**
 - Instantiate components & connect ports
 - **ComponentRepository**
 - A default place where components are found
- Frameworks must be able to load components
 - Typically shared object libraries, can be statically linked
- Frameworks must provide a way to compose applications from components

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CCA Supports Local, Parallel and Distributed Computing

- “**Direct connection**” preserves high performance of local (“in-process”) components
 - Framework makes **connection**
 - But is not involved in **invocation**
- **Distributed computing** has same uses/provides pattern, but **framework intervenes** between user and provider
 - Framework provides a *proxy* provides port local to the *uses* port
 - Framework conveys invocation from proxy to actual provides port

The diagram shows two scenarios. In the 'Direct Connection' scenario, an 'Integrator' box and a 'Linear Fun' box are shown side-by-side. A single oval labeled 'Provides/Uses Port' is positioned between them, indicating a direct interface. In the 'Network Connection' scenario, the 'Integrator' box has an oval labeled 'Provides Port'. A green lightning bolt, labeled 'Network Connection', points from this oval to another oval labeled 'Proxy Provides/ UsesPort' which is inside the 'Linear Fun' box.

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CCA Concepts: “Direct Connection” Maintains Local Performance

- Calls **between** components equivalent to a C++ **virtual function call**: lookup function location, invoke it
 - Cost equivalent of **~2.8 F77 or C function calls**
 - ~48 ns vs 17 ns on 500 MHz Pentium III Linux box
- **Language interoperability** can impose additional overheads
 - Some arguments require conversion
 - Costs vary, but small for typical scientific computing needs
- Calls **within** components have **no CCA-imposed overhead**
- **Implications**
 - **Be aware of costs**
 - Design so inter-component calls **do enough work** that overhead is negligible

More about performance in the “Applications” module

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CCA Concepts: Framework Stays “Out of the Way” of Component Parallelism

- Single component multiple data (SCMD) model is component analog of widely used SPMD model
- Each process loaded with the same set of components wired the same way
- Different components in same process “talk to each” other via ports and the framework
- **Same component in different processes talk to each other through their favorite communications layer (i.e. MPI, PVM, GA)**

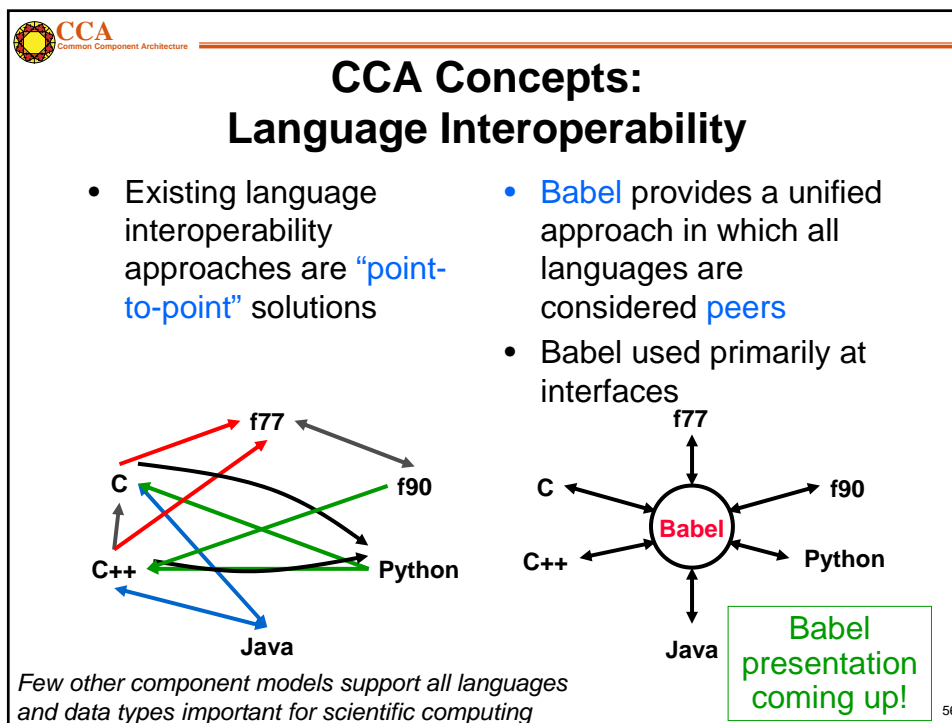
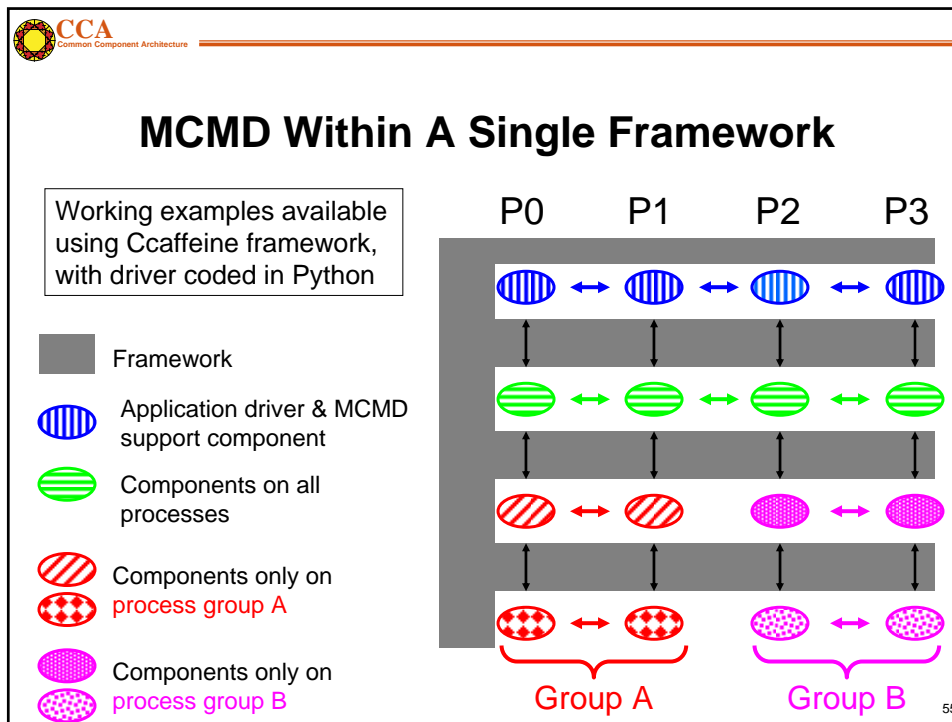
Components: Blue, Green, Red
Framework: Gray
MCMD/MPMD also supported
Other component models ignore parallelism entirely

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“Multiple-Component Multiple-Data” Applications in CCA

- Simulation composed of multiple SCMD sub-tasks
- Usage Scenarios:
 - Model coupling (e.g. Atmosphere/Ocean)
 - General multi-physics applications
 - Software licensing issues
- Approaches
 - Run single parallel framework
 - Driver component that partitions processes and builds rest of application as appropriate (through BuilderService)
 - Run multiple parallel frameworks
 - Link through specialized communications components
 - Link as components (through AbstractFramework service; highly experimental at present)

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Advanced CCA Concepts

- Frameworks provide a **BuilderService** which allows **programmatic composition** of components
- Frameworks may **present themselves as components** to other frameworks
- A “traditional” application can treat a CCA framework as a **library**
- **Meta-component models** enable bridging between CCA components and other component(-like) environments
 - e.g. SCIRun Dataflow, Visualization Toolkit (VTK), ...

No time to go into detail on these, but ask us for more info after the tutorial

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Component Lifecycle

Additional material in notes

- **Composition Phase (assembling application)**
 - Component is **instantiated** in framework
 - Component interfaces are **connected** appropriately
- **Execution Phase (running application)**
 - Code in components uses functions provided by another component
- **Decomposition Phase (termination of application)**
 - **Connections** between component interfaces may be **broken**
 - Component may be **destroyed**

In an application, individual components may be in different phases at different times

Steps may be under human or software control

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Supplementary material for handouts

User Viewpoint: Loading and Instantiating Components

- Components are code + metadata
- Using metadata, a **Palette** of available components is constructed
- Components are instantiated by user action (i.e. by dragging from **Palette** into **Arena**)
- Framework calls component's **constructor**, then **setServices**
- Details are **framework-specific!**
- Ccaffeine** currently provides both command line and GUI approaches

create
create
create

Driver
LinearFunction
MonteCarloIntegrator

Driver
LinearFunction
MonteCarloIntegrator

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Common Component Architecture

Supplementary material for handouts

User Connects Ports

- Can only connect uses & provides
 - Not uses/uses or provides/provides
- Ports connected by type, not name
 - Port names must be unique within component
 - Types must match across components
- Framework puts info about *provider* of port into *using* component's Services object

connect
connect
...

Driver
MonteCarloIntegrator

IntegratorPort
FunctionPort

MonteCarloIntegrator
LinearFunction

IntegratorPort
FunctionPort

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Common Component Architecture

Supplementary material for handouts

Component's View of Instantiation

- Framework calls component's **constructor**
- Component initializes internal data, etc.
 - Knows *nothing* outside itself
- Framework calls component's **setServices**
 - Passes setServices an object representing everything "outside"
 - setServices declares ports component *uses* and *provides*
- Component *still* knows nothing outside itself
 - But Services object provides the means of communication w/ framework
- Framework now knows how to "decorate" component and how it might connect with others

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Common Component Architecture

Supplementary material for handouts

Component's View of Connection

- Framework puts info about provider into **user component's** Services object
 - MonteCarloIntegrator's** Services object is aware of connection
 - NonlinearFunction** is not!
- MCI's** integrator code cannot yet call functions on FunctionPort

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Supplementary material for handouts

Component's View of Using a Port

- User calls `getPort` to obtain (handle for) port from Services
 - Finally user code can “see” provider
- `Cast` port to expected type
 - OO programming concept
 - Insures type safety
 - Helps enforce declared interface
- `Call` methods on port
 - e.g.
 $\text{sum} = \text{sum} + \text{function} \rightarrow \text{evaluate}(x)$
- `Release` port

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What the CCA isn't...

- CCA doesn't specify who owns “main”
 - CCA components are peers
 - Up to application to define component relationships
 - “Driver component” is a common design pattern
- CCA doesn't specify a parallel programming environment
 - Choose your favorite
 - Mix multiple tools in a single application
- CCA doesn't specify I/O
 - But it gives you the infrastructure to create I/O components
 - Use of `stdio` may be problematic in mixed language env.
- CCA doesn't specify interfaces
 - But it gives you the infrastructure to define and enforce them
 - CCA Forum supports & promotes common interface efforts
- CCA doesn't require (but does support) separation of algorithms/physics from data
 - Generic programming

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What the CCA is...

- CCA is a *specification* for a component environment
 - Fundamentally, a design pattern
 - Multiple “reference” implementations exist
 - Being used by applications
- CCA is designed for interoperability
 - Components within a CCA environment
 - CCA environment with other tools, libraries, and frameworks
- CCA provides an environment in which domain-specific application frameworks can be built
 - While retaining opportunities for software reuse at multiple levels


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Concept Review

- **Ports**
 - [Interfaces](#) between components
 - [Uses/provides](#) model
- **Framework**
 - Allows [assembly](#) of components into applications
- **Direct Connection**
 - Maintain [performance](#) of local inter-component calls
- **Parallelism**
 - Framework [stays out of the way](#) of parallel components
- **Language Interoperability**
 - [Babel](#), Scientific Interface Definition Language ([SIDL](#))


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Common Component Architecture

Distributed Computing with the CCA

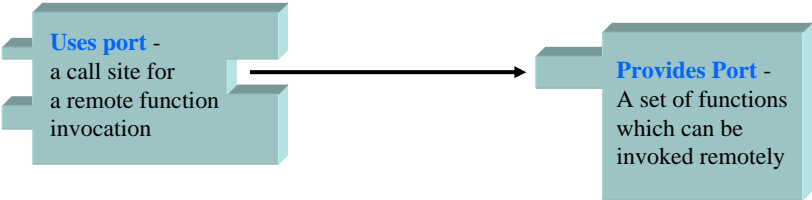
CCA Forum Tutorial Working Group
<http://www.cca-forum.org/tutorials/tutorial-wg@cca-forum.org>

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 **CCA**
Common Component Architecture

Component Composition

- Components can be linked along shared interfaces (ports) where one component invokes the services of another
 - Two types of **Ports**
 - Provides Ports – implements a remote interface
 - Uses Ports – uses a remote interface
 - A user and a provider of the same type can be linked
 - Details of run-time substrate shielded in **stubs and skeletons**
 - Similar in concept to the files generated by Babel



Uses port -
a call site for
a remote function
invocation

Provides Port -
A set of functions
which can be
invoked remotely

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CCA
Common Component Architecture

How Distributed Frameworks are Different

Remote Creation

- Launch components in remote address spaces
- Heterogeneity management
- Use resource managers to service requests on each remote resource
- Store, move and replicate component binaries

Remote Invocation

- Need [global pointers](#) and not local pointers
- Invoke methods across machine boundaries
- Need [global namespace](#) for names of components and services
- Mechanism for implementing [remote method invocation \(RMI\)](#)
- Introspection mechanisms to allow ports and services to be discovered and accessed

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CCA
Common Component Architecture

CCA Concepts that Influence Design of Distributed Frameworks (1)

- Ports
 - References to *provides* ports can move across address spaces
 - *Uses* ports are local to each component
- Services Object is present in each component
 - Manages all the ports
 - Hides details of framework-specific bindings for ports
- ComponentID: opaque handle to the component
 - Should be [serializable](#) and [deserializable](#)
 - Usually points to the [services](#) object

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CCA Concepts that Influence Design of Distributed Frameworks (2)

- Builder Service: charged with following operations
 - Create Components in remote address spaces
 - Return a **ComponentID** of instantiated components
 - Hide details of heterogeneous remote environments
 - Connect ports of components
 - Facilitate connection between uses and provides ports
 - Only if they are of the same SIDL type
 - Place provides port reference in the uses port table
- Introspection
 - Allow remote querying of a component
 - How many and what type of ports does the component have?

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Key Design Choices for Distributed CCA Frameworks (1)

- How is the CCA **ComponentID** represented in a distributed environment?
 - Handle that can be passed to remote components
 - Serialize and deserialize ComponentID
 - Belong to a namespace understood in the entire framework
 - Should enable optimized communication for co-located components
- How is the **PortType** represented?
 - *Provides* port should be designed as a remote service
 - *Uses* port should be a local object

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Key Design Choices for Distributed CCA Frameworks (2)

- Where can the key CCA functions be called from?
Are they remote or local?
 - getPort() call on the services object
 - Should return a remote reference for provides ports
 - Note that the same call in the [Ccaffeine](#) framework returns a local object
 - Details of remote and local calls should be hidden
 - Framework should internally distinguish local and remote calls
- How can components be connected?
 - Need internal mechanism for uses port to obtain remote reference of the provides port
 - Information can be stored in a central table, facilitate development of GUIs to show component assembly
 - Distributed across components so they are aware of who they are connected to

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Supplementary material for handouts

Key Design Choices for Distributed CCA Frameworks (3)

- Should Builder Service be centralized or distributed?
 - A component can have its own builder service if
 - The builder service is lightweight
 - The components has special create/connect requirements

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Current CCA Distributed Frameworks

- SCIRun2
 - University of Utah
- LegionCCA
 - Binghamton University - State University of New York (SUNY)
- XCAT (Java and C++)
 - Indiana University and Binghamton University
- DCA
 - Indiana University
 - A research framework for MXN
- Frameworks address the design questions in different ways
 - Each has a different set of capabilities
 - Specialized for different kinds of applications

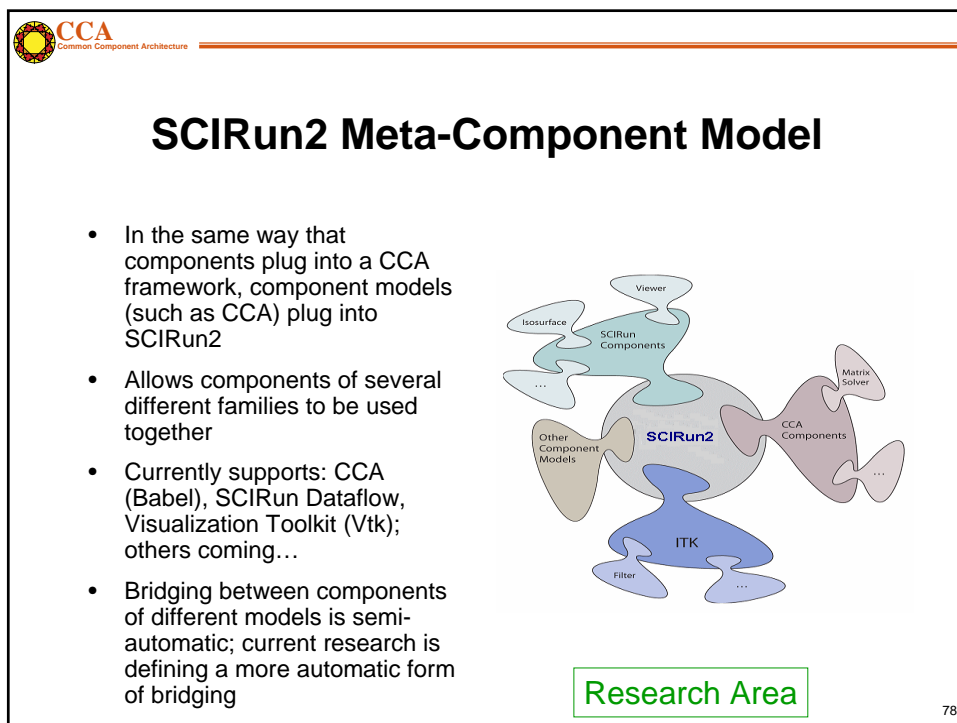
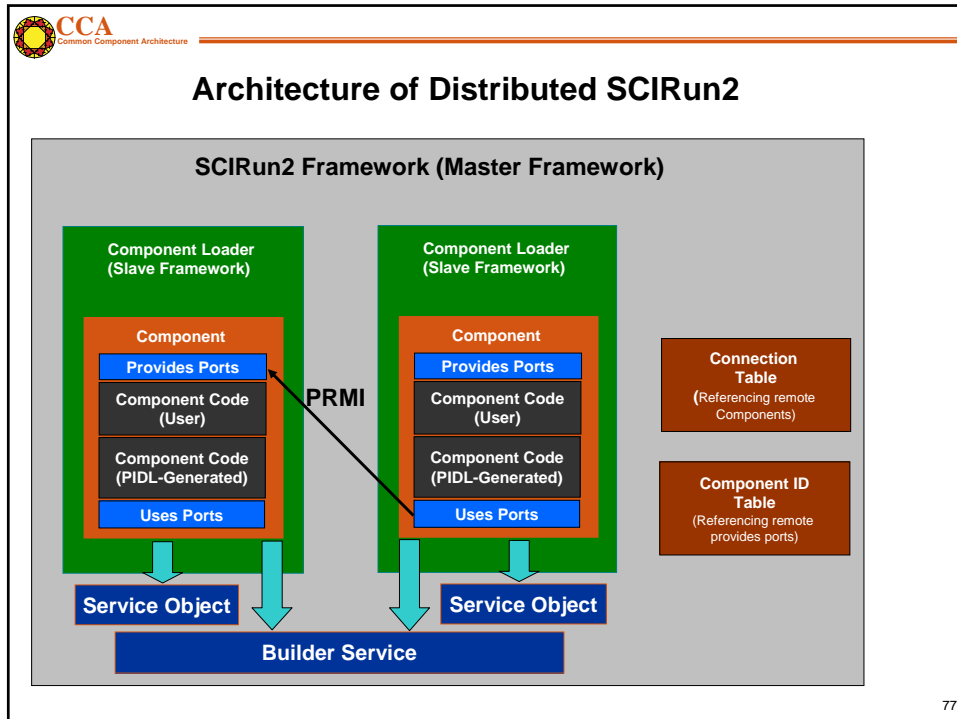
75



SCIRun2

- Communication
 - C++ RMI that uses an in-house SIDL compiler
 - Co-location optimization
- Remote creation of distributed components
 - A [slave framework](#) resides in each remote address space
 - Uses [ssh](#) to start the slave framework
 - CCA BuilderService communicates with [master framework](#) which coordinates [slave frameworks](#)
- Support for distributed and parallel components
 - Can launch MPI-parallel components
 - Components interact via [Parallel Remote Method Invocation](#)
 - Each MPI process may contain multiple threads

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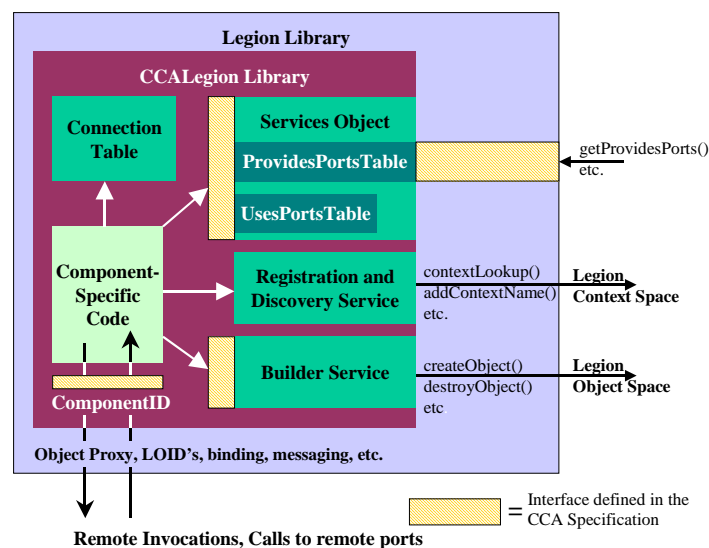
LegionCCA

- Legion is a collection of software services for the Grid
 - Provides illusion of a virtual machine for geographically-distributed resources
- LegionCCA: models CCA components as Legion objects
- Component Communication
 - Uses Legion's built-in RPC mechanisms, based on Unix sockets
- ComponentID: based on Legion LOID
 - LOID: globally unique object id

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Anatomy of a LegionCCA Component



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CCA
Common Component Architecture

XCAT

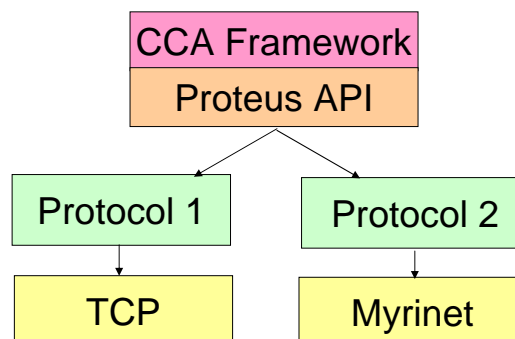
- Based on Web Services Standards
 - Remote reference format is WSDL
 - Remote Communication is based on XSOAP
 - An implementation of the [SOAP](#) protocol from Indiana Univ.
- Remote creation of distributed components
 - Creation can currently be done via [GRAM](#) or [SSH](#)
 - GRAM: Grid Resource Allocation and Management
- XCAT-Java
 - Consistent with standards in Grid Web Services
- XCAT-C++
 - Uses [Proteus](#) for high performance remote communication
 - Proteus: multi-protocol library for messaging and RMI
 - Currently has two protocols: binary and SOAP

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CCA
Common Component Architecture

Proteus: Multi-Protocol Library

- One protocol does not suit all applications
- Proteus provides single-protocol abstraction to components
 - Allows users to dynamically switch between protocols
 - Example: Protocol 1 & Protocol 2, in the picture
 - Facilitates use of specialized implementations of [serialization](#) and [deserialization](#)



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CCA
Common Component Architecture

Babel RMI

Research!

- Allows Babel objects to be accessed through remote Babel stubs.
- Underlying RMI uses Proteus.
- Objects that can be transmitted (serializable) inherent from Serializable.
- Actual implementation of serialization functions is by users, since only they know what needs to be serialized.

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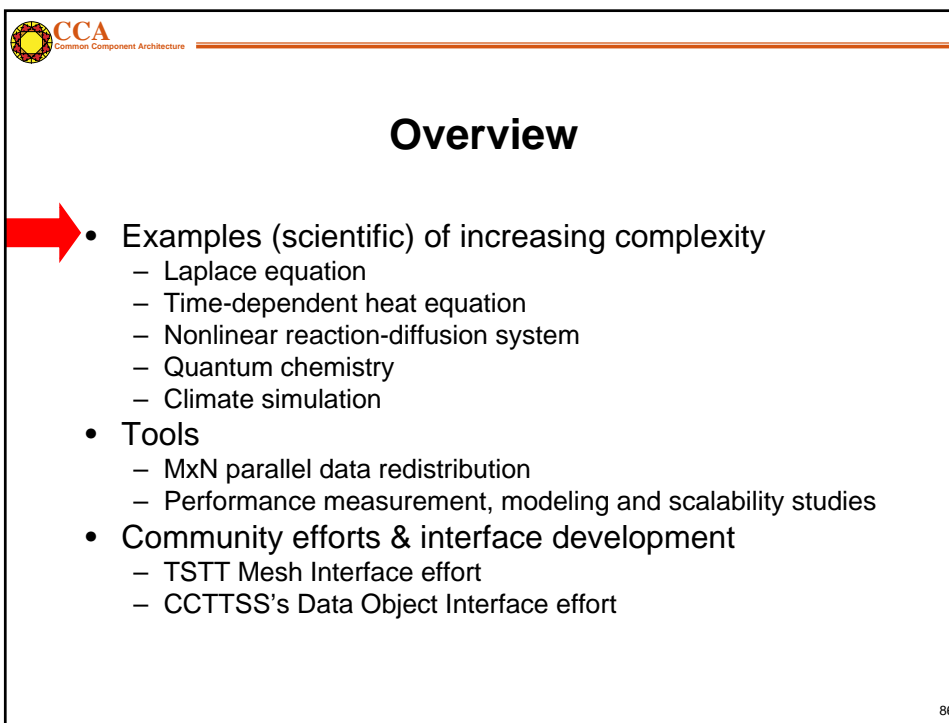
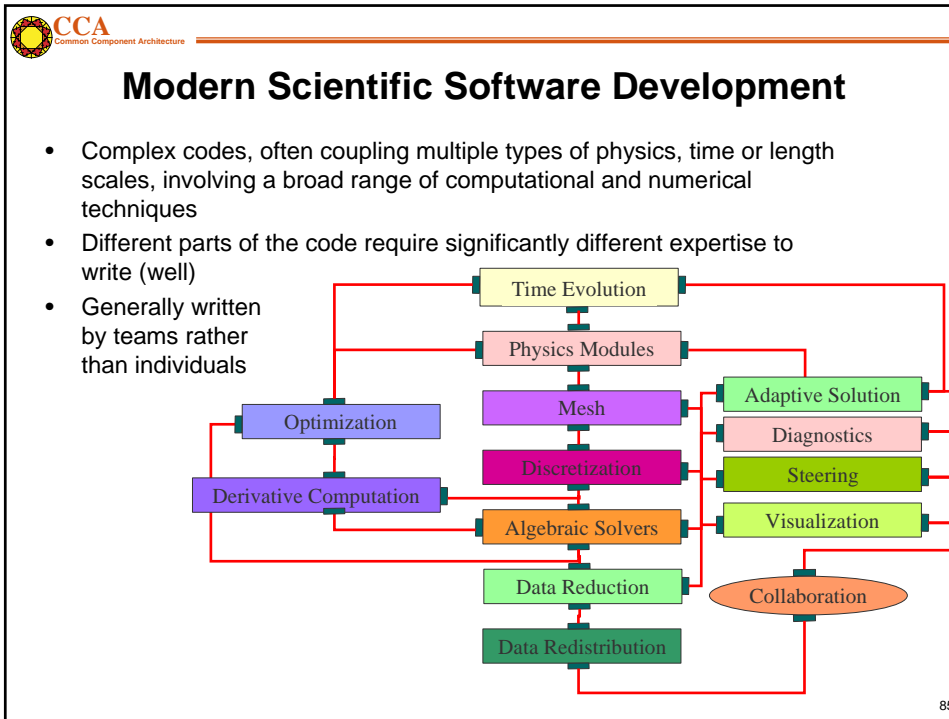
CCA
Common Component Architecture

CCA Applications

CCA Forum Tutorial Working Group

<http://www.cca-forum.org/tutorials/>
tutorial-wg@cca-forum.org

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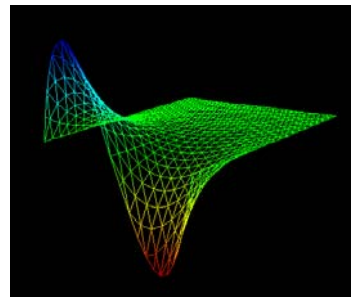
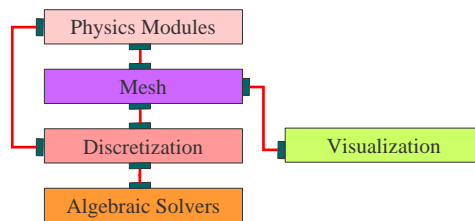
Common Component Architecture

Laplace Equation

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

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

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



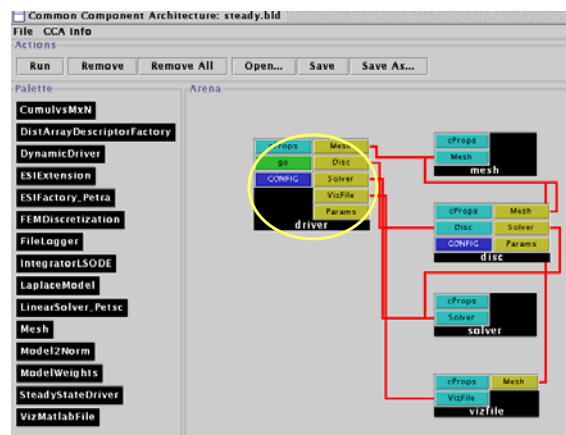
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Common Component Architecture

Laplace Equation with Components

- 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

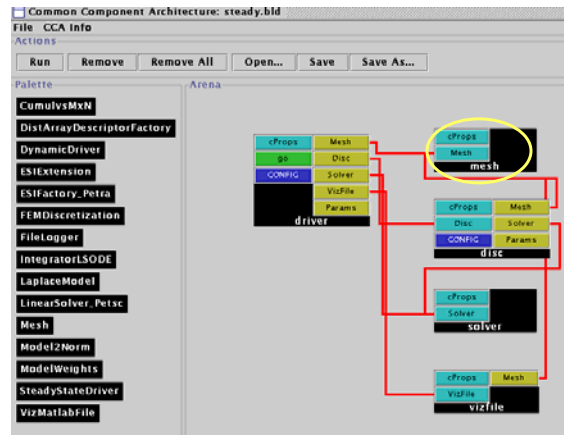


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Laplace Equation with Components

- The Driver
 - 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

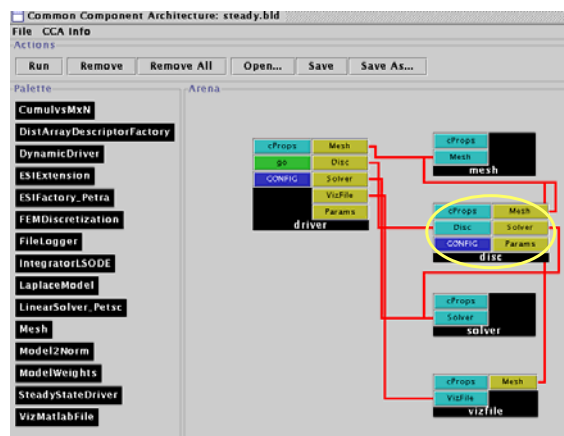


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Laplace Equation with Components

- The Driver
 - The Mesh
 - The Discretization Component
 - Provides a finite element discretization of basic operators (gradient, Laplacian, scalar terms)
 - Driver determines which terms are included and their coefficients
 - BC, Assembly etc



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CCA
Common Component Architecture

Laplace Equation with Components

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

Common Component Architecture: steady.bld

File CCA Info

Actions: Run Remove Remove All Open... Save Save As...

Palette: CumulusMxN, DistArrayDescriptorFactory, DynamicDriver, ESExtension, ESFactory_Petra, FEMDiscretization, FileLogger, IntegratorLSODE, LaplaceModel, LinearSolver_Petsc, Mesh, Model2Norm, ModelWeights, SteadyStateDriver, VizMatlabFile

Arena: driver, Mesh, Disc, Solver, VizFile

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CCA
Common Component Architecture

Laplace Equation with Components

- The Driver
- The Mesh
- The Discretization
- The Solver
- 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

Common Component Architecture: steady.bld

File CCA Info

Actions: Run Remove Remove All Open... Save Save As...

Palette: CumulusMxN, DistArrayDescriptorFactory, DynamicDriver, ESExtension, ESFactory_Petra, FEMDiscretization, FileLogger, IntegratorLSODE, LaplaceModel, LinearSolver_Petsc, Mesh, Model2Norm, ModelWeights, SteadyStateDriver, VizMatlabFile

Arena: driver, Mesh, Disc, Solver, VizFile

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CCA
Common Component Architecture

Time-Dependent Heat Equation

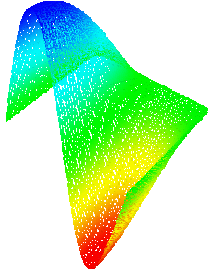
$$\delta\phi/\delta t = \nabla^2\phi \quad (x,y,t) \in [0,1] \times [0,1]$$
$$\phi(0,y,t)=0 \quad \phi(1,y,t)=.5\sin(2\pi y)\cos(t/2)$$
$$\delta\phi/\delta y(x,0) = \delta\phi/\delta y(x,1) = 0$$
$$\phi(x,y,0)=\sin(.5\pi x) \sin(2\pi y)$$


Diagram illustrating the components of the Time-Dependent Heat Equation solver:

- Time Evolution
- Physics Modules
- Mesh
- Discretization
- Algebraic Solvers
- Distributed Arrays
- Data Redistribution
- Visualization

The components are interconnected in a flow from top to bottom, with a feedback loop from Visualization back to Discretization. Distributed Arrays and Data Redistribution are connected to the bottom of the main flow.

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CCA
Common Component Architecture

Some things change...

- Requires a time integration component
 - Based on the LSODE library
- Uses a new visualization component
 - Based on AVS
- The visualization component requires a Distributed Array Descriptor component
 - Similar to HPF arrays
- The driver component changes to accommodate the new physics

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 Common Component Architecture

... and some things stay the same

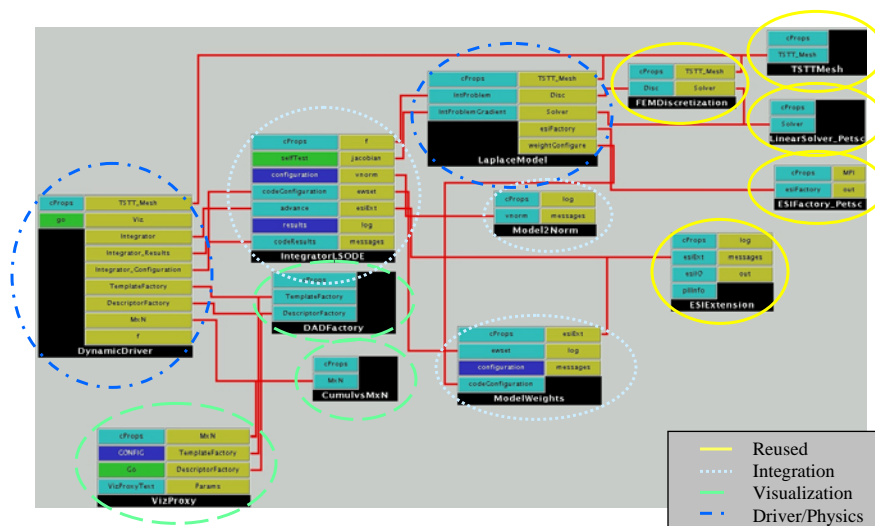
- The mesh component doesn't change
- The discretization component doesn't change
- The solver component doesn't change
 - What we use from the solver component changes
 - Only vectors are needed

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Common Component Architecture

Heat Equation Wiring Diagram



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What did this exercise teach us?

- Easy to incorporate the functionalities of components developed at other labs and institutions given a well-defined interface.
 - 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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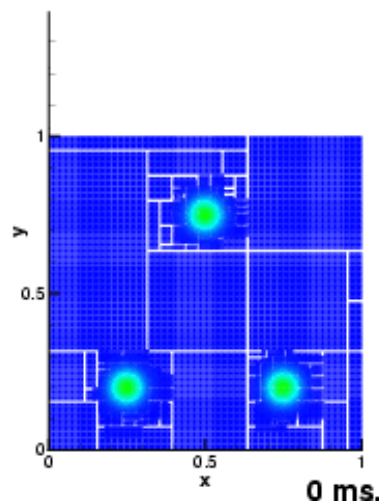
Nonlinear Reaction-Diffusion Equation

Temperature (K)

- 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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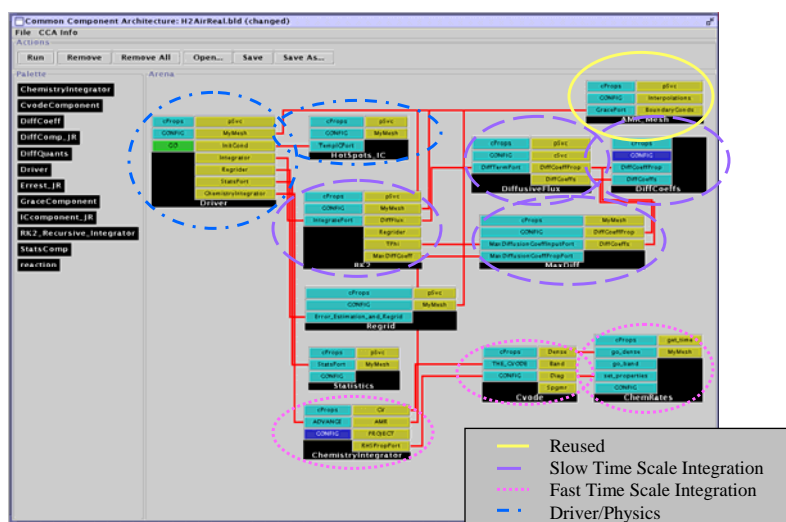
Numerical Solution

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

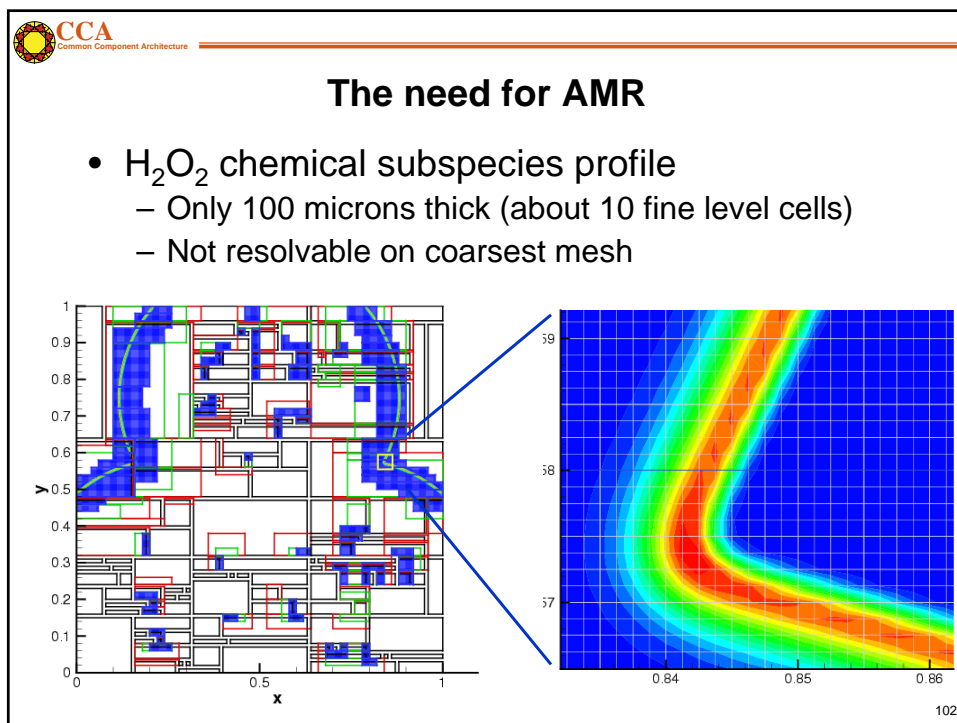
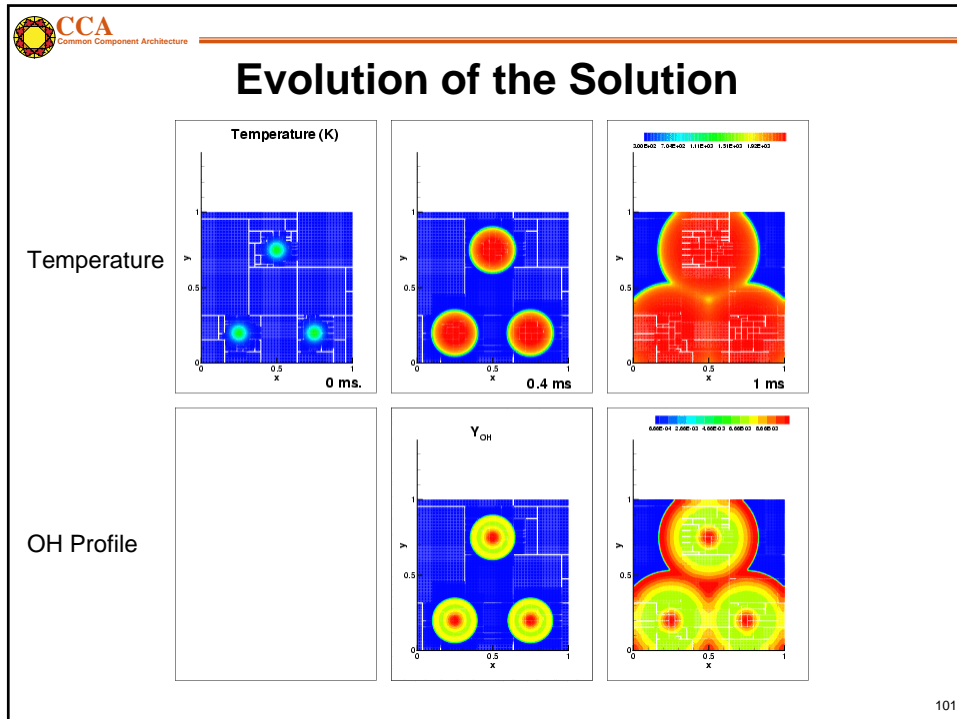
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Reaction-Diffusion Wiring Diagram

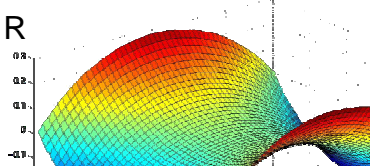


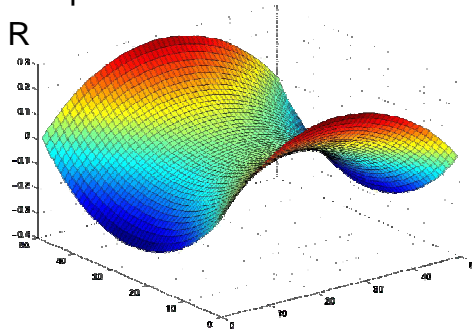
100





Unconstrained Minimization Problem

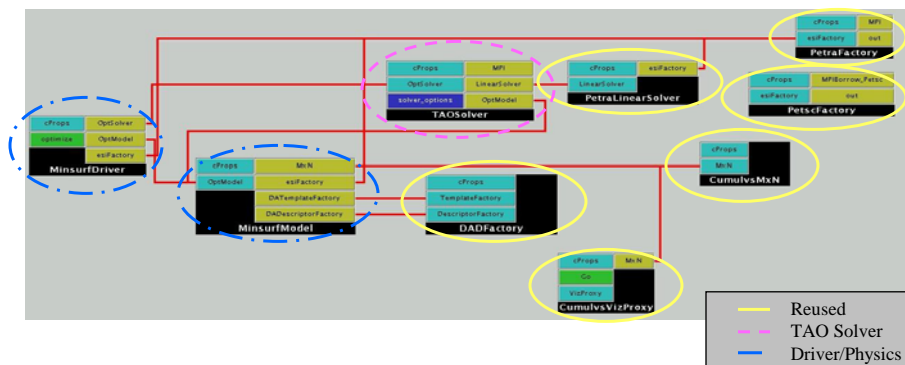
- Given a rectangular 2-dimensional domain and boundary values along the edges of the domain
 - Find the surface with minimal area that satisfies the boundary conditions, i.e., compute $\min f(x)$, where $f: \mathbb{R} \rightarrow \mathbb{R}$
 - Solve using optimization components based on TAO (ANL)
- 



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Unconstrained Minimization Using a Structured Mesh

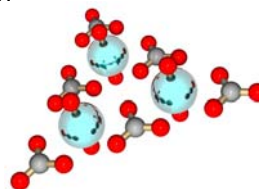


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Computational Chemistry: Molecular Optimization

- **Investigators:** Yuri Alexeev (PNNL), Steve Benson (ANL), Curtis Janssen (SNL), Joe Kenny (SNL), Manoj Krishnan (PNNL), Lois McInnes (ANL), Jarek Nieplocha (PNNL), Jason Sarich (ANL), Theresa Windus (PNNL)
- **Goals:** Demonstrate interoperability among software packages, develop experience with large existing code bases, seed interest in chemistry domain
- **Problem Domain:** Optimization of molecular structures using quantum chemical methods

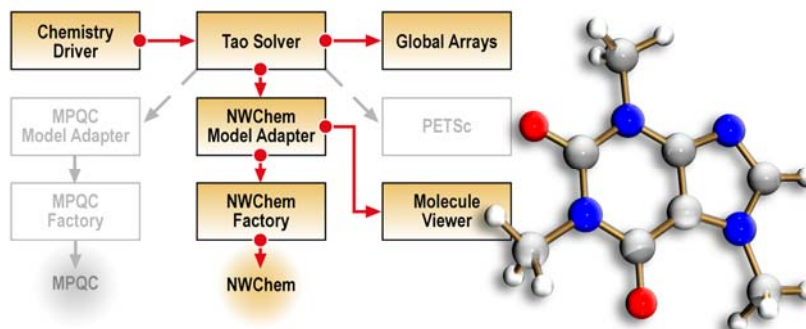


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Molecular Optimization Overview

- Decouple geometry optimization from electronic structure
- Demonstrate interoperability of electronic structure components
- Build towards more challenging optimization problems, e.g., protein/ligand binding studies



Components in gray can be swapped in to create new applications with different capabilities.

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CCA
Common Component Architecture

Wiring Diagram for Molecular Optimization

- Electronic structures components:
 - MPQC (SNL)
<http://aros.ca.sandia.gov/~cljanss/mpqc>
 - NWChem (PNNL)
<http://www.emsl.pnl.gov/pub/docs/nwchem>
- Optimization components: TAO (ANL)
<http://www.mcs.anl.gov/tao>
- Linear algebra components:
 - Global Arrays (PNNL)
<http://www.emsl.pnl.gov:2080/docs/global/ga.html>
 - PETSc (ANL)
<http://www.mcs.anl.gov/petsc>

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CCA
Common Component Architecture

Actual Improvements

Molecule	NWChem	NWChem/TAO	MPQC	MPQC/TAO
Glycine	33	19	26	19
Isoprene	56	45	75	43
Phosposerine	79	67	85	62
Aspirin	43	51	54	48
Cholesterol	33	30	27	30

Function and gradient evaluations

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Componentized Climate Simulations

- NASA's ESMF project has a component-based design for Earth system simulations
 - ESMF components can be assembled and run in CCA compliant frameworks such as Ccaffeine.
- Zhou et al (NASA Goddard) has integrated a simple coupled Atmosphere-Ocean model into Ccaffeine and is working on the Cane-Zebiak model, well-known for predicting *El Nino* events.
- Different PDEs for ocean and atmosphere, different grids and time-stepped at different rates.
 - Synchronization at ocean-atmosphere interface; essentially, interpolations between meshes
 - Ocean & atmosphere advanced in sequence
- Intuitively : Ocean, Atmosphere and 2 coupler components
 - 2 couplers : atm-ocean coupler and ocean-atm coupler.
 - Also a Driver / orchestrator component.

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Coupled Atmosphere-Ocean Model Assembly

• Climate Component :

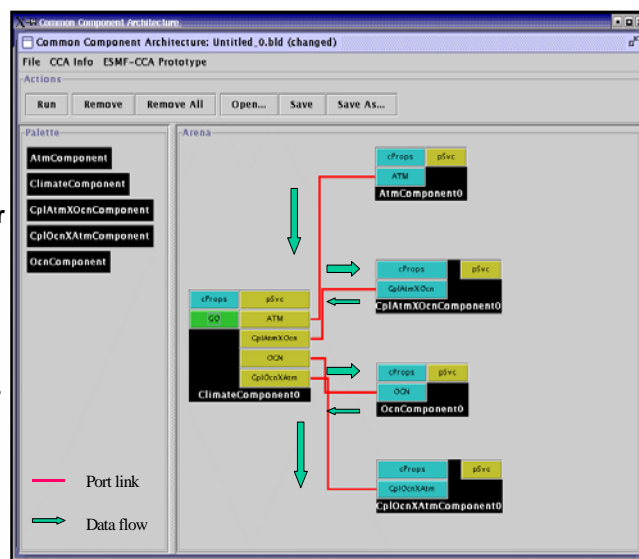
- Schedule component coupling

• Data flow is via pointer NOT data copy.

- All components in C++; run in CCAFFEINE.

• Multiple ocean models with the same interface

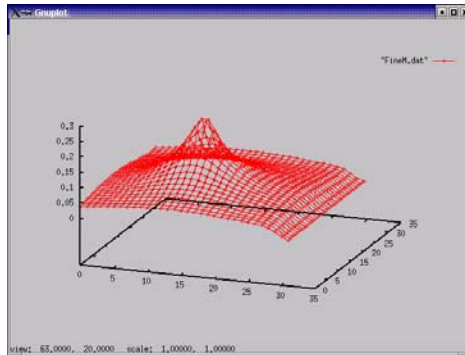
- Can be selected by a user at runtime



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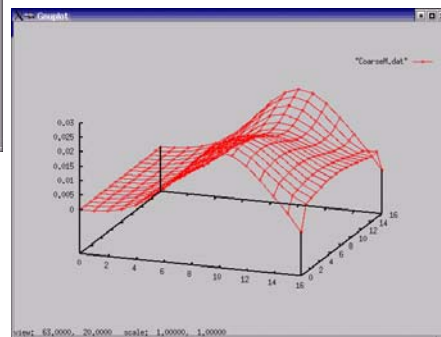


Simulation Results



A non-uniform ocean field variable
(e.g., current)

...changes a field variable (e.g., wind)
in the atmosphere !

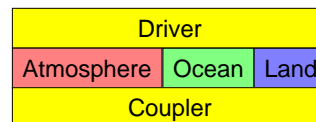


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Concurrency At Multiple Granularities

- Certain simulations need multi-granular concurrency
 - Multiple Component Multiple Data, multi-model runs
- Usage Scenarios:
 - Model coupling (e.g. Atmosphere/Ocean)
 - General multi-physics applications
 - Software licensing issues
- Approaches
 - Run single parallel framework
 - Driver component that partitions processes and builds rest of application as appropriate (through BuilderService)
 - Run multiple parallel frameworks
 - Link through specialized communications components
 - Link as components (through AbstractFramework service; highly experimental at present)



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Overview

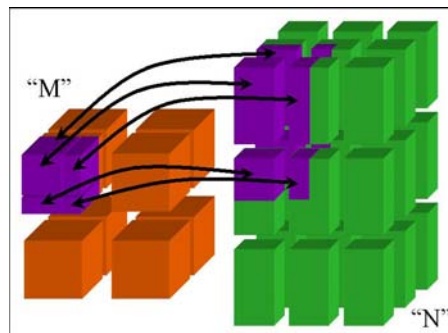
- Examples (scientific) of increasing complexity
 - Laplace equation
 - Time-dependent heat equation
 - Nonlinear reaction-diffusion system
 - Quantum chemistry
 - Climate simulation
- • Tools
 - MxN parallel data redistribution
 - Performance measurement, modeling and scalability studies
- Community efforts & interface development
 - TSTT Mesh Interface effort
 - CCTSS's Data Object Interface effort

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“MxN” Parallel Data Redistribution: The Problem...

- Create complex scientific simulations by coupling together multiple parallel component models
 - Share data on “M” processors with data on “N”
 - $M \neq N \sim$ Distinct Resources (Pronounced “M by N”)
 - Model coupling, e.g., climate, solver / optimizer
 - Collecting data for visualization
 - Mx1; increasingly MxN (parallel rendering clusters)
- Define common interface
 - Fundamental operations for any parallel data coupler
 - Full range of synchronization and communication options



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Hierarchical MxN Approach

- Basic MxN Parallel Data Exchange
 - Component implementation
 - Initial prototypes based on CUMULVS & PAWS
 - Interface generalizes features of both
- Higher-Level Coupling Functions
 - Time & grid (spatial) interpolation, flux conservation
 - Units conversions...
- “Automatic” MxN Service via Framework
 - Implicit in method invocations, “parallel RMI”



<http://www.csm.ornl.gov/cca/mxn/>

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CCA Delivers Performance

Local

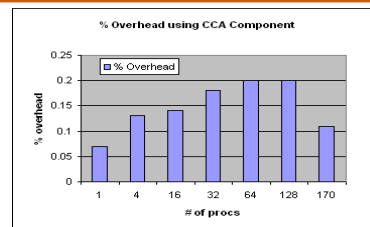
- No CCA overhead *within* components
- Small overhead *between* components
- Small overhead for *language interoperability*
- Be aware of costs & design with them in mind
 - Small costs, easily amortized

Parallel

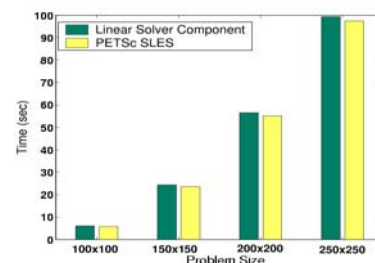
- No CCA overhead on *parallel computing*
- Use *your favorite* parallel programming model
- Supports SPMD and MPMD approaches

Distributed (remote)

- No CCA overhead – performance depends on networks, protocols
- CCA frameworks support OGSA/Grid Services/Web Services and other approaches



Maximum 0.2% overhead for CCA vs native C++ code for parallel molecular dynamics up to 170 CPUs



Aggregate time for linear solver component in unconstrained minimization problem w/ PETSc

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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

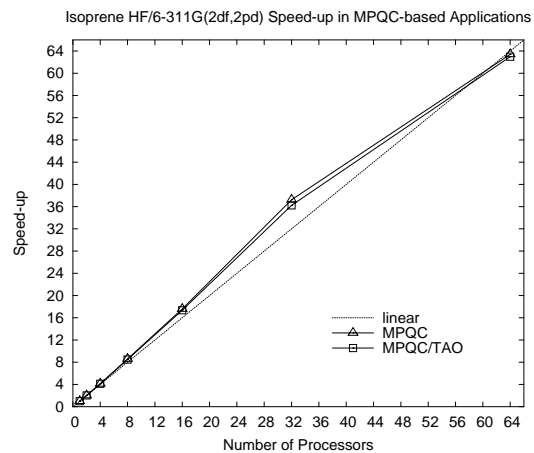
Function arg type	f77	Component
Array	80 ns	224ns
Complex	75ns	209ns
Double complex	86ns	241ns

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Scalability : Component versus Non-component. I

- QC simulation
- Sandia's MPQC code
 - Both componentized and non-componentized versions
- Componentized version used TAO's optimization algorithms
- Problem :Structure of isoprene HF/6-311G(2df,2pd)



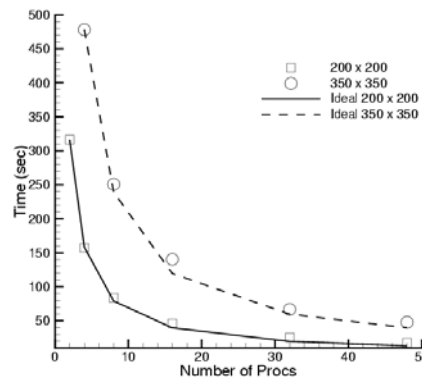
Parallel Scaling of MPQC w/ native and TAO optimizers

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Scalability : Component versus Non-component. II

- Hydrodynamics; uses CFRFS set of components
- Uses GrACEComponent
- Shock-hydro code with no refinement
- 200 x 200 & 350 x 350 meshes
- Cplant cluster
 - 400 MHz EV5 Alphas
 - 1 Gb/s Myrinet
- Negligible component overhead
- Worst perf : 73% scaling efficiency for 200x200 mesh on 48 procs



Reference: S. Lefantzi, J. Ray, and H. Najm, Using the Common Component Architecture to Design High Performance Scientific Simulation Codes, *Proc of Int. Parallel and Distributed Processing Symposium*, Nice, France, 2003.

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Performance Measurement In A Component World

- CCA provides a novel means of profiling & modeling **component** performance
- Need to collect incoming inputs and match them up with the corresponding performance, but how ?
 - Need to “instrument” the code
 - But has to be non-intrusive, since we may not “own” component code
- What kind of performance infrastructure can achieve this?
 - Previous research suggests proxies
 - Proxies serve to intercept and forward method calls

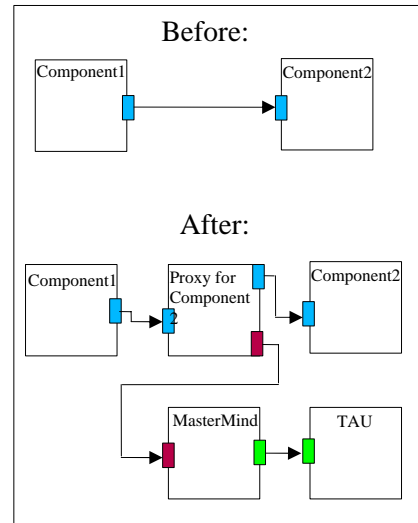
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“Integrated” Performance Measurement Capability

Measurement infrastructure:

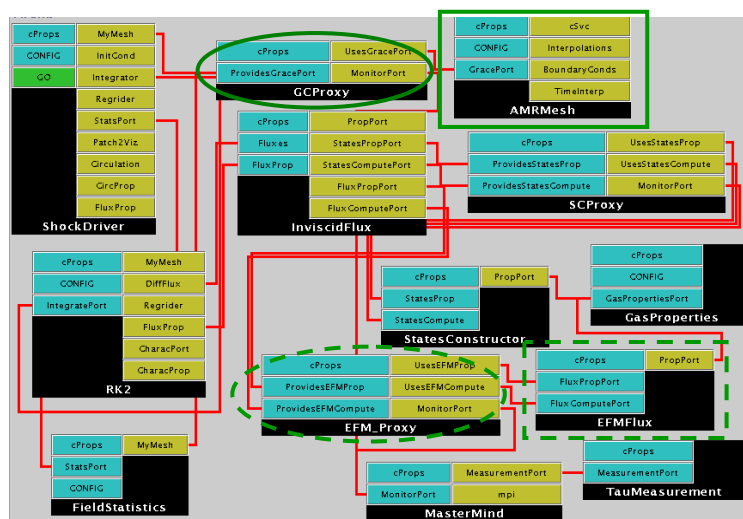
- **Proxy**
 - Notifies MasterMind of all method invocations of a given component, along with performance dependent inputs
 - Generated automatically using PDT
- **MasterMind**
 - Collects and stores all measurement data
- **TAU**
 - Makes all performance measurements



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Component Application With Proxies



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Overview

- Examples (scientific) of increasing complexity
 - Laplace equation
 - Time-dependent heat equation
 - Nonlinear reaction-diffusion system
 - Quantum chemistry
 - Climate simulation
- Tools
 - MxN parallel data redistribution
 - Performance measurement, modeling and scalability studies
- • Community efforts & interface development
 - TSTT Mesh Interface effort
 - CCTSS's Data Object Interface effort

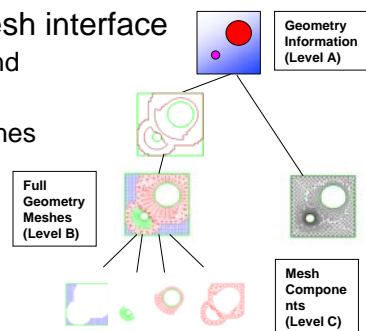
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The Next Level



- 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



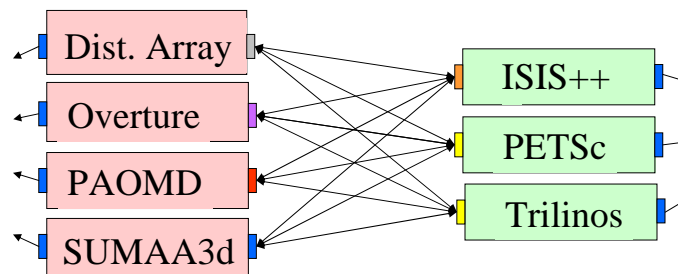
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Proliferations of interfaces – the N^2 problem

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



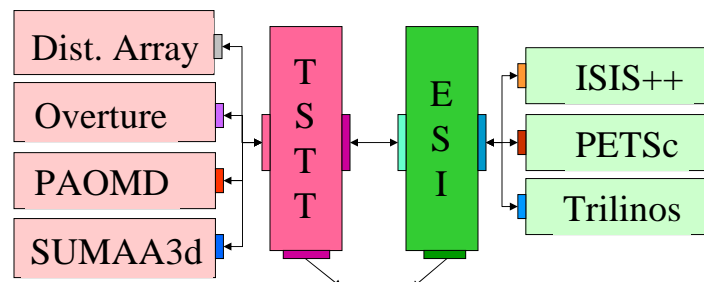
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Common Interface Specification

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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Common Component Architecture

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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Common Component Architecture



CCTTSS Research Thrust Areas and Main Working Groups

- Scientific Components
Lois Curfman McInnes, ANL (curfman@mcs.anl.gov)
- “MxN” Parallel Data Redistribution
Jim Kohl, ORNL (kohlja@ornl.gov)
- Frameworks
 - Language Interoperability / Babel / SIDL
Gary Kumfert, LLNL (kumfert@llnl.gov)
- User Outreach
David Bernholdt, ORNL (bernholdtde@ornl.gov)

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CCA
Common Component Architecture

Summary

- Complex applications that use components are possible
 - Combustion
 - Chemistry applications
 - Optimization problems
 - Climate simulations
- 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, LSODE, 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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CCA
Common Component Architecture

Language Interoperable CCA Components via



CCA Forum Tutorial Working Group

<http://www.cca-forum.org/tutorials/>
tutorial-wg@cca-forum.org

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Common Component Architecture

Goal of This Module

Legacy codes → Babelized CCA Components

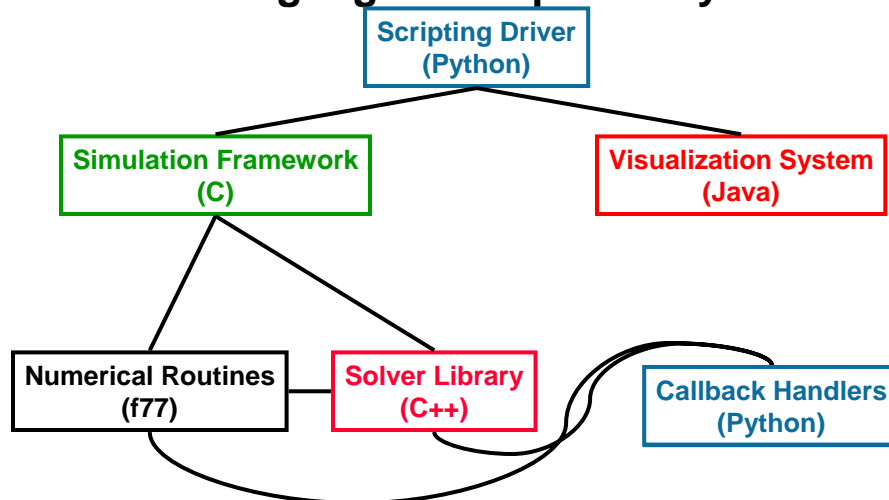
- Introduction To:
 - Babel
 - SIDL
- See Babel in use
 - “Hello World” example
- Babel aspects of writing a CCA component

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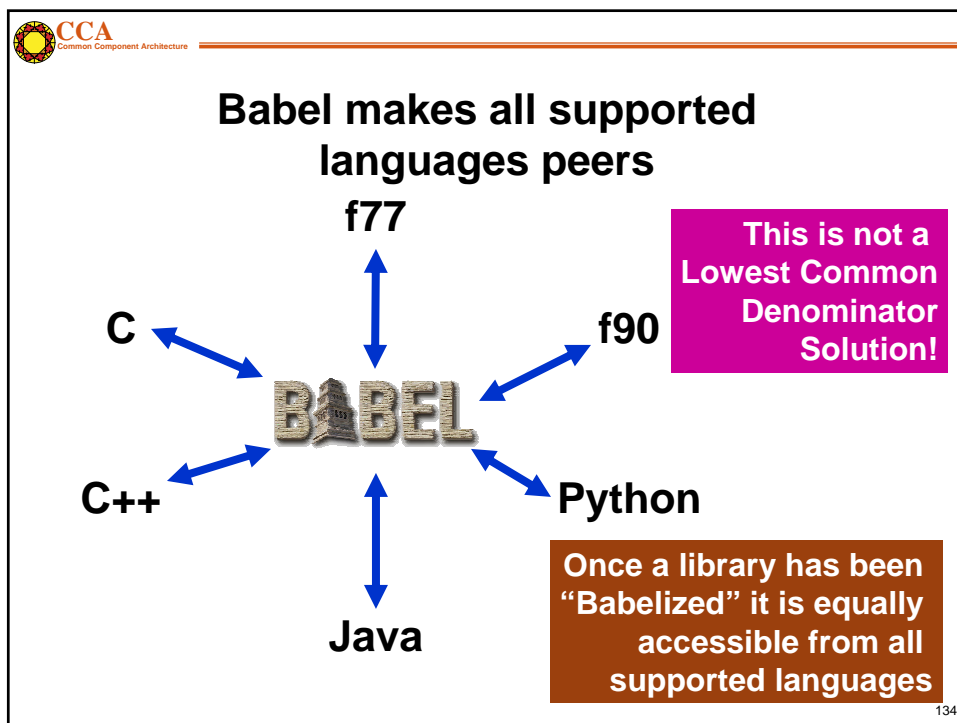
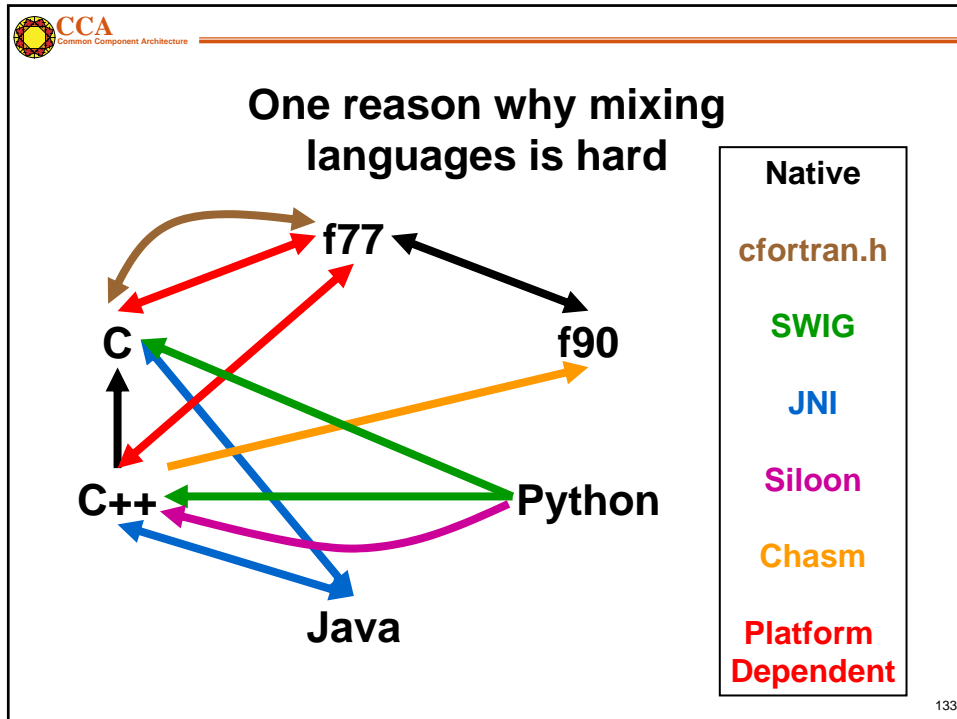



Common Component Architecture

What I mean by “Language Interoperability”



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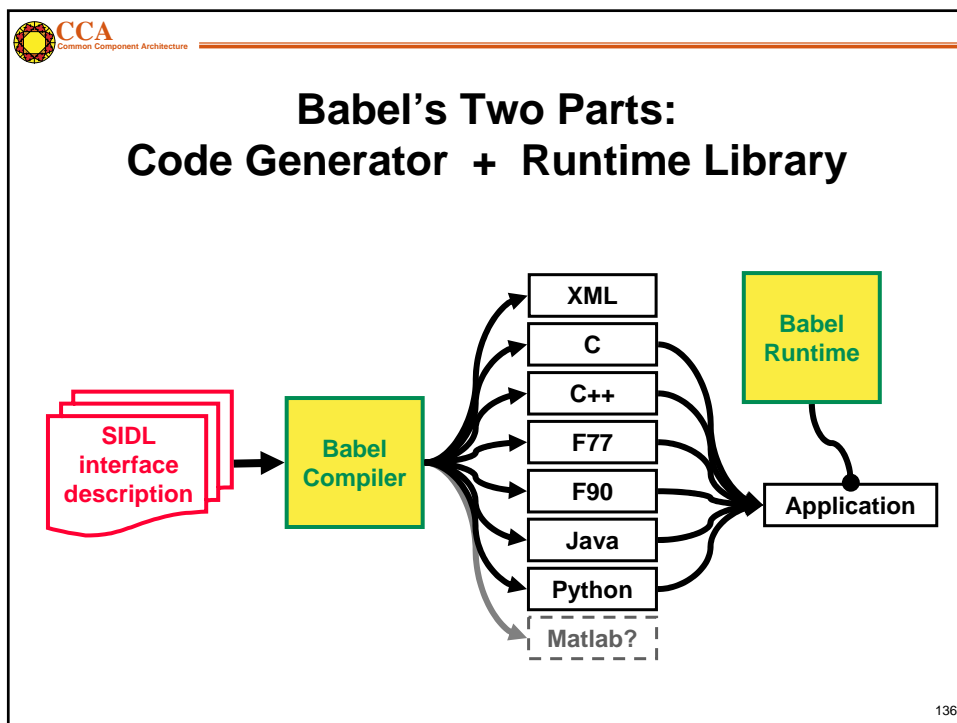


 **CCA**
Common Component Architecture

Babel Module's Outline

- Introduction
- **Babel Basics**
 - How to use Babel in a “Hello World” Example
 - SIDL Grammar
 - Wrapping legacy code
- Babel aspects of writing a CCA component

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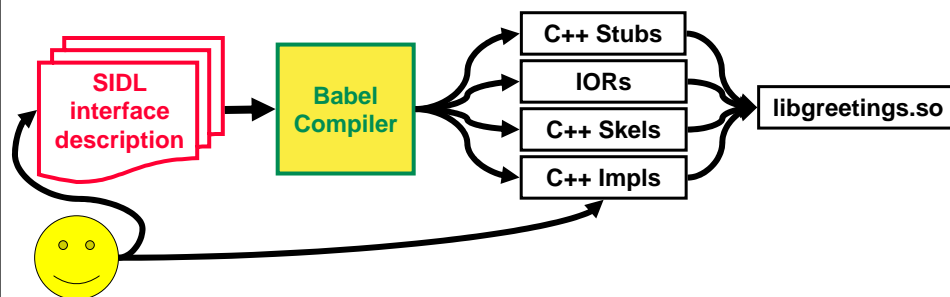
greetings.sidl: A Sample SIDL File

```
package greetings version 1.0 {  
  interface Hello {  
    void setName( in string name );  
    string sayIt ( );  
  }  
  class English implements-all Hello { }  
}
```

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Library Developer Does This...



1. `babel --server=C++ greetings.sidl`
2. Add implementation details
3. Compile & Link into Library/DLL

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CCA
Common Component Architecture

Adding the Implementation

```
namespace greetings {
class English_impl {
private:
    // DO-NOT-DELETE spl i cer. begi n(greeti ngs. Engl i sh. _i mpl )
    string d_name;
    // DO-NOT-DELETE spl i cer. end(greeti ngs. Engl i sh. _i mpl )

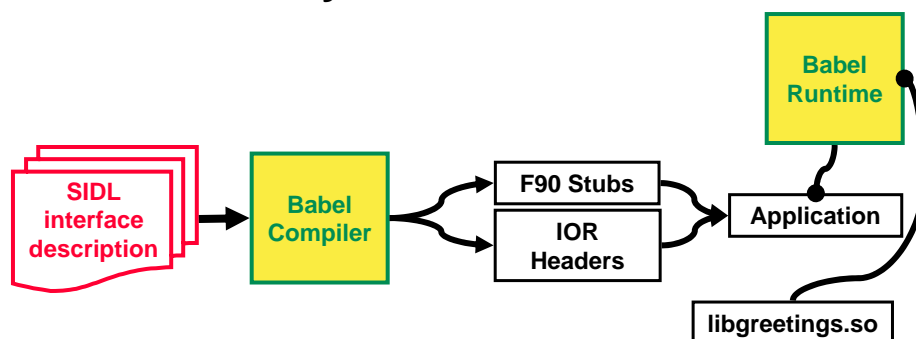
string
greeti ngs::Engl i sh_i mpl::sayl t()
throw ()
{
    // DO-NOT-DELETE spl i cer. begi n(greeti ngs. Engl i sh. sayl t)
    string msg("Hello ");
    return msg + d_name + "!";
    // DO-NOT-DELETE spl i cer. end(greeti ngs. Engl i sh. sayl t)
}
```

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Common Component Architecture

Library User Does This...



1. `babel --client=F90 greetings.sidl`
2. Compile & Link generated Code & Runtime
3. Place DLL in suitable location

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F90/Babel “Hello World” Application

```

program hellocient
  use greetings_English
  implicit none
  type(greetings_English_t) :: obj
  character (len=80)          :: msg
  character (len=20)          :: name

  name=' World'
  call new( obj )
  call setName( obj, name )
  call sayIt( obj, msg )
  call deleteRef( obj )
  print *, msg
end program hellocient

```

These subroutines
come from directly
from the SIDL

Some other subroutines
are “built in” to every
SIDL class/interface



SIDL Grammar (1/3): Packages and Versions

You'll use
SIDL in the
hands-on

- Packages can be nested

```
package foo version 0.1 { package bar { ... } }
```

- Versioned Packages
 - defined as packages with explicit version number
OR packages enclosed by a versioned package
 - Reentrant by default, but can be declared final
 - May contain interfaces, classes, or enums
- Unversioned Packages
 - Can only enclose more packages, not types
 - Must be re-entrant. Cannot be declared final



SIDL Grammar (2/3): Classes & Interfaces

- SIDL has 3 user-defined objects
 - **Interfaces** – APIs only, no implementation
 - **Abstract Classes** – 1 or more methods unimplemented
 - **Concrete Classes** – All methods are implemented
- Inheritance (like Java/Objective C)
 - Interfaces may **extend** Interfaces
 - Classes **extend** no more than one Class
 - Classes can **implement** multiple Interfaces
- Only concrete classes can be instantiated

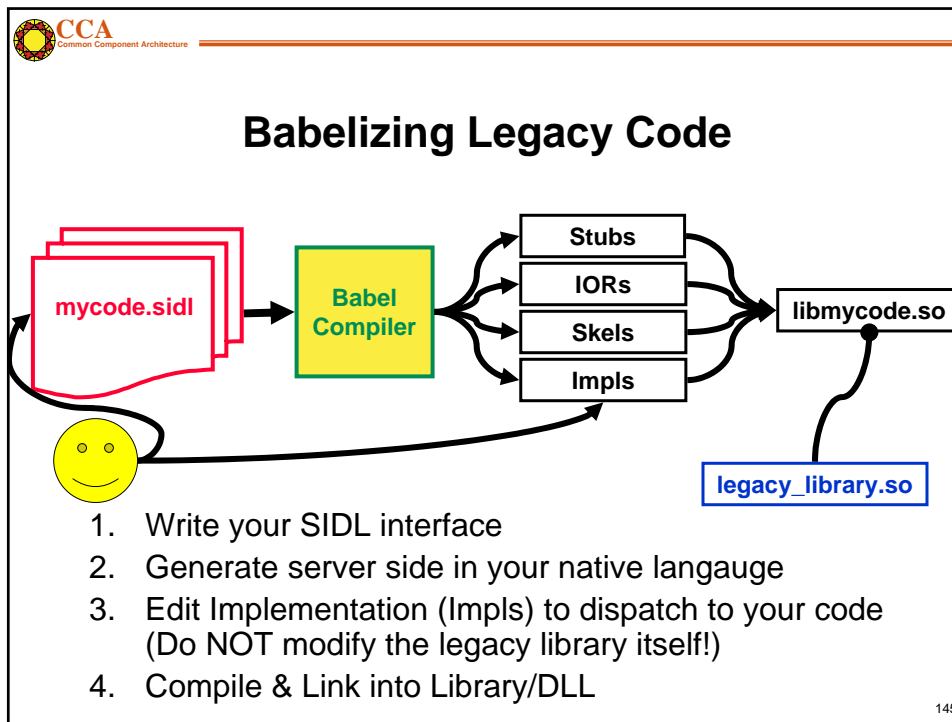
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SIDL Grammar (3/3): Methods and Arguments

- Methods are **public virtual** by default
 - **static** methods are not associated with an object instance
 - **final** methods can not be overridden
- Arguments have 3 parts
 - Mode: can be **in**, **out**, or **inout** (like CORBA, but semantically different than F90)
 - Type: one of (bool, char, int, long, float, double, fcomplex, dcomplex, array<*Type*,*Dimension*>, enum, interface, class)
 - Name

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Known Projects Using Babel
(see www.llnl.gov/CASC/components/gallery.html for more)

ALPS

research.cs.vt.edu/lacsa

I implemented a Babel-based interface for the hydre library of linear equation solvers. The Babel interface was straightforward to write and gave us interfaces to several languages for less effort than it would take to interface to a single language.

--Jeff Painter, LLNL.

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Investing in Babelization can **improve** the interface to the code.


“When Babelizing LEOS [an equation of state library at LLNL], I completely ignored the legacy interface and wrote the SIDL the way I thought the interface should be. After running Babel to generate the code, I found all the hooks I needed to connect LEOS without changing any of it. Now I’ve got a clean, new, object-oriented python interface to legacy code. Babel is doing much more than just wrapping here.”

-- Charlie Crabb, LLNL
(conversation)

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Babel Module’s Outline

- Introduction
 - Babel Basics
 - How to use Babel in a “Hello World” Example
 - SIDL Grammar
-  Babel aspects of writing a CCA component

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CCA
Common Component Architecture

How to Write and Use Babelized CCA Components

1. Define “Ports” in SIDL
2. Define “Components” that implement those Ports, again in SIDL
3. Use Babel to generate the glue-code
4. Write the guts of your component(s)

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CCA
Common Component Architecture

How to Write A Babelized CCA Component (1/3)

1. Define “Ports” in SIDL
 - CCA Port =
 - a SIDL Interface
 - extends gov.cca.Port

```
package functions version 1.0 {  
  interface Function extends gov.cca.Port {  
    double evaluate( in double x );  
  }  
}
```

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How to Write A Babelized CCA Component (2/3)

2. Define “Components” that implement those Ports

- CCA Component =
 - SIDL Class
 - implements gov.cca.Component (& any provided ports)

```
class LinearFunction implements functions.Function,  
                                gov.cca.Component {  
    double evaluate( in double x );  
    void setServices( in cca.Services svcs );  
}
```

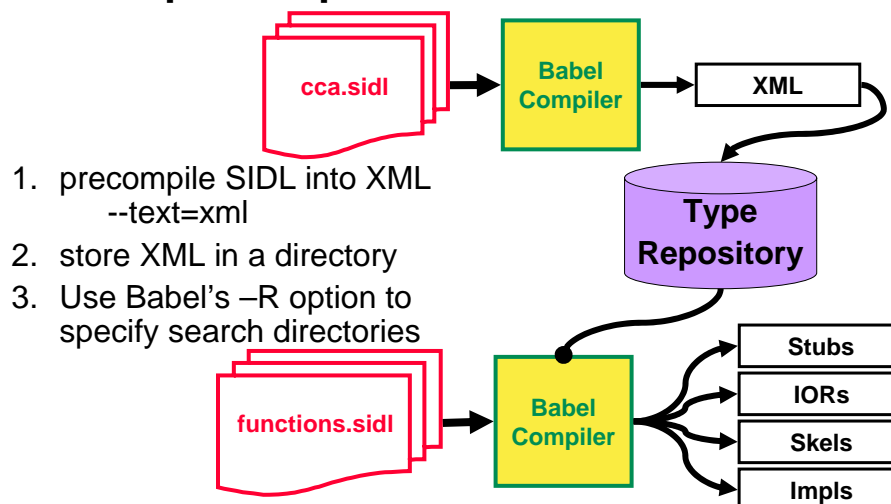
```
class LinearFunction implements-all  
    functions.Function, gov.cca.Component { }
```

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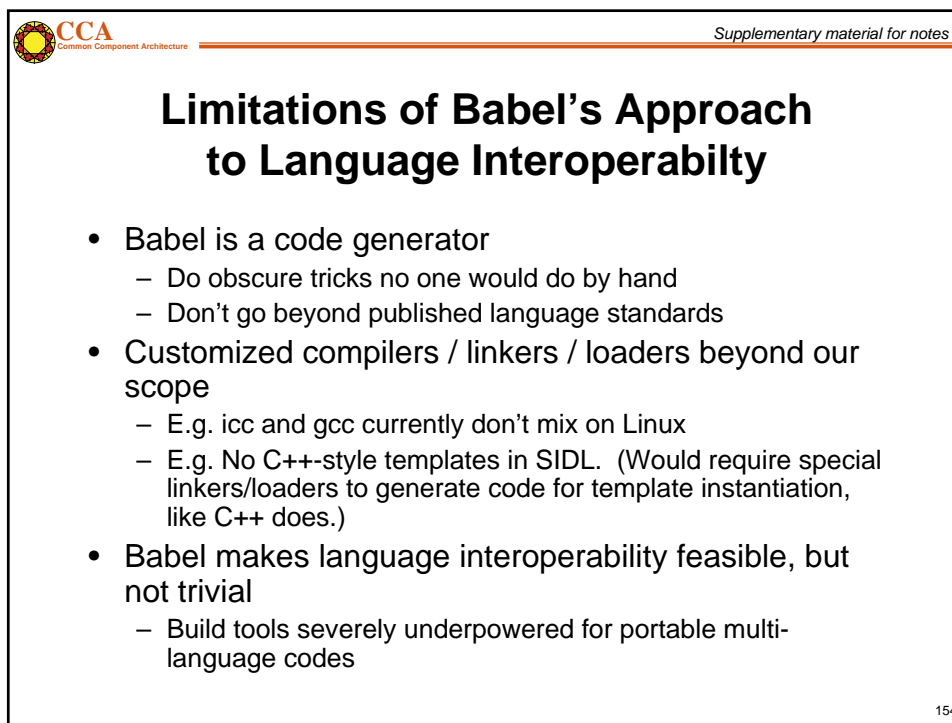
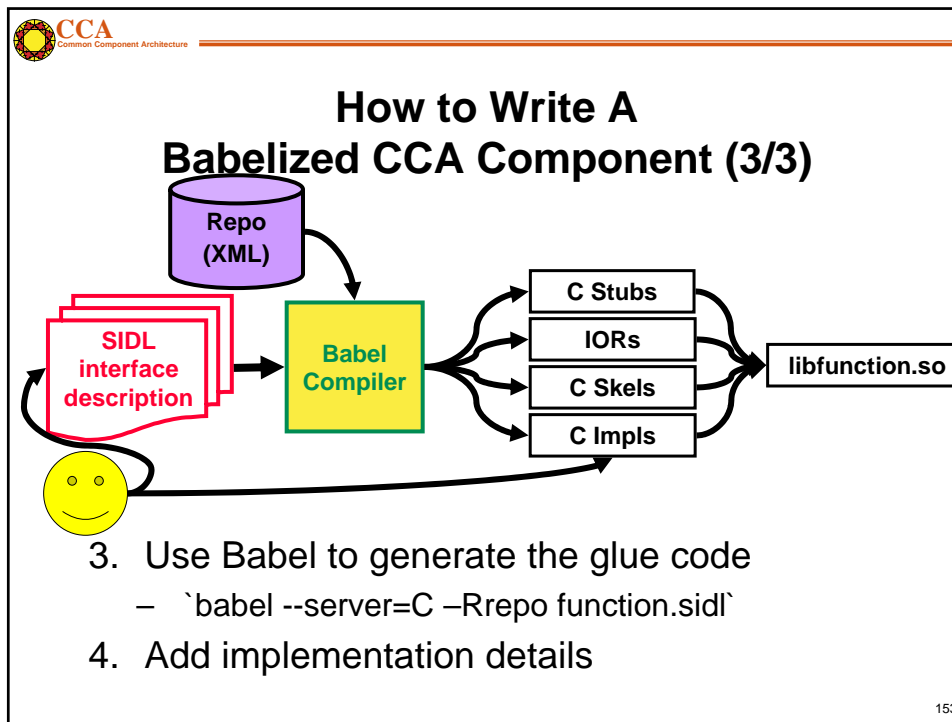


Supplementary material for notes

Tip: Use Babel's XML output like precompiled headers in C++



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Common Component Architecture

Contact Info

- Project: <http://www.llnl.gov/CASC/components>
 - Babel: language interoperability tool
 - Alexandria: component repository
 - Quorum: web-based parliamentary system
 - Gauntlet (coming soon): testing framework
- Bug Tracking: <http://www-casc.llnl.gov/bugs>
- Project Team Email: components@llnl.gov
- Mailing Lists: majordomo@lists.llnl.gov
 - subscribe babel-users *[email address]*
 - subscribe babel-announce *[email address]*