



CCA
Common Component Architecture

Welcome to the Common Component Architecture Tutorial

Eighth DOE ACTS Collection Workshop
24 August 2007

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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 - CCA Forum Tutorial Working Group, Common Component Architecture Tutorial, 2007, <http://www.cca-forum.org/tutorials/>



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 CCA Common Component Architecture			
<h2>Agenda & Table of Contents</h2>			
Time	Title	Slide No.	Presenter
9:30-9:35am	Welcome	1	David Bernholdt, ORNL
9:35-10:20am	What Can Component Technology do for Scientific Computing	5	David Bernholdt, ORNL
	An Intro to Components & the CCA	16	David Bernholdt, ORNL
10:20-10:40am	CCA Tools	71	Ben Allan, SNL
10:40-11:10am	Break		
11:10-11:40am	Language Interoperable CCA Components with Babel	108	Tom Epperly, LLNL
11:40am-12:25pm	Using CCA: Approaches & Experience	135	Jaideep Ray, SNL
12:25-12:30pm	Closing	182	Jaideep Ray, SNL
12:30-2:00pm	Lunch		
2:00-3:00pm	TAU hands-on (212 Wheeler, UCB)		
3:00-6:00pm	CCA hands-on (212 Wheeler, UCB)	Separate handouts	Rob Armstrong, SNL

 CCA Common Component Architecture	
<h2>Who We Are: The Common Component Architecture (CCA) Forum</h2>	
<ul style="list-style-type: none">• Combination of standards body and user group for the CCA• Define specifications for high-performance scientific components & frameworks• Promote and facilitate development of tools for component-based software development, components, and component applications• Open membership, quarterly meetings...	
General mailing list: cca-forum@cca-forum.org	
Web: http://www.cca-forum.org/	
<ul style="list-style-type: none">• Center for Technology for Advanced Scientific Component Software (TASCS)<ul style="list-style-type: none">– Funded by the US DOE SciDAC program– Core development team for CCA technologies	



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What Can Component Technology do for Scientific Computing?

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Managing Code Complexity

Some Common Situations:

- Your code is so large and complex it has become fragile and hard to keep running
- You have a simple code, and you want to extend its capabilities
 - rationally
- You want to develop a computational “toolkit”
 - Many modules that can be assembled in different ways to perform different scientific calculations
 - Gives users w/o programming experience access to a flexible tool for simulation
 - Gives users w/o HPC experience access to HPC-ready software

How CCA Can Help:

- Components help you think about software in manageable chunks that interact only in well-defined ways
- Components provide a “plug-and-play” environment that allows easy, flexible application assembly

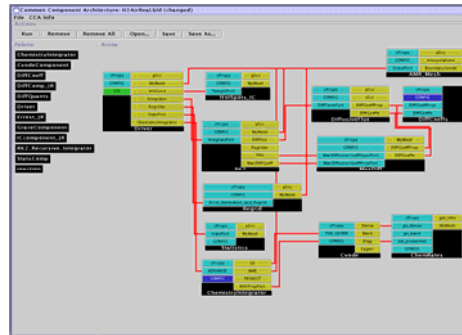


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Example: Computational Facility for Reacting Flow Science (CFRFS)

- A toolkit to perform simulations of unsteady flames
- Solve the Navier-Stokes with detailed chemistry
 - Various mechanisms up to ~50 species, 300 reactions
 - Structured adaptive mesh refinement
- CFRFS today:
 - 61 components
 - 7 external libraries
 - 9 contributors



“Wiring diagram” for a typical CFRFS simulation, utilizing 12 components.

CCA tools used: Ccaffeine, and ccafe-gui

Languages: C, C++, F77

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Helping Groups Work with Software

Some Common Situations:

- Many (geographically distributed) developers creating a large software system
 - Hard to coordinate, different parts of the software don't work together as required
- Groups of developers with different specialties
- Forming communities to standardize interfaces or share code

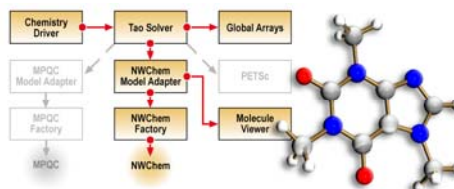
How CCA Can Help:

- Components are natural units for
 - Expressing software architecture
 - Individuals or small groups to develop
 - Encapsulating particular expertise
- Some component models (including CCA) provide tools to help you think about the *interface* separately from the *implementation*

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Example: Quantum Chemistry

- Integrated state-of-the-art optimization technology into two quantum chemistry packages to explore effectiveness in chemistry applications
- Geographically distributed expertise:
 - California - chemistry
 - Illinois - optimization
 - Washington – chemistry, parallel data management
- Effective collaboration with minimal face-to-face interaction



Schematic of CCA-based molecular structure determination quantum chemistry application.

Components based on: MPQC, NWChem (quantum chem.), TAO (optimization), Global Arrays, PETSc (parallel linear algebra)

CCA tools used: Babel, Ccaffeine, and ccafe-qui

Languages: C, C++, F77, Python

Example: TSTT Unstructured Mesh Tool Interoperability

- Common interface for unstructured mesh geometry and topology
 - 7 libraries: FMDB, Frontier, GRUMMP, Mesquite, MOAB, NWGrid, Overture
 - 6 institutions: ANL, BNL/SUNY-Stony Brook, LLNL, PNNL, RPI, SNL
- Reduces need for N^2 pairwise interfaces to just N

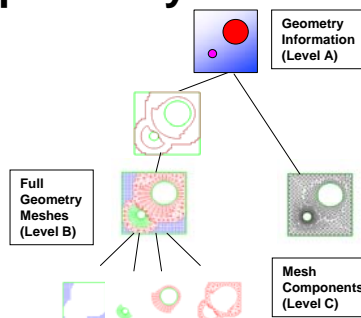


Illustration of geometry domain hierarchy used in TSTT mesh interface.

CCA tools used: Babel (SIDL), Chasm

Library languages: C, C++, F77, F90

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Language Interoperability

Some Common Situations:

- Need to use existing code or libraries written in multiple languages in the same application?
- Want to allow others to access your library from multiple languages?
- Technical or sociological reasons for wanting to use multiple languages in your application?

How CCA Can Help:

- Some component models (including CCA) allow transparent mixing of languages
- Babel (CCA's language interop. tool) can be used separately from other component concepts



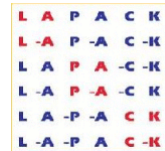
hypre

- High performance preconditioners and linear solvers
- Library written in C
- Babel-generated object-oriented interfaces provided in C, C++, Fortran

Examples

LAPACK07

- Update to LAPACK linear algebra library
 - To be released 2007
 - Library written in F77, F95
- Will use Babel-generated interfaces for: C, C++, F77, F95, Java, Python
- Possibly also ScaLAPACK (distributed version)



"I implemented a Babel-based interface for the hypre 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. 2 June 2003

CCA tools used: Babel, Chasm





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Coupling Codes

Some Common Situations:

- Your application makes use of numerous third-party libraries
 - Some of which interact (version dependencies)
- You want to develop a simulation in which your code is coupled with others
 - They weren't designed with this coupling in mind
 - They must remain usable separately too
 - They are all under continual development, individually
 - They're all parallel and need to exchange data frequently

How CCA Can Help:

- Components are isolated from one another
 - Interactions via well-defined interfaces
 - An application can include multiple versions of a component
- Components can be composed flexibly, hierarchically
 - Standalone application as one assembly, coupled simulation as another
- CCA can be used in SPMD, MPMD, and distributed styles of parallel computing
- CCA is developing technology to facilitate data and functional coupling of parallel applications

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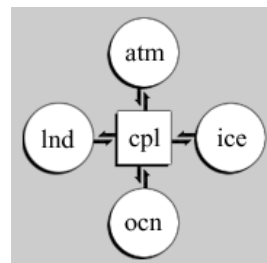


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Example: Global Climate Modeling and the Model Coupling Toolkit (MCT)



- MCT is the basis for Community Climate System Model (CCSM3.0) coupler (cpl6)
- Computes interfacial fluxes and manages redistribution of data among parallel processes
- Written in F90, Babel-generated bindings for C++, Python
- **CCA tools used:** Babel, Chasm



Schematic of CCSM showing coupler managing data exchanges between atmosphere, sea ice, ocean, and land models.
(From <http://www.cesm.ucar.edu/models/ccsm3.0/cpl6/>)

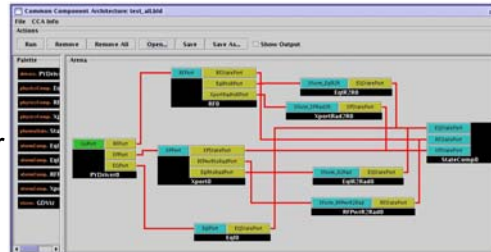
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Example: Integrated Fusion Simulation

- Proof-of-principle of using CCA for integrated whole-device modeling needed for the ITER fusion reactor
- Couples radio frequency (RF) heating of plasma with transport modeling
- Coarse-grain encapsulation of pre-existing programs
- Follow-on plans for RF, transport, and magneto-hydrodynamics



"Wiring diagram" for integrated fusion simulation.

Components based on: AORSA, Houlberg's transport library

New components: Driver, State

CCA tools used: Babel, Chasm, Ccaffeine, ccafe-gui

Languages: C++, F90, Python

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An Introduction to Components and the Common Component Architecture

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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
- Give you sufficient **understanding** of the CCA to begin **evaluating** whether it would be useful to you



What are Components?

- No universally accepted definition in computer science research, but key features include...
- 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**





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 components are composed to form an application and executed (**framework**)
 - The rights and responsibilities of the framework

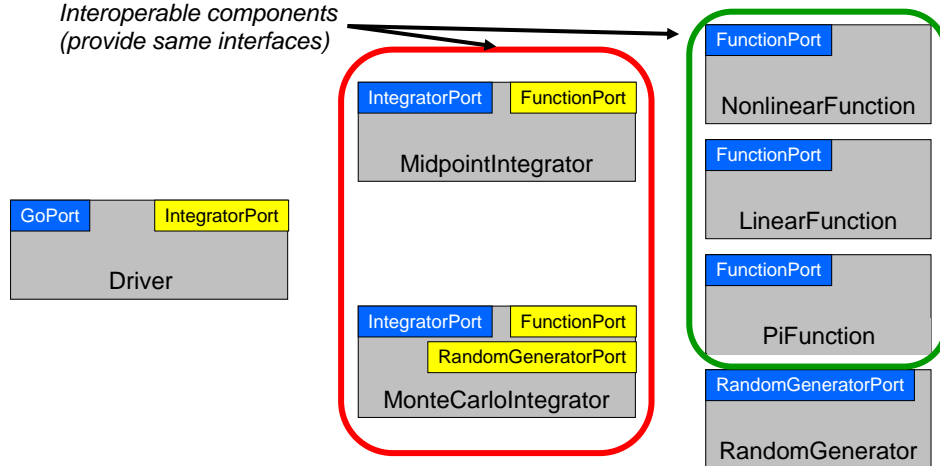


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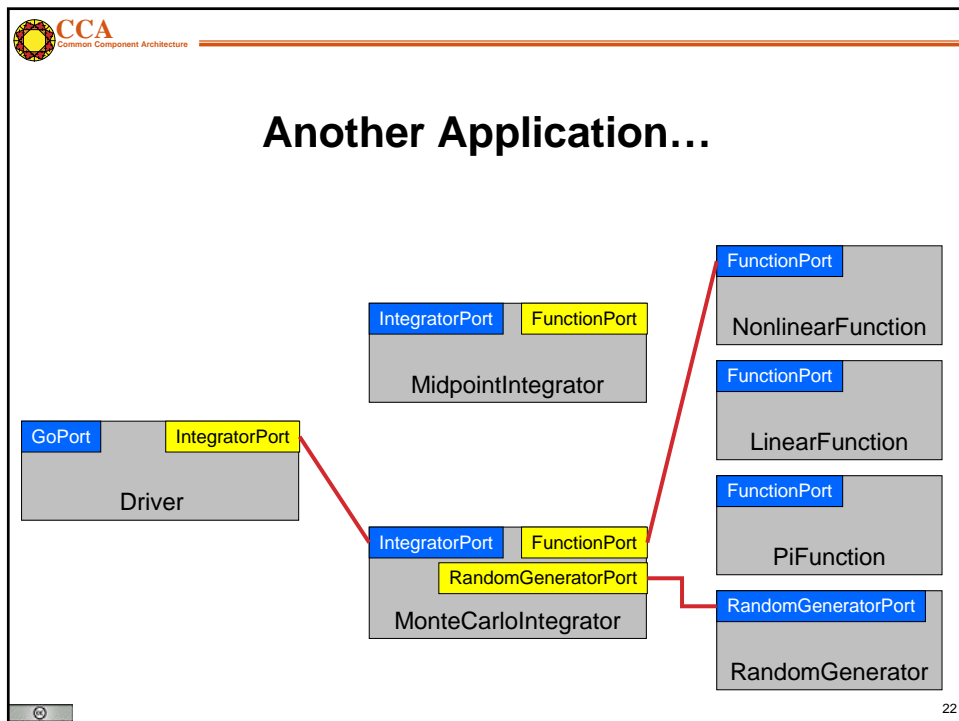
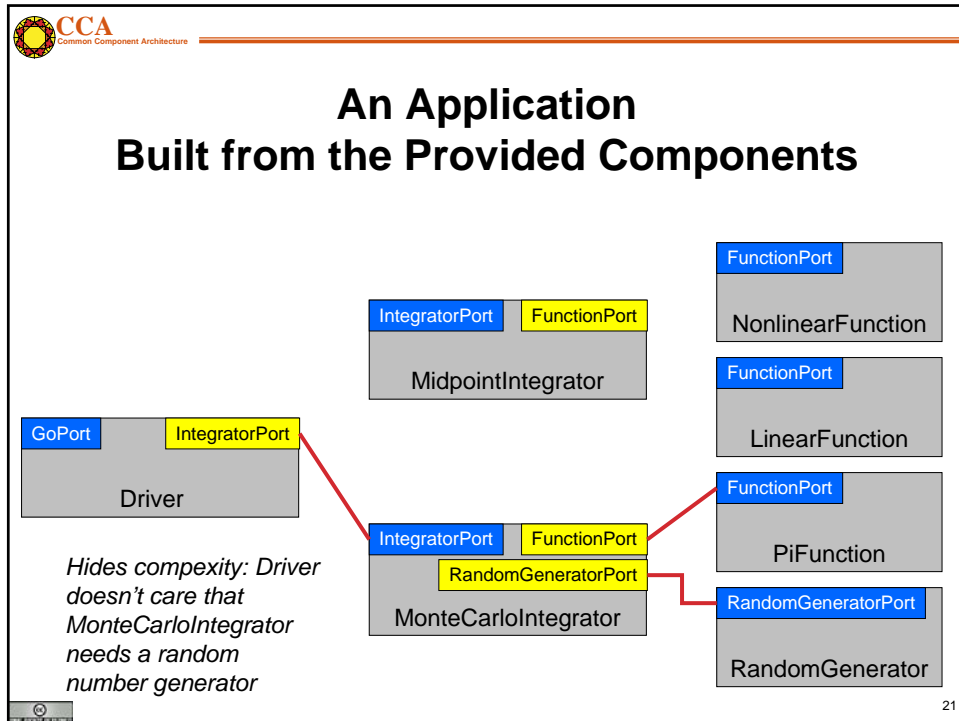


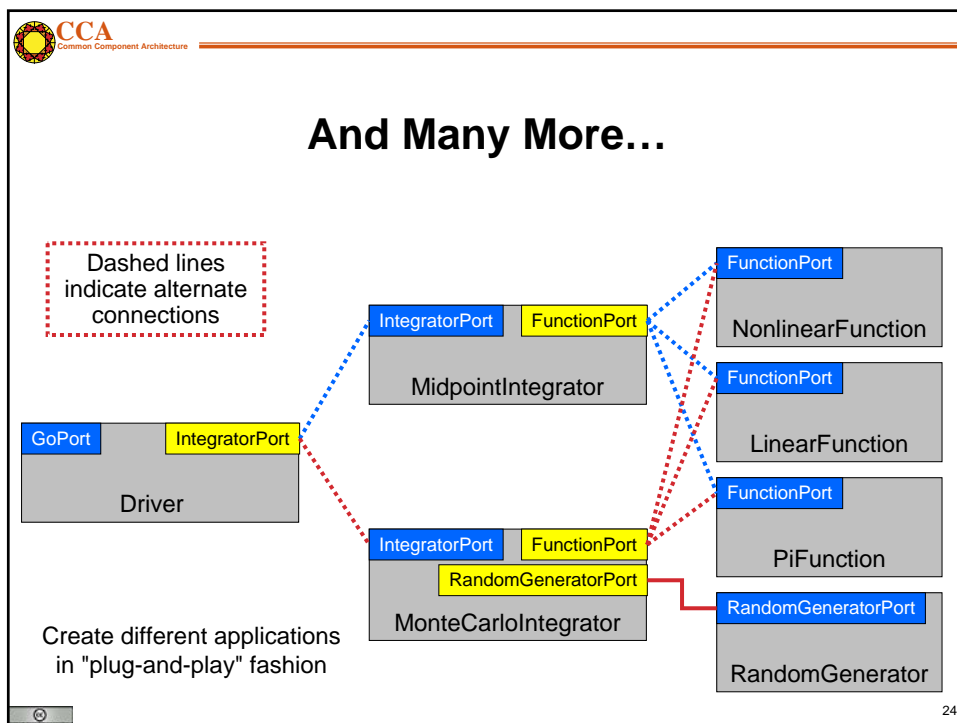
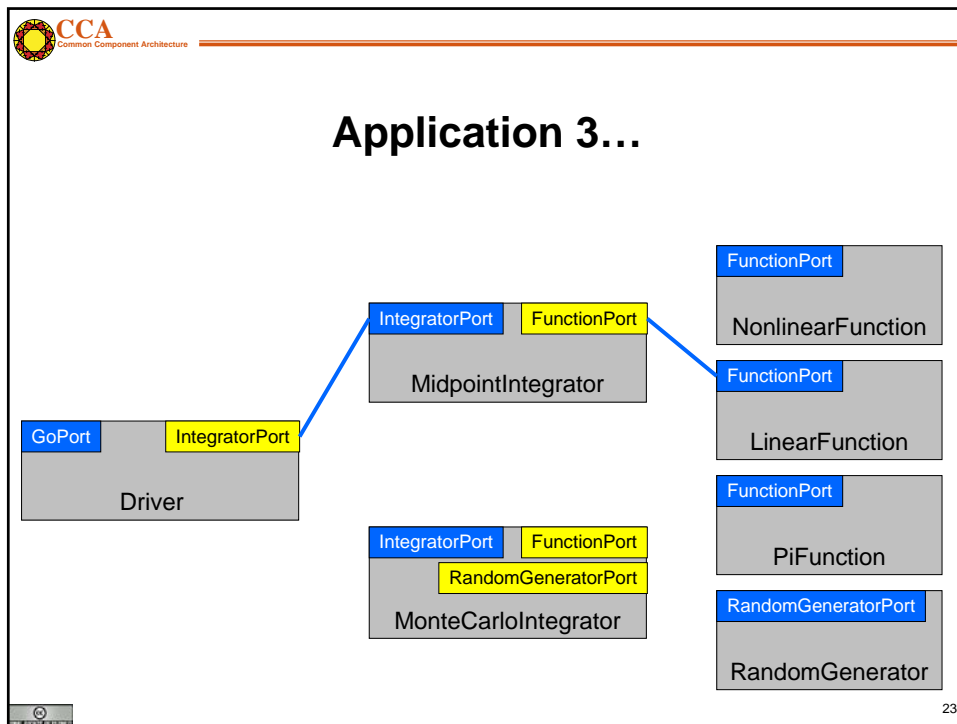
A Simple Example: Numerical Integration Components


*Interoperable components
(provide same interfaces)*



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Comparison of Application Development Approaches

Characteristics	Monolithic Simulation Code	Simulation Frameworks	Library -Based	Component -Based
Support for specific workflows and information flows	High	High	Low	Low
Flexibility w.r.t. workflow and information flow	Low	Medium	High	High
User-level extensibility	Low	Medium	High	High
Ease of incorporation of outside code (code reuse)	Low	Low-Medium	Medium	High
Ease of experimentation	Low	Medium	Medium	High
Amount of new code required to create a complete simulation	Low	Medium	High	High (reuse can reduce)
Breadth of current “ecosystem” for “plugins”	Low	Medium	High	Low (but growing)
Ease of coupling simulations	Low	Low	Medium	High

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Be Aware: “Framework” Describes Many Things

- Currently in scientific computing, this term means different things to different people
- **Basic software composition environment**
 - Examples: CCA, CORBA Component Model, ...
- An environment facilitating development of applications in **a particular scientific domain** (i.e. fusion, computational chemistry, ...)
 - Example: Earth System Modeling Framework, <http://www.esmf.ucar.edu>
 - Example: Computational Facility for Reacting Flow Science, <http://cfrfs.ca.sandia.gov>
- An environment for managing complex **workflows** needed to carry out calculations
 - Example: Kepler: <http://kepler-project.org>
- **Integrated data analysis and visualization environments** (IDAVEs)
- Lines are often fuzzy
 - Example: Cactus, <http://www.cactuscode.org>
- Others types of frameworks *could* be built based on a **basic software composition environment**

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Relationships: Components, Objects, and Libraries

- Components are typically discussed as **objects** or collections of objects
 - **Interfaces** generally designed in **OO** terms, but...
 - Component **internals need not be OO**
 - **OO languages are not required**
- Component environments can **enforce** the use of **published interfaces** (prevent access to internals)
 - Libraries can not
- It is possible to load **several instances** (versions) of a component in a single application
 - Impossible with libraries
- Components *must* include some code to **interface with the framework/component environment**
 - Libraries and objects do not

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What is the CCA?

- Component-based software engineering has been developed in other areas of computing
 - Especially business and internet
 - Examples: CORBA Component Model, COM, Enterprise JavaBeans
- Many of the needs are similar to those in HPC scientific computing
- But scientific computing imposes special requirements not common elsewhere
- **CCA is a component environment specially designed to meet the needs of HPC scientific computing**

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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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CCA: Concept and Practice

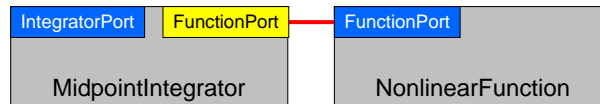
- In the following slides, we explain important **concepts** of component-based software from the CCA perspective
- We also sketch how these concepts are **manifested in code** (full details in the Hands-On)
- The **CCA Specification** is the mapping between concept and code
 - A standard established by the CCA Forum
 - Expressed in the Scientific Interface Definition Language (SIDL) for language neutrality (syntax similar to Java)
 - SIDL can be translated into bindings for specific programming languages using, e.g., the Babel language interoperability tool



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CCA Concepts: Components

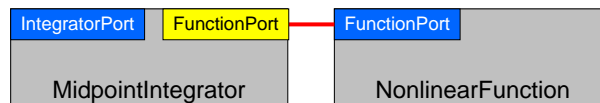


- A component encapsulates some computational functionality
- Components provide/use one or more interfaces
 - A component with no interfaces is formally okay, but isn't very interesting or useful
- In SIDL, a component is a **class** that **implements** (inherits from) **gov.cca.Component**
 - This means it must implement the **setServices** method to tell framework what ports this component will **provide** and **use**
 - **gov.cca.Component** is defined in the CCA specification

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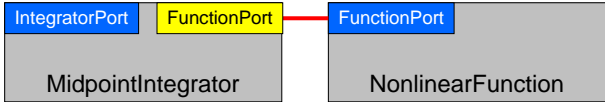
CCA Concepts: Ports



- Components interact through well-defined **interfaces**, or **ports**
 - A port expresses some **computational functionality**
 - In Fortran, a port is a bunch of subroutines or a **module**
 - In OO languages, a port is an **abstract class** or **interface**
- Ports and connections between them are a procedural (caller/callee) relationship, **not dataflow!**
 - e.g., *FunctionPort* could contain a method like **evaluate(in Arg, out Result)** with data flowing both ways

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CCA Concepts: *Provides* and *Uses* Ports



The diagram shows two components: **MidpointIntegrator** and **NonlinearFunction**. **MidpointIntegrator** has two ports: **IntegratorPort** (blue) and **FunctionPort** (yellow). **NonlinearFunction** has one port: **FunctionPort** (blue). A red line connects the **FunctionPort** of **MidpointIntegrator** to the **FunctionPort** of **NonlinearFunction**, indicating a "Provides" relationship.

- Components may **provide** ports – **implement** the class or subroutines of the port (**"Provides" Port**)
 - Providing* a port implies certain inheritance relationships between the component and the abstract definition of the interface (**more details shortly**)
 - A component can *provide* multiple ports
 - Different "views" of the same functionality, or
 - Related pieces of functionality
- Components may **use** ports – **call** methods or subroutines in the port (**"Uses" Port**)
 - Use* of ports is just like calling a method normally except for a little additional work due to the "componentness" (**more details shortly**)
 - No inheritance relationship implied between caller and callee
 - A component can *use* multiple ports

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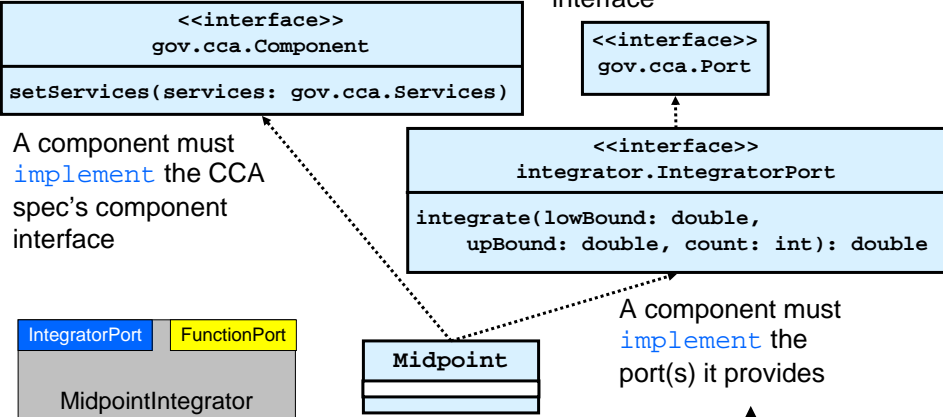
Components and Ports (in UML)

Note that only the **provides** ports appear in the component's inheritance hierarchy. **Uses** ports do not.

A port must **extend** the CCA spec's port interface

A component must **implement** the CCA spec's component interface

A component must **implement** the port(s) it provides



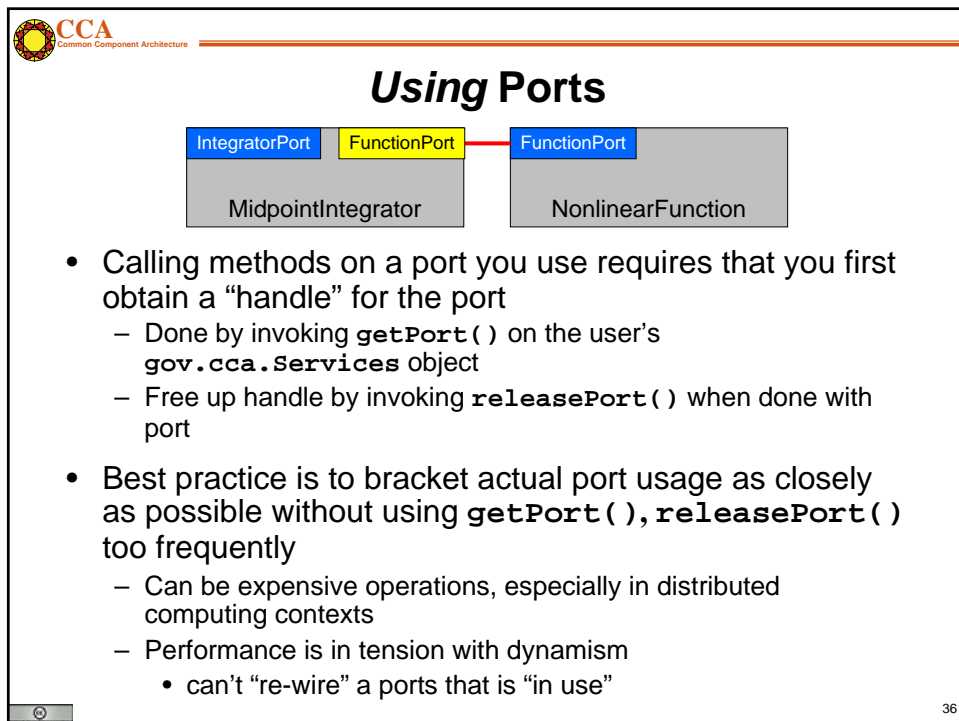
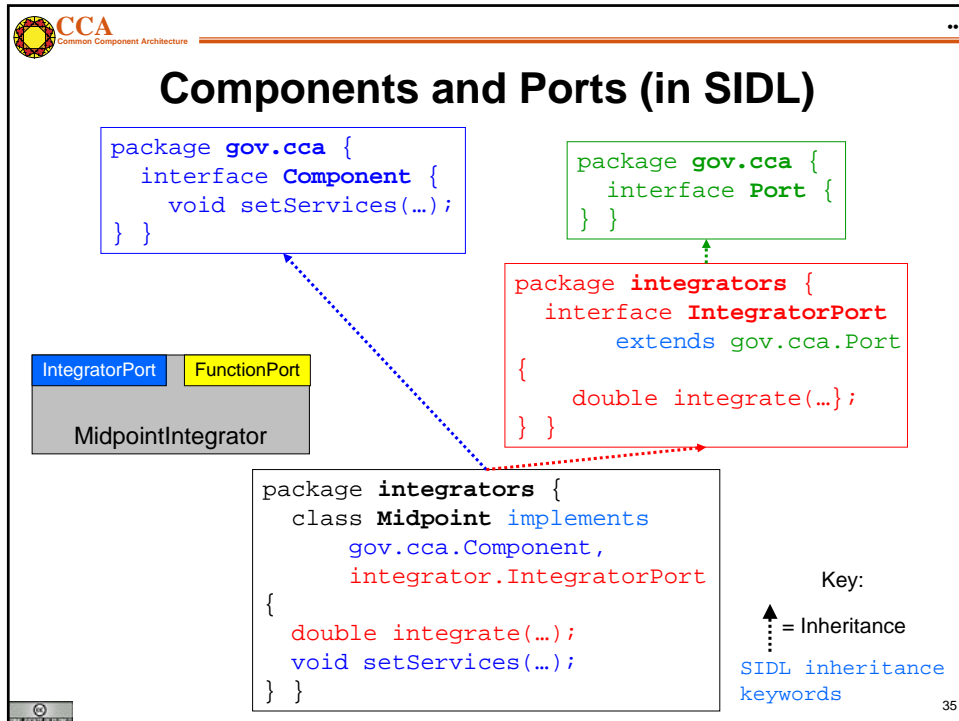
The UML diagram shows the following elements and relationships:

- gov.cca.Component**: An interface with the method `setServices(services: gov.cca.Services)`. It is the base interface for all components.
- gov.cca.Port**: An interface that is the base for all ports.
- integrator.IntegratorPort**: A port interface that extends **gov.cca.Port** (indicated by a dashed arrow) and has the method `integrate(lowBound: double, upBound: double, count: int): double`.
- MidpointIntegrator**: A component class that implements **gov.cca.Component** (indicated by a solid arrow) and provides **IntegratorPort** and **FunctionPort**.
- Midpoint**: A class that implements **integrator.IntegratorPort** (indicated by a solid arrow).

Class for Midpoint Integrator component

Key:
 ↑ = Inheritance
 ... = SIDL keywords

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Where Do Ports Come From?

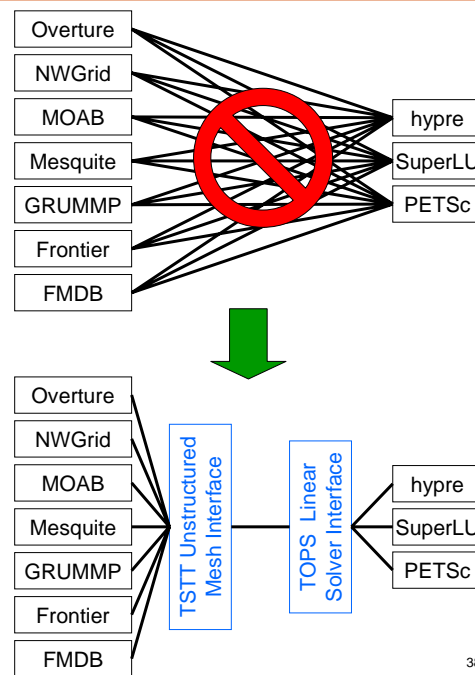
- Most ports are designed and implemented by **users** of CCA
 - May be specific to an application or used more broadly (i.e. community-wide)
- The **CCA specification** defines a *small* number of ports
 - Most are services CCA frameworks must provide for use by components
 - Some are intended for users to implement in their components, and have a special meaning recognized by the framework
 - *E.g. `gov.cca.ports.GoPort`* provides a very simple protocol to start execution of component-based applications

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Interfaces are Key to Reuse and Interoperability of Code

- **Interoperability** -- multiple implementations conforming to the same interface
- **Reuse** – ability to use a component in many applications
- The larger the community that agrees to the interface, the greater the opportunity for interoperability and reuse



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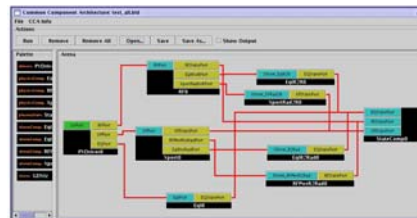
Interfaces are an Investment

- The larger the community, the greater the time & effort required to obtain agreement
 - Equally true in component and non-component environments
 - MPI 1.0 (well understood at the start) took 8 months, meeting every six weeks
 - MPI 2.0 (not well understood at the start) took 1.5 years, meeting every six weeks
 - Convenient communities are often “project” and “scientific domain”
- Formality of “standards” process varies
- 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**

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CCA Concepts: Frameworks

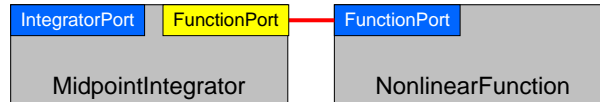


- The framework provides the means to “hold” components and **compose** them into applications
- Frameworks allow **connection of ports** without exposing component implementation details
- Frameworks provide a small set of **standard services** to components
 - Framework services are CCA ports, just like on components
 - Additional (non-standard) services can also be offered
 - Components can register ports as services using the *ServiceProvider* port
- *Currently:* specific frameworks are specialized for specific computing models (parallel, distributed, etc.)
- *Future:* better integration and interoperability of frameworks

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Components Must Keep Frameworks Informed



- Components must tell the framework about the ports they are providing and using
 - Framework will not allow connections to ports it isn't aware of
- Register them using methods on the component's `gov.cca.Services` object
 - `addProvidesPort()` and `removeProvidesPort()`
 - `registerUsesPort()` and `unregisterUsesPort()`
 - All are defined in the CCA specification
- Ports are usually registered in the component's `setServices()` method
 - Can also be added/removed dynamically during execution

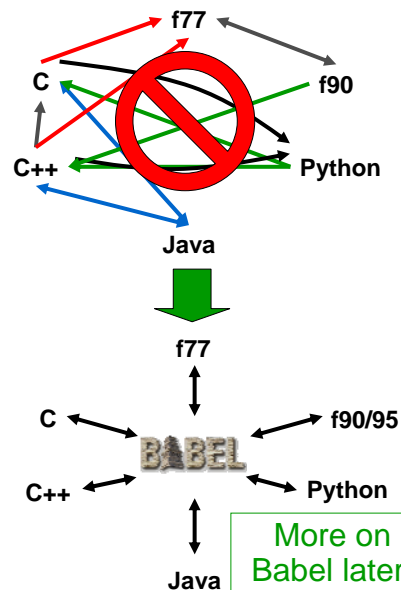


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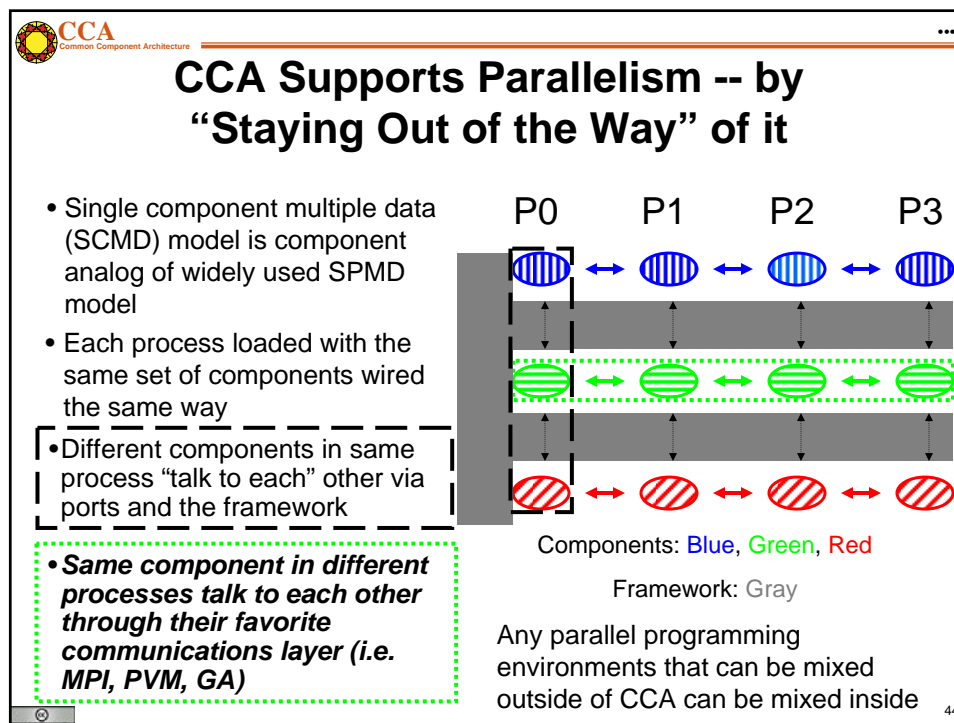
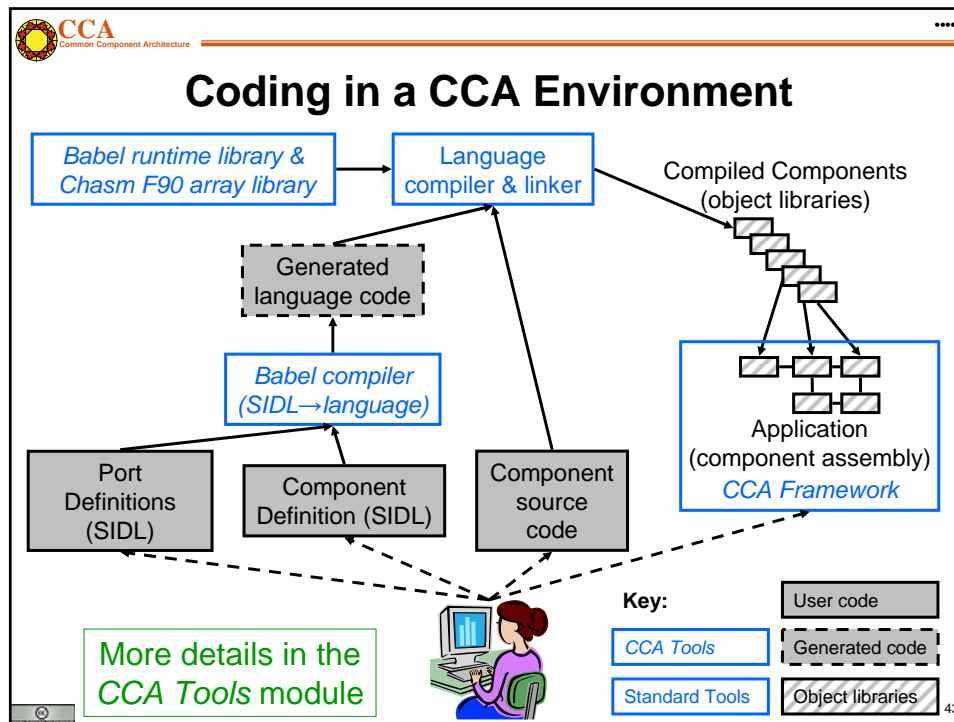



CCA Concepts: Language Interoperability

- Scientific software is increasingly diverse in use of programming languages
- In a component environment, users should not care what language a component is implemented in
- “Point-to-point” solutions to language interoperability are not suitable for a component environment
- The [Babel](#) language interoperability tool provides a common solution for all supported languages
- [Scientific Interface Definition Language](#) provides language-neutral way of expressing interfaces



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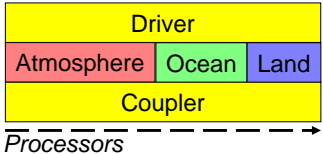





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“Multiple-Component Multiple-Data” Applications in CCA

- Simulation composed of multiple SCMD sub-tasks
- Usage Scenarios:
 - Model coupling (e.g. Atmosphere/Ocean)
 - General multi-physics applications
 - Software licensing issues
 - i.e. limited number of instances
- 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)



Processors →







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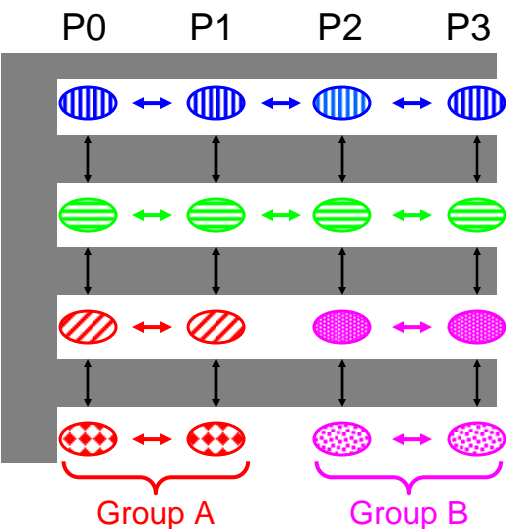



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MCMD Within A Single Framework

See example in the *Using CCA* module (multilevel parallelism in quantum chemistry)

-  Framework
-  Application driver & MCMD support component
-  Components on all processes
-  Components only on process group A
-  Components only on process group B

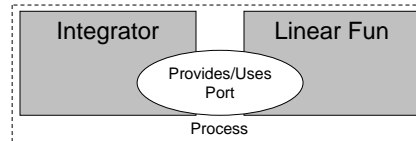



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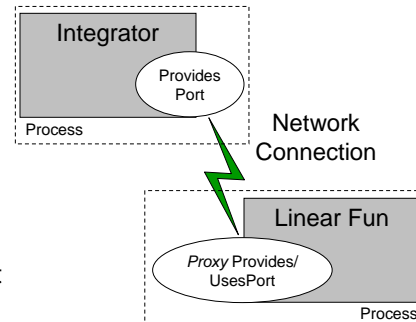


CCA Supports High-Performance Local and Distributed Computing

- “**Direct connection**” preserves high performance of local (“in-process”) and parallel 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



Direct Connection




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“Direct Connection” Details

- Directly connected components are in the **same address space**
 - Data can be passed by reference instead of copying
 - Just like “traditional” programs
 - Framework involved in **connecting** components, but **not invocations** on ports
- Cost of “CCAness” in a direct connect environment is **one level of indirection** on calls **between** components
 - Equivalent to a C++ **virtual function call**: lookup function location, invoke it
 - Overhead is on the **invocation only** (i.e. latency), not the total execution time
 - Cost equivalent of ~2.8 F77 or C function calls
 - ~48 ns vs 17 ns on 500 MHz Pentium III Linux box

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CCA
Common Component Architecture

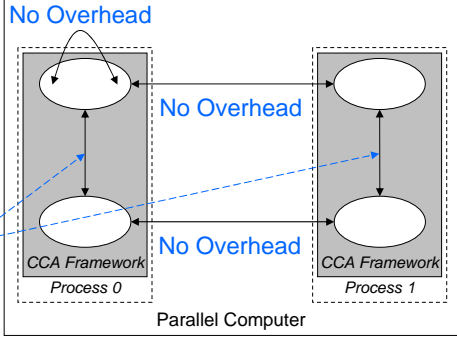
Performance, the Big Picture

Direct-Connect, Parallel

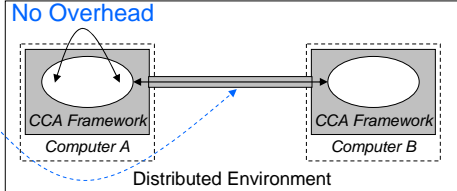
- No CCA overhead on...
 - calls within component
 - parallel communications across components
- Small overheads on invocations on ports
 - Virtual function call (CCAness)
 - Language Interoperability (some data types)

Distributed

- No CCA overhead on calls within component
- Overheads on invocations on ports
 - Language interoperability (some data types)
 - Framework
 - (Wide area) network




Parallel Computer



Distributed Environment

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CCA
Common Component Architecture

Maintaining HPC Performance

- The performance of your application is as important to us as it is to you
- The CCA is designed to provide maximum performance
 - But the best we can do is to make your code perform **no worse**
- Facts:
 - Measured overheads per function call are **low**
 - Most overheads **easily amortized** by doing enough work per call
 - Other changes made during componentization may also have performance impacts
 - **Awareness** of costs of abstraction and language interoperability facilitates design for high performance

More about performance in notes

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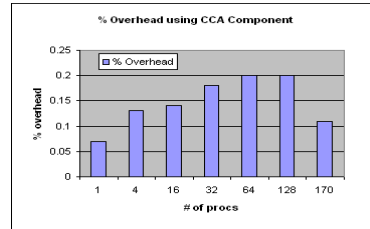


Common Component Architecture

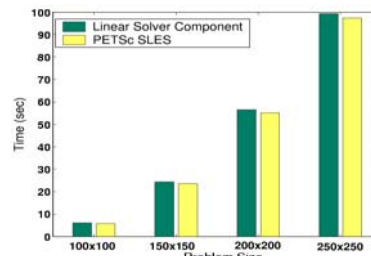
Supplementary material for handouts

Some Performance Results and References

- Lois Curfman McInnes, et al. **Parallel PDE-Based Simulations Using the Common Component Architecture**. In Are Magnus Bruaset, Petter Bjorstad, and Aslak Tveito, editors, *Numerical Solution of PDEs on Parallel Computers*. Springer-Verlag, 2005. Invited chapter, in press.
- S. Benson, et al. **Using the GA and TAO Toolkits for Solving Large-Scale Optimization Problems on Parallel Computers**. Technical report ANL/MCS-P1084-0903, Argonne National Laboratory, September 2003.
- Boyana Norris, et al. **Parallel Components for PDEs and Optimization: Some Issues and Experiences**. *Parallel Computing*, 28:1811--1831, 2002.
- David E. Bernholdt, et al. **A Component Architecture for High-Performance Computing**. In *Proceedings of the Workshop on Performance Optimization via High-Level Languages and Libraries (POHLL-02)*, 2002.



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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Common Component Architecture

Supplementary material for handouts

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

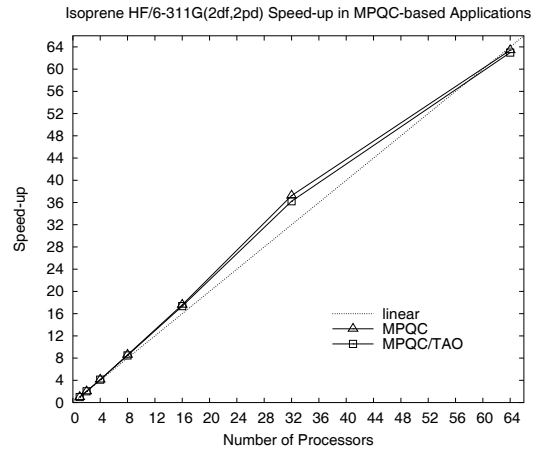
Function arg type	f77	Component
Array	80 ns	224ns
Complex	75ns	209ns
Double complex	86ns	241ns

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Scalability : Component versus Non-component. I

- Quantum chemistry 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)



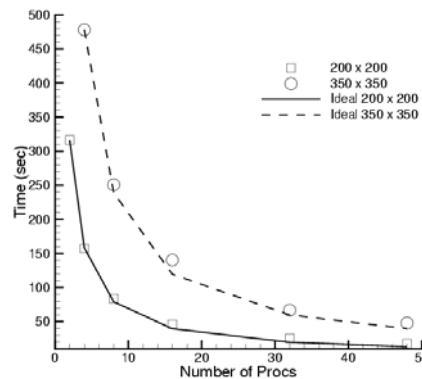
Parallel Scaling of MPQC w/ native and TAO optimizers

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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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Advanced CCA Concepts

Brief introductions only, but more info is available – just ask us!

- Leveraging the component environment to provide additional capabilities to software developers
- The Proxy Component pattern (Hands-On Ch. 6, papers)
- Component lifecycle (tutorial notes, Hands-On)
- Components can be dynamic (papers)
- Improving the quality of component software (papers)
- Support for advanced parallel/high-performance computing (papers)



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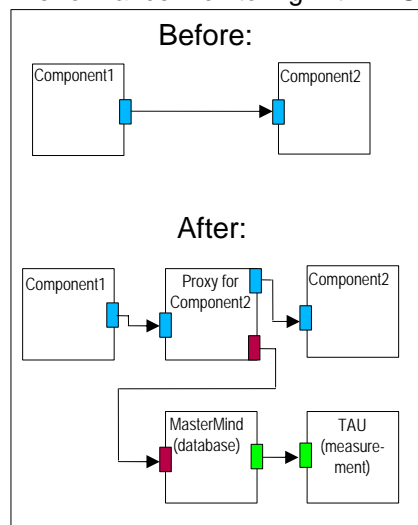
The Proxy Component Pattern

- A “proxy” component can be inserted between the user and provider of a port without either being aware of it (non-invasive)
- Proxy can observe or act on all invocations of the interface
- Similar to aspect-oriented programming
- For many purposes, proxies can be generated automatically from SIDL definition of the port

Sample uses for proxy components:

- **Performance:** instrumentation of method calls
- **Debugging:** execution tracing, watching data values
- **Testing:** Capture/replay

Performance Monitoring with TAU



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Common Component Architecture

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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Common Component Architecture

Supplementary material for handouts

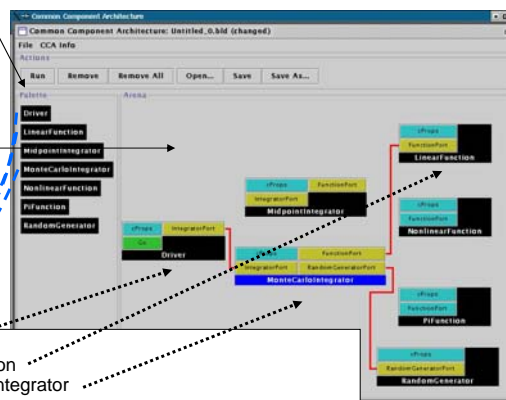
User Viewpoint: Loading and Instantiating Components

- 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

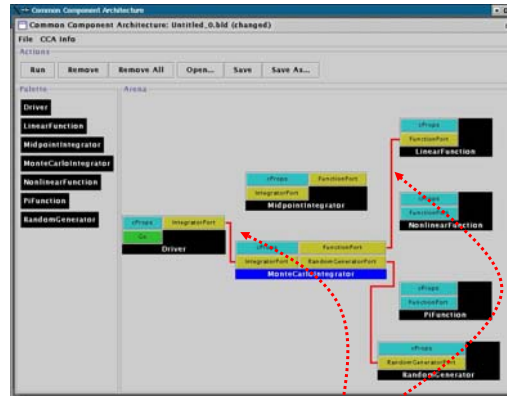


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User Connects Ports

- 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



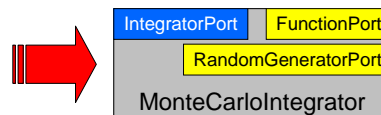
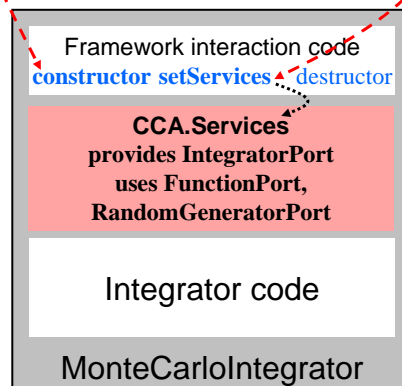
connect connect Driver MonteCarloIntegrator IntegratorPort FunctionPort MonteCarloIntegrator IntegratorPort FunctionPort

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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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CCA 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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CCA Common Component Architecture 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.
sum = sum + **function->evaluate(x)**
- Call **releasePort**

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Dynamic Component Assemblies

- `gov.cca.BuilderService` allows **programmatic composition** of components
 - Components can be instantiated/destroyed, and connected/disconnected under program control

Sample uses of *BuilderService*:

- Python “**driver**” **script** which can assemble and control an application
 - i.e. MCMD climate model
- **Adaptation** to changing conditions
 - Swap components in and out to give better performance, numerical accuracy, convergence rates, etc.
 - TASCs project “**Computational Quality of Service**” activity



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Enhancing Software Quality

- Current component architectures define **syntax** of interfaces
- Extend interface to include **semantics** (behavior) for more complete definition

– “Design by contract”

– Help ensure component **performs correctly**

– Help ensure component **is used correctly**

- Selective enforcement to control impact

- TASCs project “**Software Quality and Verification**” activity

```
package vector version 1.0 {
  class Utils { ...
    static double norm(in array<double> u,
                      in double tol,
                      in int badLevel)
      require /* Preconditions */
        not_null : u != null;
        u_is_1d : dimen(u) == 1;
        non_negative_tolerance : tol >= 0.0;
      ensure /* Postconditions */
        no_side_effects : is pure;
        non_negative_result : result >= 0.0;
        nearEqual(result, 0.0, tol)
        iff isZero(u, tol);
    ... }
}
```



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Supporting Emerging HPC Hardware Environments

- CCA does not dictate a specific approach to parallelism
- Different approaches and tools can be provided via components and custom frameworks

Examples...

- Uintah Computational Framework (Utah) provides a multi-threaded parallel execution environment based on task graphs
 - Specialized to certain structured adaptive mesh refinement problems
- TASCs developing services to manage groups of parallel components/tasks (MCMD)

Also...

- TASCs developing support for heterogeneous processor environments
 - FPGAs, GP-GPUs, accelerators, and other co-processors
 - Accelerator code encapsulated as components, interacting w/ components on primary processors
- Integration of fault tolerance capabilities with CCA under development (CIFTS-TASCs collaboration)



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Is CCA for You?

- Much of what CCA does can be done without such tools *if* you have sufficient discipline
 - The larger a group, the harder it becomes to impose the necessary discipline
- Projects may use different aspects of the CCA
 - CCA is *not* monolithic – use what *you* need
 - Few projects use all features of the CCA... initially
- Evaluate what *your* project needs against CCA's capabilities
 - Other groups' criteria probably differ from yours
 - CCA continues to evolve, so earlier evaluations may be out of date
- Evaluate CCA against other ways of obtaining the desired capabilities
- Suggested starting point:
 - CCA tutorial “hands-on” exercises



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Take an Evolutionary Approach

- The CCA is designed to allow selective use and incremental adoption
- “SIDLize” interfaces incrementally
 - Start with essential interfaces
 - Remember, only externally exposed interfaces need to be Babelized
- Componentize at successively finer granularities
 - Start with whole application as one component
 - Basic feel for components without “ripping apart” your app.
 - Subdivide into finer-grain components as appropriate
 - Code reuse opportunities
 - Plans for code evolution



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View it as an Investment

- CCA is a long-term investment in your software
 - Like most software engineering approaches
- There is a cost to adopt
- The payback is longer term
- Remember Biggerstaff’s Rule of Threes
 - Look at three systems, requires three times the effort, payback after third release



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CCA is Still Under Development

- We've got...
 - A stable component model
 - Working tools
 - Active users
- But...
 - We know its not perfect
 - We're not "done" by any stretch
- Talk to us...
 - If you're evaluating CCA and need help or have questions
 - If you don't think CCA meets your needs
 - If you've got suggestions for things we might do better



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What Can CCA Do Today?

- Ccaffeine framework for HPC/parallel
 - XCAT and other options for distributed computing
- Language interoperability
 - Fortran 77/90/95, C, C++, Java, Python
 - Support for Fortran/C user-defined data structures under development
- CCA Tools working on a variety of platforms
 - Linux most widely used
 - Mac OS X second
 - Some IBM AIX users
 - Works on Cray XT series, port to IBM BlueGene in progress
 - Porting is driven by user needs, so let us know!



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CCA Tools – Language Interoperability and Frameworks

CCA Forum Tutorial Working Group

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



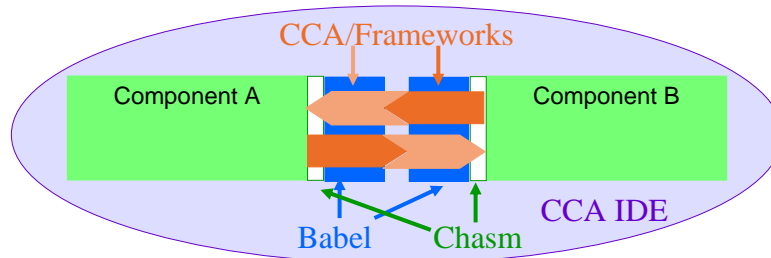
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Goal of This Module

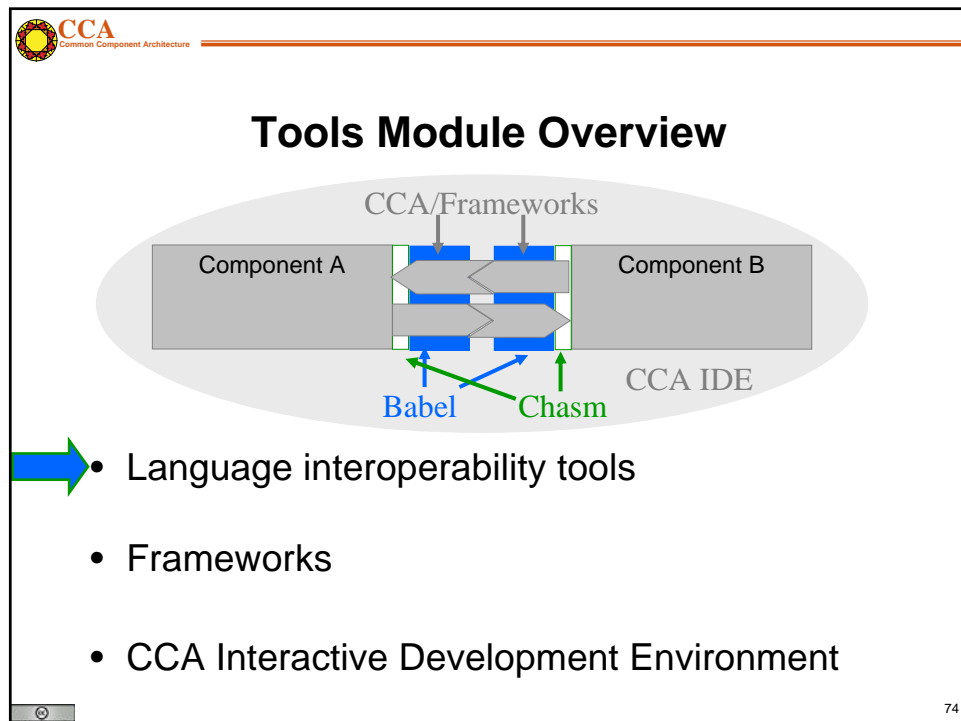
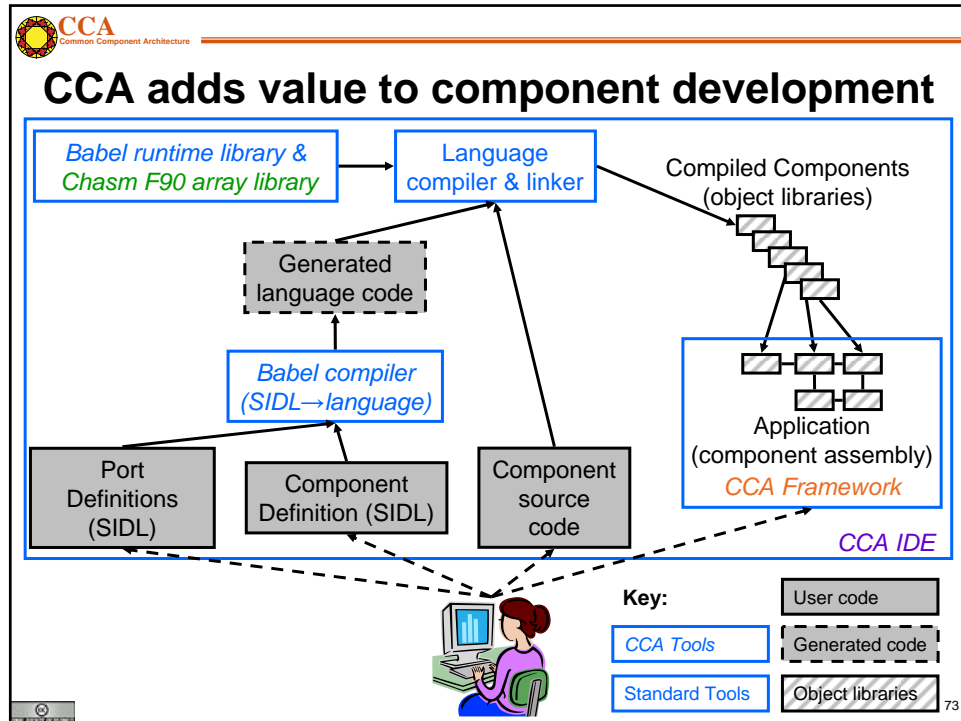



- Describe **tools** for multi-lingual, scientific component 'plug-and-play'



IDE = Interactive Development Environment

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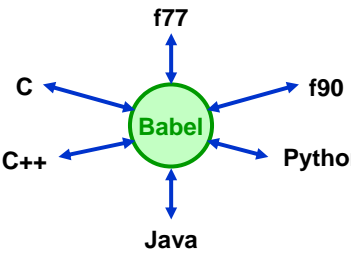
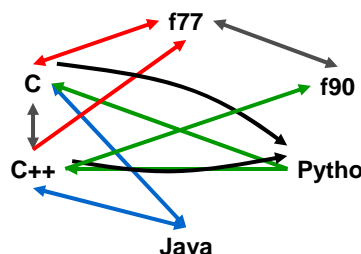



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Babel


Babel Facilitates *Scientific* Programming Language Interoperability

- Programming language-neutral interface descriptions
- Native support for basic scientific data types
 - Complex numbers
 - Multi-dimensional, multi-strided arrays
- Automatic object-oriented wrapper generation


vs.


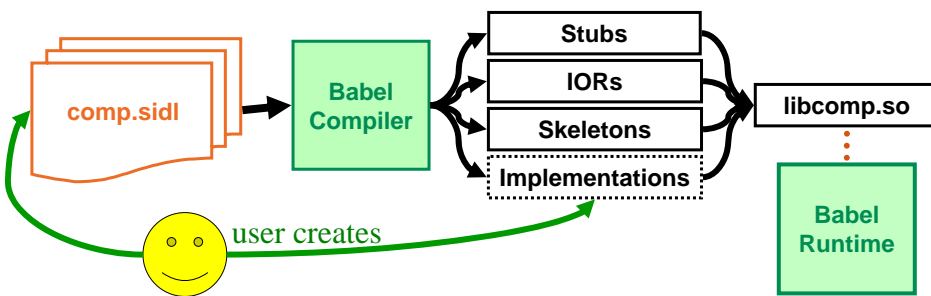
Supported on Linux, AIX, works on OSX, catamount;
 C (ANSI C), C++ (GCC), F77 (g77, Sun f77), F90 (Intel, Lahey, GNU, Absoft, PGI), Java (1.4)

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Babel

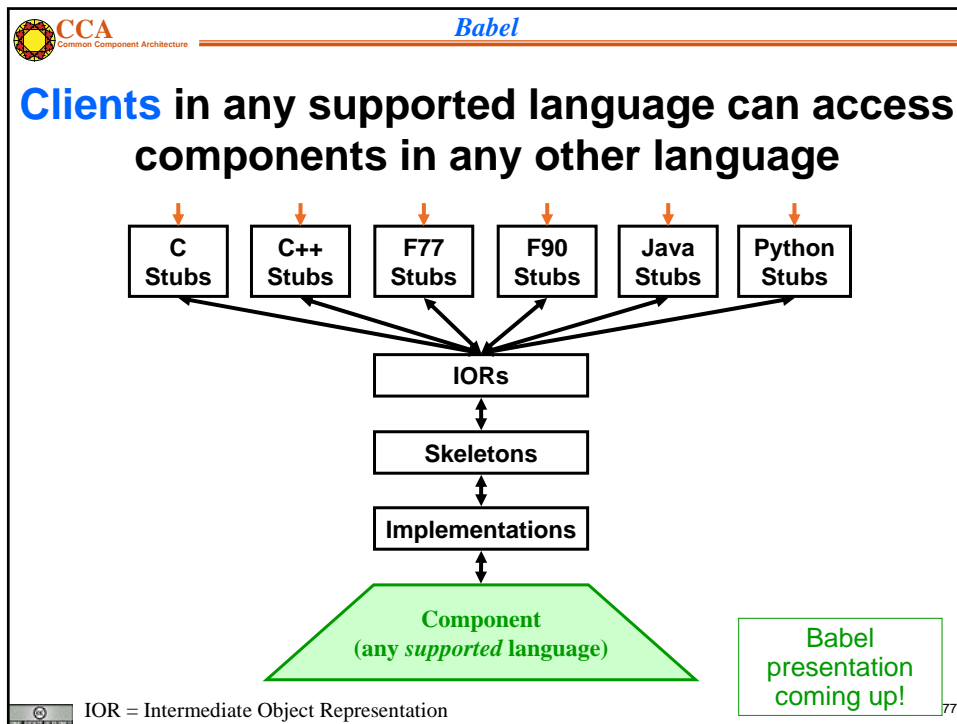
Babel Generates Object-Oriented Language Interoperability Middleware



1. Write your SIDL file to define public methods
2. Generate server side in your native language using Babel
3. Edit Implementations as appropriate
4. Compile and link into library/DLL


 IOR = Intermediate Object Representation SIDL = Scientific Interface Definition Language


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Recent and Upcoming Features

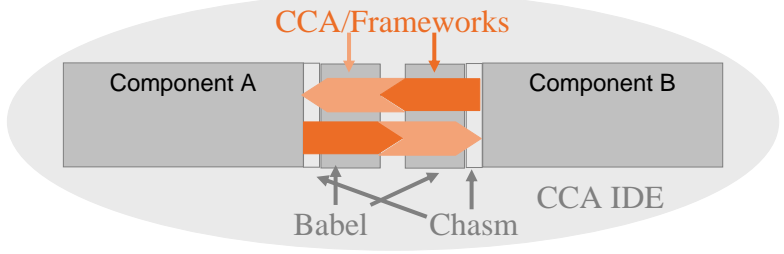
- Remote Method Invocation (Babel RMI)
Kumfert, Leek, & Epperly IPDPS'07
ALPHA – Babel 1.0. (aka “stable branch”)*
*BETA – Babel 1.1.**
Final – Future Stable Branch (Babel 1.2?)
- Design-by-Contract
Dahlgren CBSE'07 (to appear)
ALPHA – Internal Babel branch
BETA – Babel 1.1.2 (expected)
- Feature requests are accepted and tracked in the open using Roundup
<http://www.cca-forum.org/bugs/babel>

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Common Component Architecture

Tools Module Overview



- Language interoperability tools
- ➔ • Frameworks
- CCA Interactive Development Environment

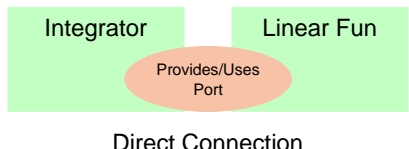

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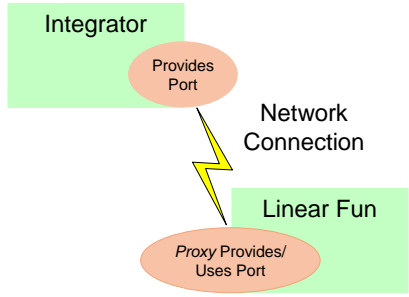
CCA
Common Component Architecture

Frameworks are Specialized to Different Computing Environments


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



Direct Connection



Network Connection


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Graphical User Interfaces (GUIs) Deliver Plug-and-Play Experience

- Plug & play for:
 - Application software assembly
 - Visualization pipelines
 - Workflow management
- Assembling “wiring” diagrams is almost universal.
 - Software assembly: Ccaffeine, XCAT, SciRUN
 - Workflow: XCAT, SciRUN
 - Visualization: SciRUN



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Ccaffeine Framework

Ccaffeine is a *Direct-Connect*, Parallel-Friendly Framework

- Supports SIDL/Babel components
 - Conforms to latest CCA specification (0.8)
 - Also supports legacy CCA specification (0.5)
 - Any C++ allowed with C and Fortran by C++ wrappers
- Provides command-line and GUI for composition
 - Scripting supports batch mode for SPMD
 - MPMD/SPMD custom drivers in any Babel language

Supported on Linux, AIX, OSX and is portable to modern UNIXes.



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Ccaffeine Involves a Minimum of Three Steps

- As easy as 1-2-3:
 - Write your component.
 - Describe it with an XML file.
 - Add a line to your Ccaffeine input file to load the component at runtime.
- Proceed to plug & play...

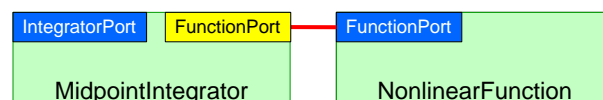
There are many details and automated tools that help manage components.




Optional

Ccaffeine GUI

- Process
 - User input is broadcast SPMD-wise from Java.
 - Changes occur in GUI *after* the C++ framework replies.
 - If your components are computing, GUI changes are blocked.
- Components interact through *port connections*
 - *provide* ports *implement* class or subroutines "Provides" Port
 - *use* ports *call* methods or subroutines in the port. "Uses" Port
 - Links denote caller/callee relationship *not* data flow



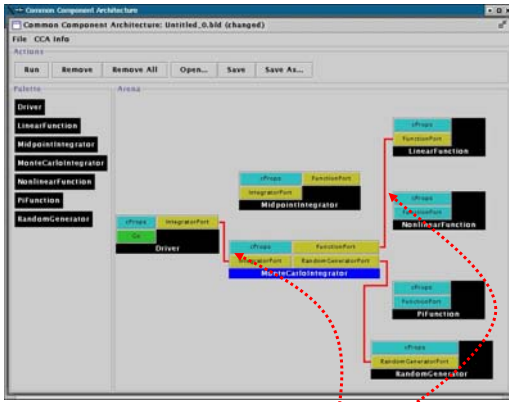


CCA
Common Component Architecture

Caffeine Framework (ccafe-gui)


User Connects Ports

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



connect	Driver	IntegratorPort	MonteCarloIntegrator	IntegratorPort
connect	MonteCarloIntegrator	FunctionPort	LinearFunction	FunctionPort
...				

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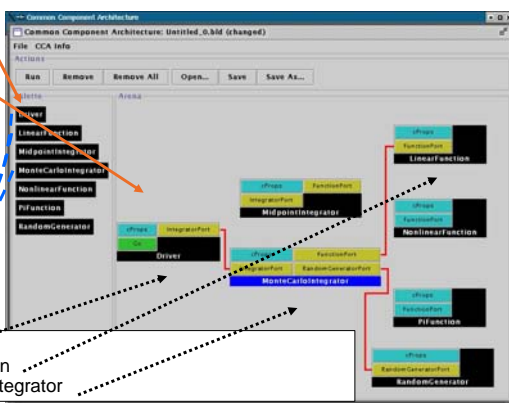


CCA
Common Component Architecture

Caffeine Framework (ccafe-gui)


Building an Application (1 of 2)

- Components are code + XML 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*



create	Driver	Driver
create	LinearFunction	LinearFunction
create	MonteCarloIntegrator	MonteCarloIntegrator

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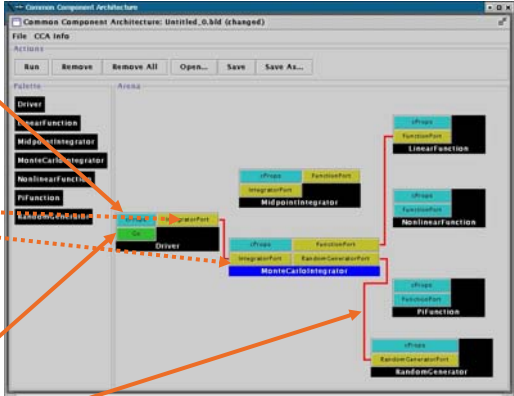


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Common Component Architecture

Ccaffeine Framework (ccafe-gui)


Building an Application (2 of 2)

1. Click *Configure* port to start parameter input dialogue.
2. For each connection:
click a *uses* port then click a *provides* port to establish a connection.
3. Click *Go* port to start the application.




Right-clicking a connection line breaks the connection -- enabling component substitution.

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Common Component Architecture


XCAT-C++ Framework



XCAT is a Web-services based *Distributed* Component Framework

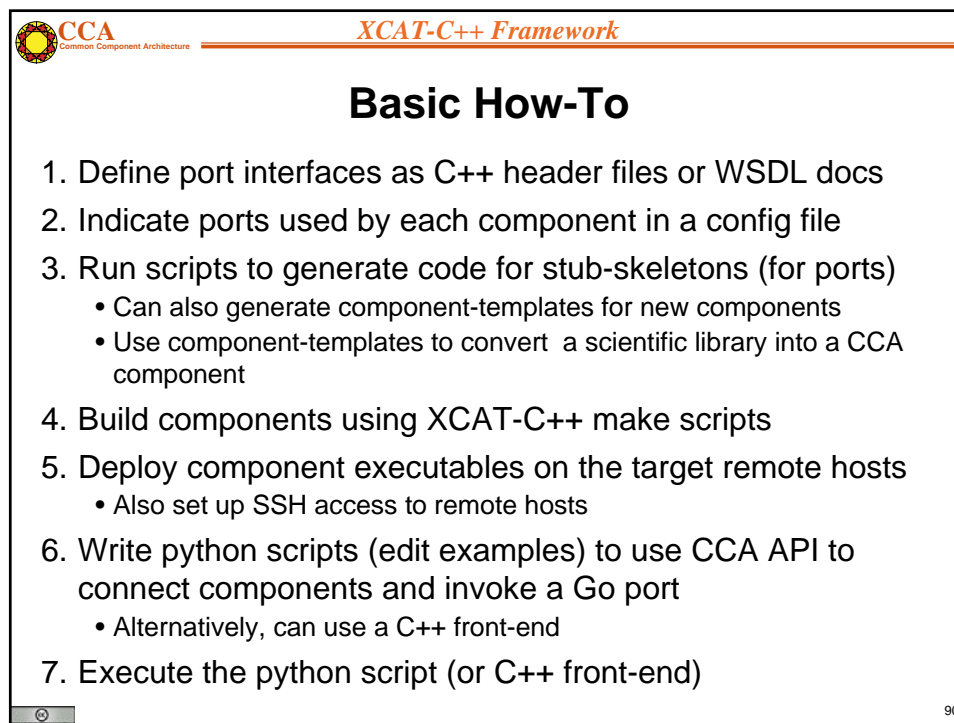
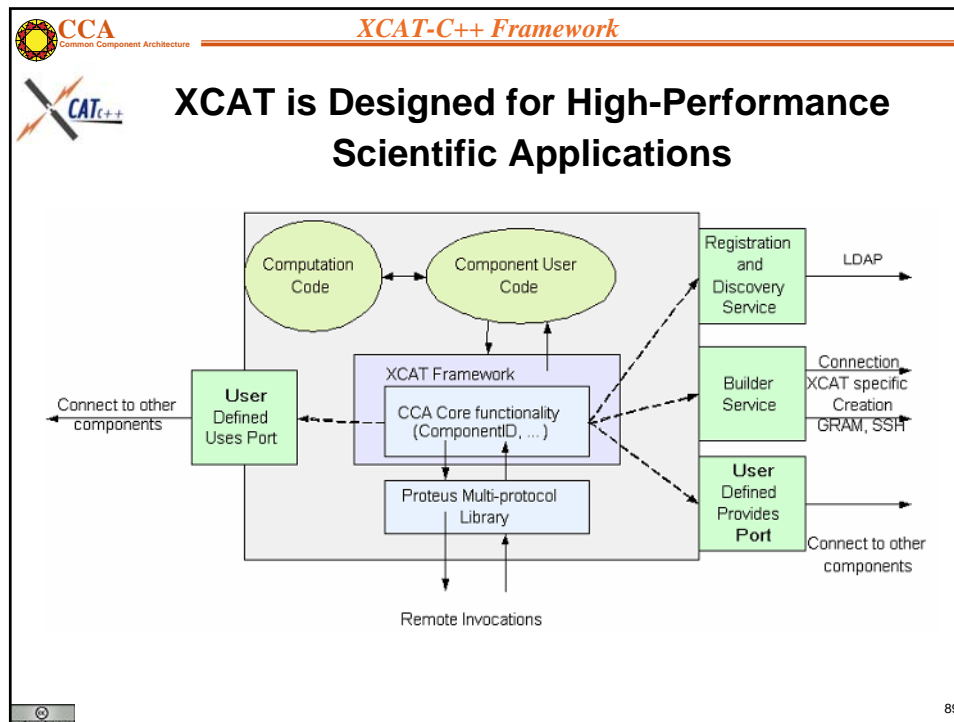
- Remote references
 - Port types described in C++ header files or in WSDL documents
- User Interface
 - C++ and Python interface to CCA *BuilderService*
 - Uses SWIG for Python-C++ translations
- Component creation
 - Remote creation via SSH
- Component communication
 - Proteus multi-protocol library
 - Communication libraries can be loaded at run-time


Tested on Linux.



WSDL = Web Service Definition Language


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Common Component Architecture


XCAT-C++ Framework



Recent and Upcoming Features

- Incorporate Babel's Remote Method Invocation
 - Allows access to Babel objects through remote Babel stubs
 - Provides direct support for SIDL in distributed applications
- Incorporate Web-services based protocols in BabelRMI
- Performance analysis of Babel-RMI based distributed communication
- Design Distributed Framework Interoperability Specification


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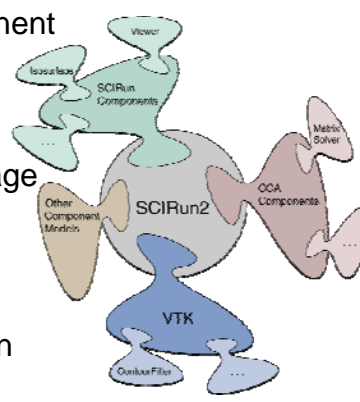


CCA
Common Component Architecture

SCIRun2 Framework


SCIRun2 is a Cross-Component Model, *Distributed Component Framework*

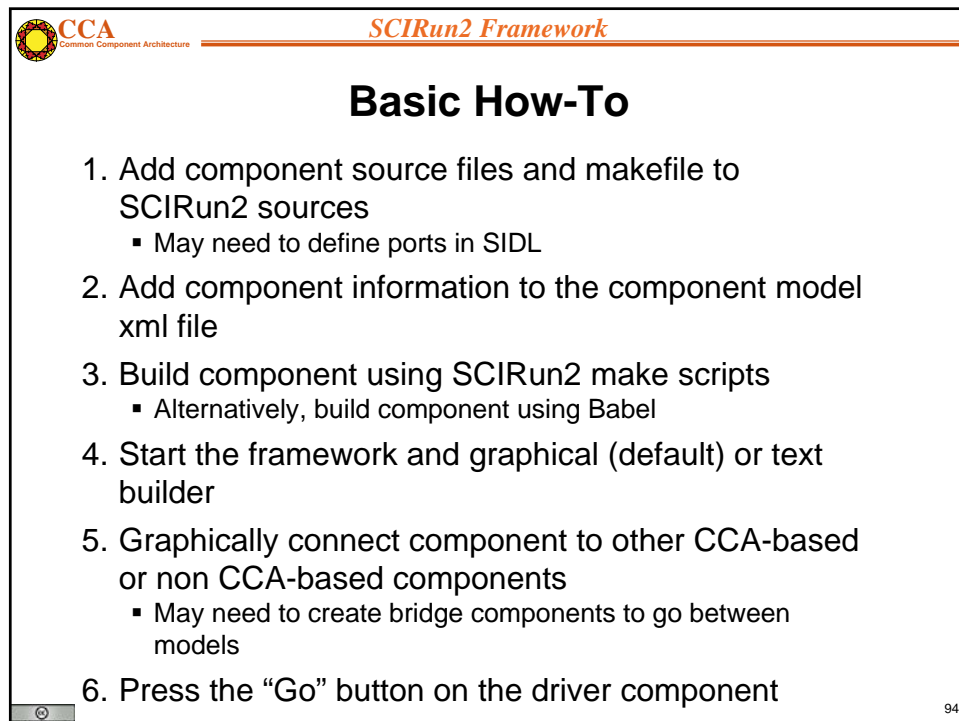
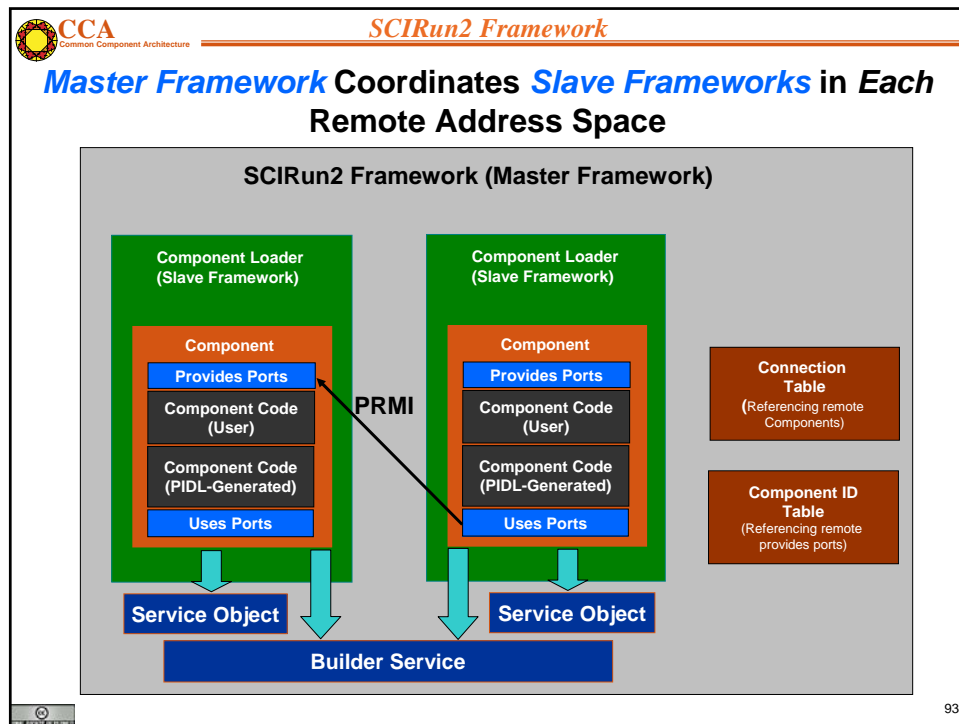
- Semi-automatically bridges component *models*
 - Templated components connected at run-time generate bridges
- Parallel Interface Definition Language (PIDL) – a SIDL variant
- User interface – GUI and textual
 - Dynamic composition
- Component and framework creation
 - Remote via SSH
- Component communication
 - C++ RMI with co-location optimization
 - MPI/ Parallel Remote Method Invocation (PRMI)



The diagram illustrates the SCIRun2 framework as a central hub. It is a large, light-blue, irregular shape labeled 'SCIRun2'. Surrounding it are several smaller, colored shapes representing different components: a green shape labeled 'Viewer' at the top, a red shape labeled 'Matrix Solver' at the top right, a yellow shape labeled 'Other Component Models' at the bottom left, a blue shape labeled 'VTK' at the bottom, and a pink shape labeled 'OCA Components' at the bottom right. Arrows indicate connections between these components and the central SCIRun2 hub.

Supported on Linux.


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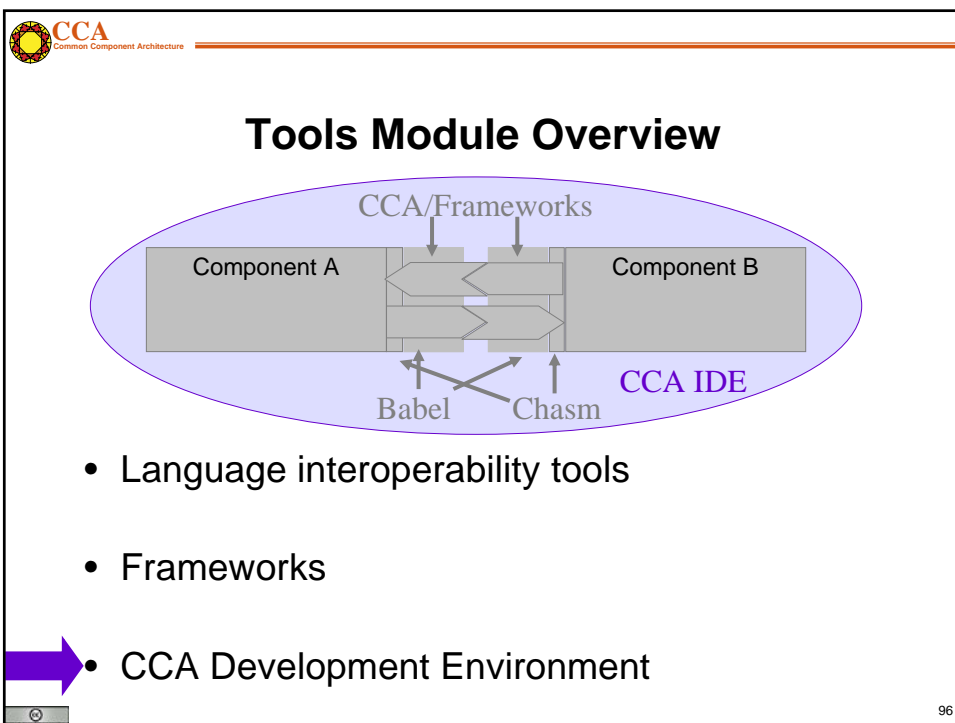


CCA	Common Component Architecture	Supplementary material for notes	
Experimental Frameworks			
Framework	Purpose	Summary	
Distributed CCA Framework (DCA)	MxN research	<ul style="list-style-type: none"> • Goal: explore MxN Parallel-Remote Method Invocation (PRMI) using MPI • Parallel data transfer and redistribution integrated into port invocation mechanism 	
LegionCCA	Grid-based research	<ul style="list-style-type: none"> • Goal: allow component-based CCA applications to run in Grid-scale environments using Legion • Supports creation, scheduling, persistence, migration, and fault notification; relies on Legion's built-in RPC mechanism (~Unix sockets) 	
XCAT-Java	Globus-based Grid research	<ul style="list-style-type: none"> • Goal: explore web interface for launching distributed applications • This (alpha) version compatible with latest CCA specification and provides built-in seamless compatibility with OGSI. 	




OGSI = Open Grid Services Infrastructure

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 **CCA**
Common Component Architecture


CCA IDE

Component Development Environments

- Bocca
 - Provides a light-weight, portable environment
- Eclipse
 - Provides a high-level graphical environment



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 **CCA**
Common Component Architecture

CCA IDE


Eclipse Environment Provided via Eclipse Plug-ins


- Provides a high-level graphical environment
 - Creating new SIDL-based components
 - Componentizing legacy codes
 - C, C++, Java and Fortran
- Automatic code generation

Supported on Linux, Windows, MacOS.



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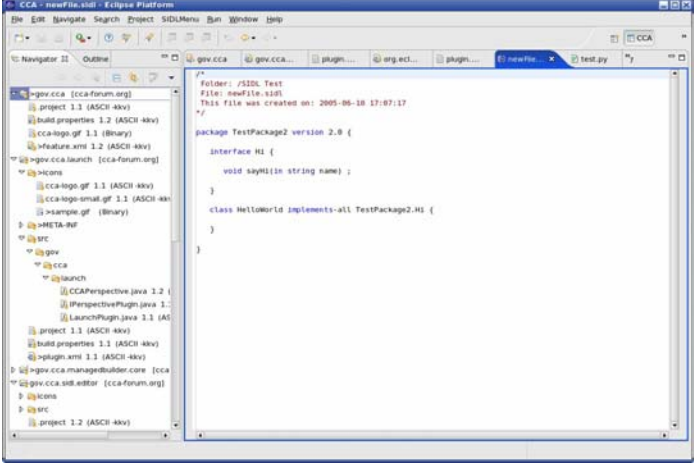




Component Development Environment Starts at the Eclipse Platform Level


Plug-ins for:


- SIDL Editor
- Wizards
- Preliminary automated build support



Imperative that you start by creating a new project!

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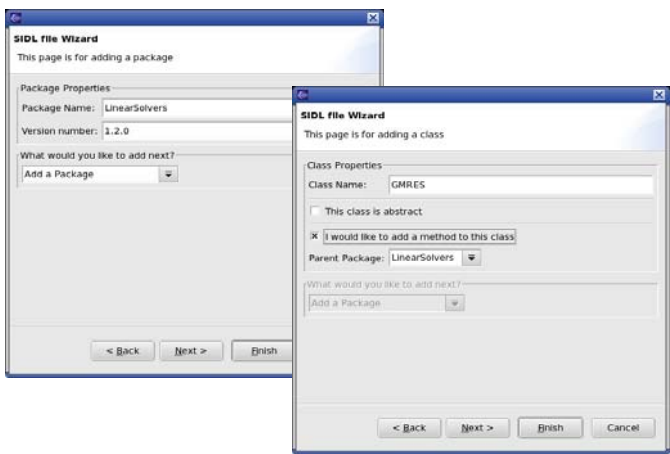




Wizards are Available for Adding Packages and Classes or Generating SIDL from Legacy Codes

• Intuitive interfaces to port and component definition

• Helper wizards for setting port, component and (in the future) application properties



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Bocca Development Environment

- Provides a text-based, portable environment
 - Create or import SIDL and CCA based codes.
 - Automatic build maintenance.
 - Easy to adopt or abandon while preserving code, build.
- No GUI required.
- Still in the early alpha stage of development
 - Being tested by managing the tutorial source.
 - Basis for common CCA toolkit installation.
 - No Java support yet. Coming soon.



Bocca is an Application Generator

- Purely command-line driven
 - Generates the glue code that enables components and language interoperability.
 - Enables rapid generation of an entire application skeleton and build system in minutes.
 - Good for full project life-cycle
 - But is meant to support very rapid prototyping.
- Complementary to Eclipse IDE
 - Does not even have an editor for creating code
 - Invoke your own editor with bocca assistance





Bocca Creates Skeletons for CCA

- Including **ports**
 - Give the SIDL name and an empty port is created.
- Including **components**
 - Give the name and an empty component is created.
 - With extra parameters the component uses/provides ports
- Including **build system**
 - For all ports/components in the project
 - Implemented in any CCA supported language
- Create applications with Ccaffeine GUI (today)
- Including **application** composition (coming soon)



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Bocca Example


```
# create an empty but buildable CCA skeleton
bocca create project myproj
cd myproj
bocca create port myJob
bocca create component myWorker --provides=myJob:job1

# fill in public functionality
bocca edit port myJob

# fill in implementation
bocca edit component -i myWorker
```



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CCA
Common Component Architecture

Supplementary material for notes

CCA Tools Contacts (1 of 2)

Tool	Purpose	More information
Babel	Scientific language interoperability tool kit	URL: www.llnl.gov/CASC/components Email: components@llnl.gov or babel-users@lists.llnl.gov
Ccaffeine	Direct-connect, parallel-friendly framework	URL: www.cca-forum.org/software/ Email: Ben Allan, ccafe-help@cca-forum.org Wiki: https://www.cca-forum.org/wiki
bocca	CCA development environment	Email: bocca-dev@cca-forum.org bocca FAQ: https://www.cca-forum.org/wiki


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CCA
Common Component Architecture

Supplementary material for notes

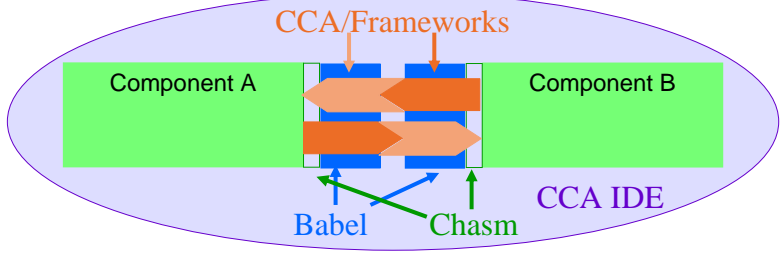
CCA Tools Contacts (2 of 2)

Tool	Purpose	More information
CCA Eclipse IDE	CCA development environment	Email: usability@cca-forum.org
SCIRun2	Cross-component model framework	URL: www.sci.utah.edu/ Email: Steve Parker, sparker@cs.utah.edu
XCAT-C++	Globus-based GRID framework	URL: grid.cs.binghamton.edu/projects/xcats/ Email: Madhu Govindaraju, mgovinda@cs.binghamton.edu


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 **CCA**
Common Component Architecture


Module Summary




The diagram illustrates the Module Summary. It shows two green rectangular boxes labeled 'Component A' and 'Component B' connected by a series of orange arrows representing 'CCA/Frameworks'. Below these, two blue arrows labeled 'Babel' and 'Chasm' point towards the connection. The entire setup is enclosed in a purple oval labeled 'CCA IDE'.

- Described **tools** for multi-lingual, scientific component 'plug-and-play'
 - Language interoperability through Babel and Chasm
 - CCA Frameworks provide mechanisms for composition
 - CCA Interactive Development Environments


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 **CCA**
Common Component Architecture



CCA Forum Tutorial Working Group

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

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Goal of This Module

Expose Attendees to How Existing Code is

- Wrapped into Babel objects, and then
- Promoted to CCA components

In the process, will also cover

- Babel Basics
- Scientific Interface Definition Language (SIDL)
- Code sample (“Hello World!”)



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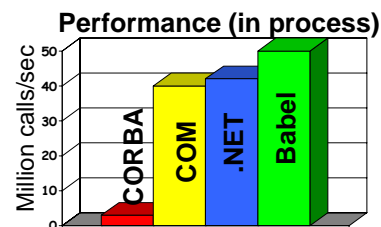


BABEL is Middleware for HPC



2006

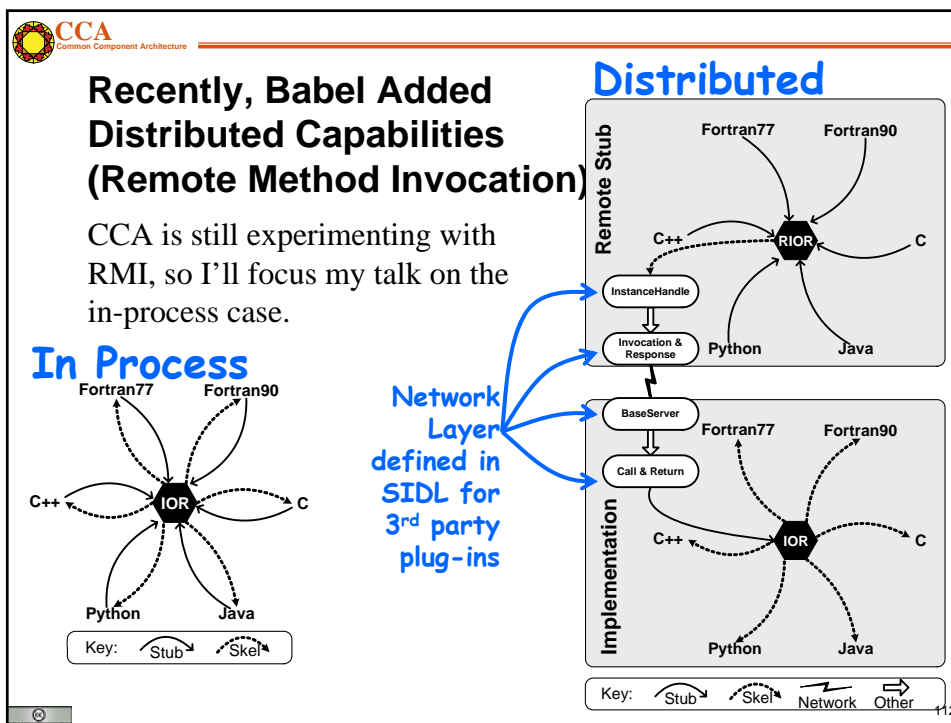
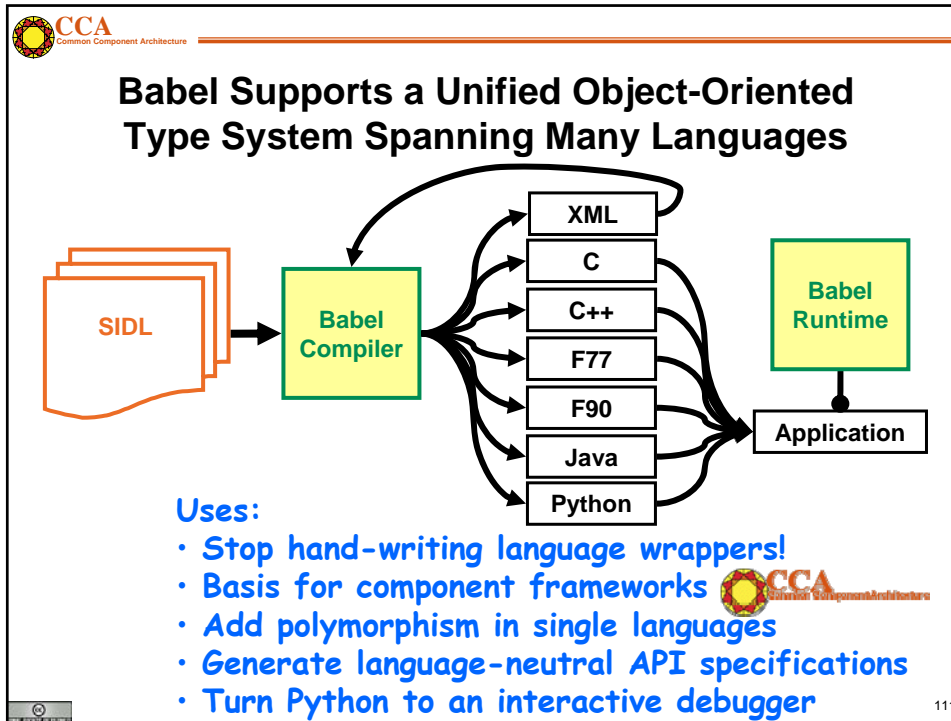
“The world’s most rapid communication among many programming languages in a single application.”

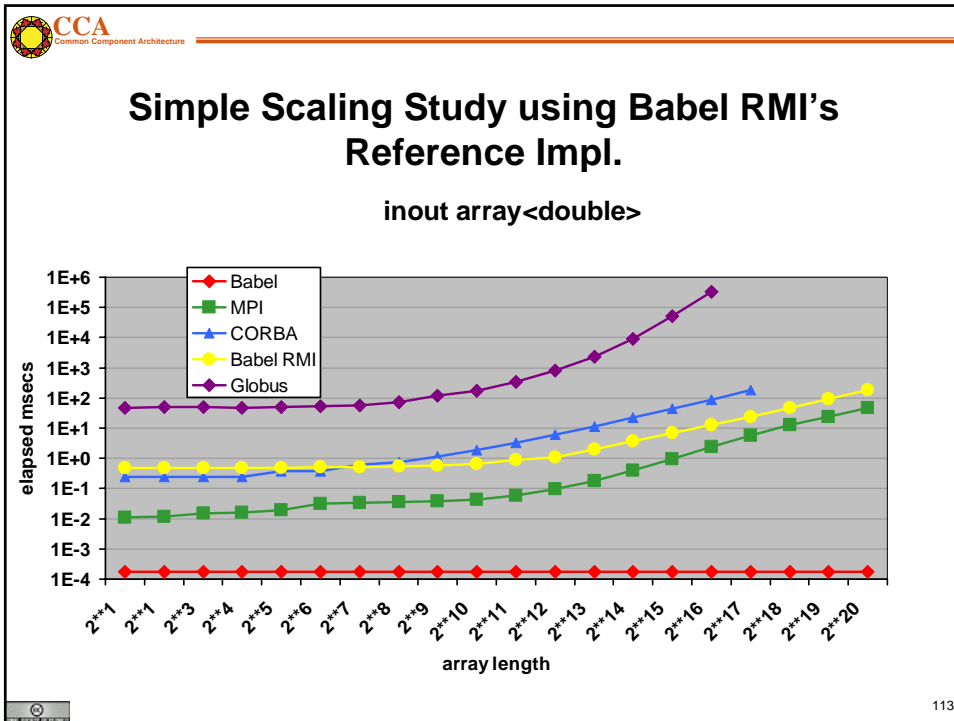


	CORBA	COM	.NET	Babel
BlueGene, Cray, Linux, AIX, & OS X	No	No	No	Yes*
Fortran	No	Limited	Limited	Yes
Multi-Dim Arrays	No	No	No	Yes
Complex Numbers	No	No	No	Yes
Licensing	Vendor Specific	Closed Source	Closed Source	Open Source

* BlueGene port expected mid 2007¹⁰







CCA
Common Component Architecture

Working Code: “Hello World” in F90 Using a Babel Type

```

program helloclient
  ① use greetings_english
  ② use siidl_BabelInterface
  implicit none
  ③ type(greetings_english_t) :: obj
  ④ type(siidl_BabelInterface_t) :: exc
  character (len=80) :: msg
  character (len=20) :: name
  ⑤ name='World'
  ⑥ call new( obj, exc )
  ⑦ call setName( obj, name, exc )
  ⑧ call sayIt( obj, msg, exc )
  ⑨ call deleteRef( obj, exc )
  print *, msg
end program helloclient
  
```

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Handout Material: Code Notes

- ① Use statement for the greetings.English type
- ② Use statement for the sidl.BaseInterface type
- ③ Obj is a F90 derived type we get from the using statement, note the “_t” extension that prevents it from colliding with the using statement.
- ④ Exc is used to hold exceptions thrown by methods
- ⑤ In C/C++ examples, this variable would be initialized by a the command-line variable “argv[1]”, but its trickier to do portably in F90 and too long, so I just initialize the name to “World”.
- ⑥ Obj is not yet initialized. The Babel idiom in F90 is to call new() to initialize the Babel type. In other languages its _create(). NOTE: good code would add error checking.
- ⑦ setName() puts data into the obj. It sets its state.
- ⑧ sayIt() returns the entire greeting including the aforementioned name.
- ⑨ deleteRef() is a subroutine that all Babel types inherit from a parent class. All Babel objects are reference counted. When there are no more outstanding references, the object is told to clean up after itself.



Working Code: “Hello World” in F90 Using a Babel Type

```

program helIoclient
  use greetings_English
  use sidl_BaseInterface
  implicit none
  type(greetings_English_t) :: obj
  type(sidl_BaseInterface_t) :: exc
  character (len=80) :: msg
  character (len=20) :: name
  name='World'
  call new( obj, exc )
  call setName( obj, name, exc )
  call sayIt( obj, msg, exc )
  call deleteRef( obj, exc )
  print *, msg
end program helIoclient

```

Looks like a native
F90 derived type

These subroutines
were specified in the
SIDL.

Other basic subroutines
are “built in” to all Babel
types.



Question: What language is “obj” really implemented in?

```

program helloclient
  use greetings_English
  use si dl _BaseInterface
  implicit none
  type(greetings_English_t) :: obj
  type(si dl _BaseInterface_t) :: exc
  character (len=80)          : msg
  character (len=20)          :
  name=' World'
  call new( obj, exc )
  call setName( obj, name, exc )
  call sayI t( obj, msg, exc )
  call deleteRef( obj, exc )
  print *, msg
end program helloclient

```

Answer: Can't Know!

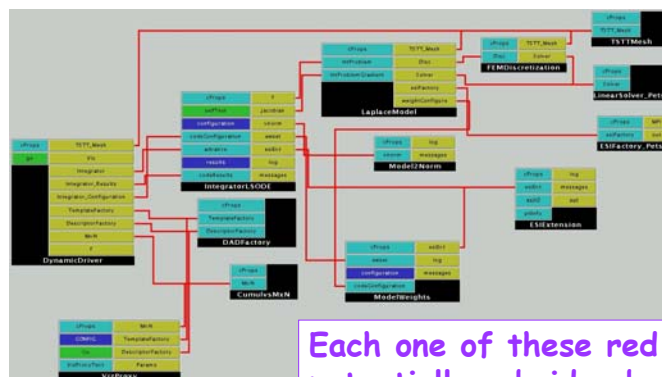
With Babel, it could be C, C++, Python, Java, Fortran77, or Fortran90/95

In fact, it could change on different runs without recompiling this code!

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CCA uses Babel for high-performance n-way language interoperability



Each one of these red lines, is potentially a bridge between two languages. No telling which language your component will be connected to when you write it.

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The SIDL File that defines the “greetings.English” type

```

①② package greetings version 1.0 {
③④   interface Hello {
⑤       void setName( in string name );
        string sayIt ( );
    }
⑥   class English implements-all Hello { }
}
```

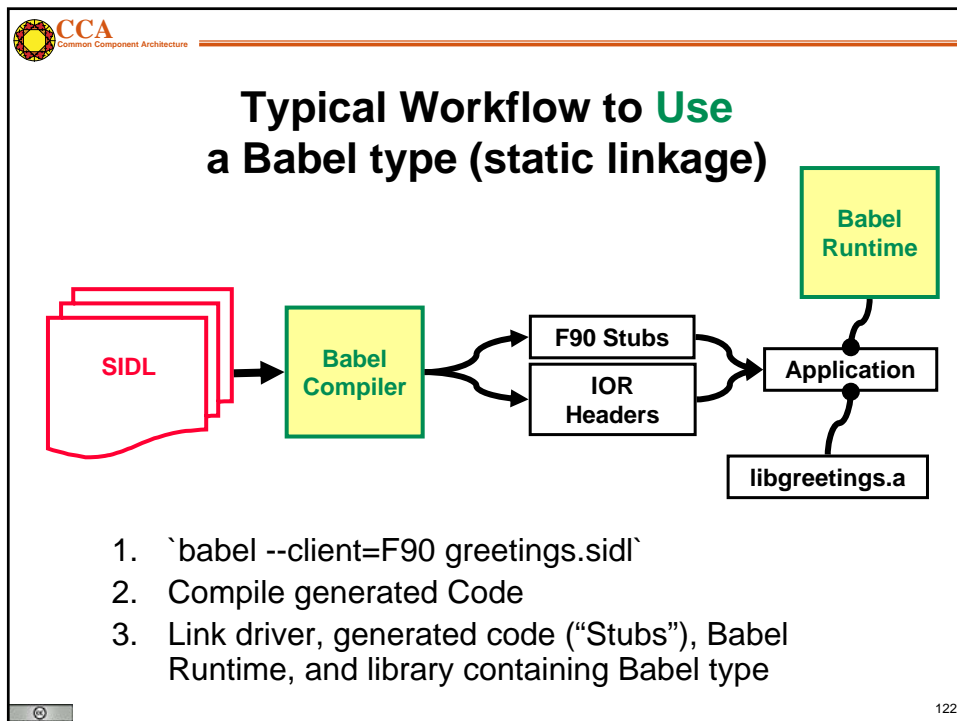
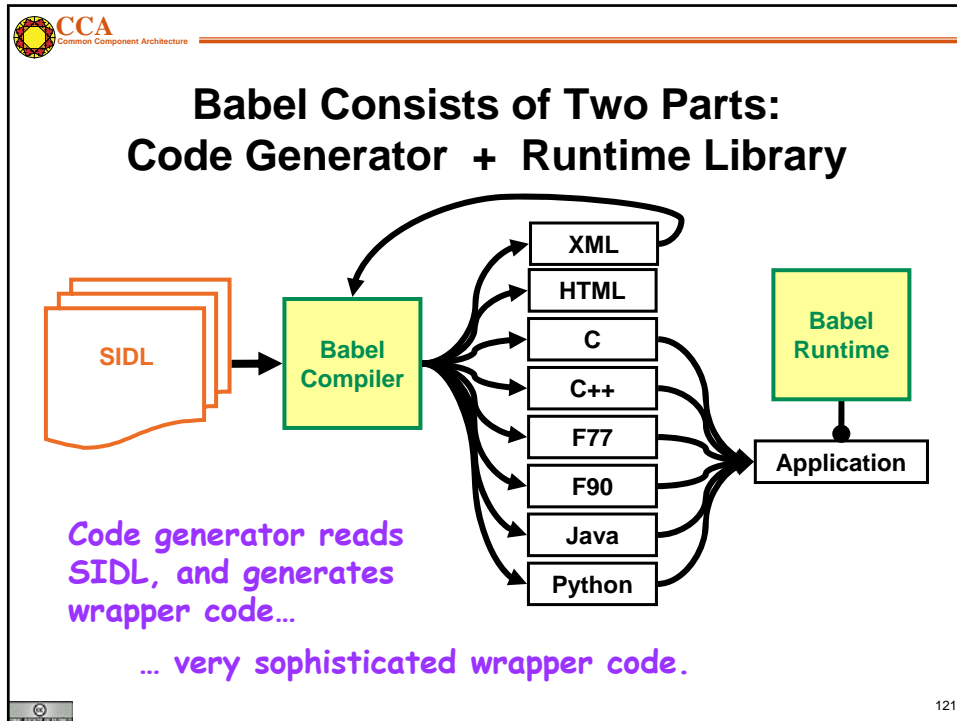
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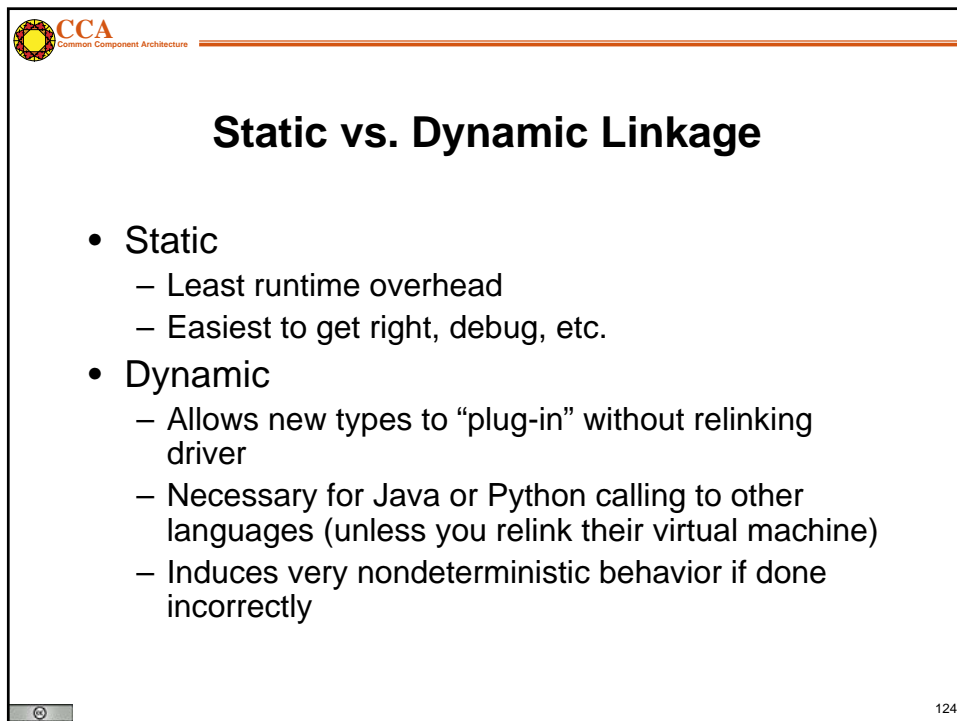
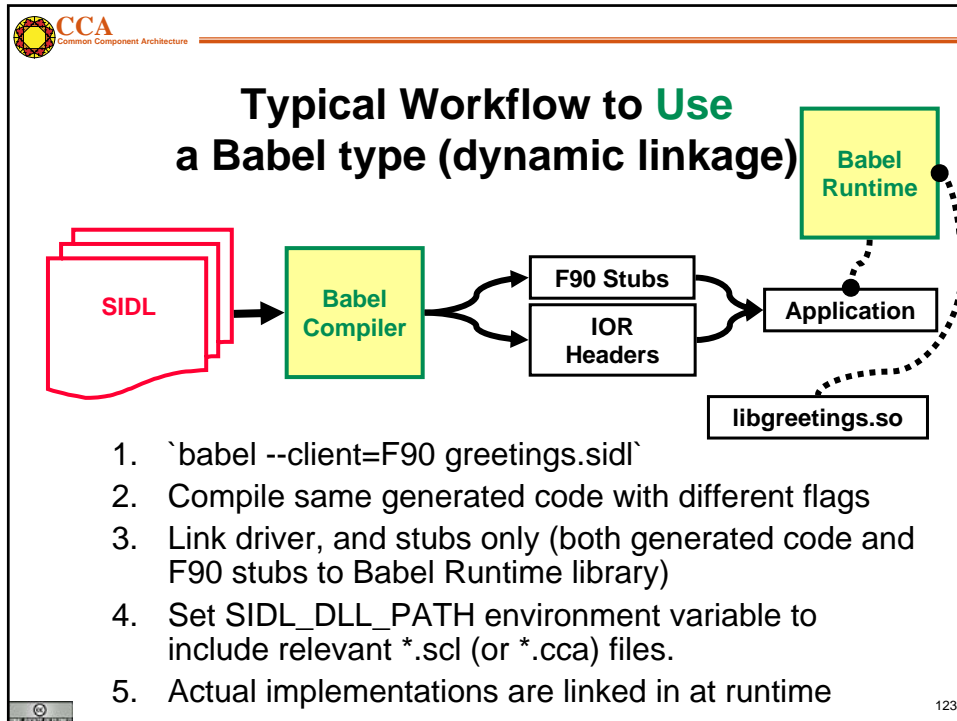


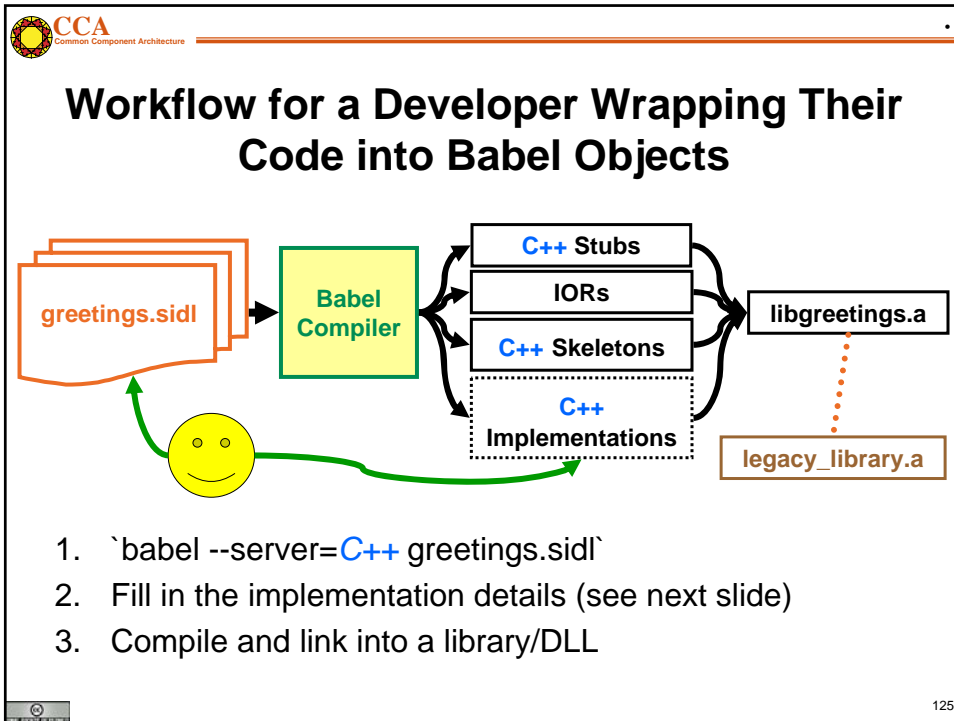
Handout Material: Code Notes

- ① Packages contain user-defined types and are used to reduce naming collisions. Packages can be nested.
- ② Packages can be versioned. User defined types must be nested inside a versioned package and gain the same version number as the innermost versioned package
- ③ SIDL has a inheritance model similar to Java and Objective C. Classes can inherit multiple interfaces, but at most one implementation (other class).
- ④ An interface describes an API, but doesn't name the implementation.
- ⑤ Note that arguments have mode, type, and name. Mode can be one of “in”, “out”, and “inout”. These SIDL modes have slightly different semantics than Fortran90 “intents”.
- ⑥ This class generates English greetings. One could imagine a strategy for internationalization that uses the Hello interface everywhere, but loads in English, French, or whatever classes based on user's preference.

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CCA
Common Component Architecture

Implementation Details Must be Filled in Between Splicer Blocks

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

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

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Quick Review of Babel in general before proceeding to CCA specifics

- Babel can be used as a standalone tool
- Each language binding strikes a balance
 - support the SIDL type system (OO, exceptions, etc.)
 - provide it in a manner “natural” to experienced programmers in the target language
- For more details about Babel and SIDL
 - SC|04 tutorial slides for Babel
<http://www.llnl.gov/CASC/components/docs/sc04.html>
 - Babel User's Guide (aka. the BUG)
http://www.llnl.gov/CASC/components/docs/users_guide/



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CCA uses SIDL to specify APIs and Type Hierarchy for Frameworks, Services, Components, & Ports

- **A CCA framework must**
 - implement gov. cca. AbstractFramework,
 - provide a gov. cca. ports. BuilderService,
 - etc.
- **A CCA port must**
 - be a SIDL interface extending gov. cca. Port
- **A CCA component must**
 - be a SIDL class implementing gov. cca. Component

The CCA Specification is a SIDL file.



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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

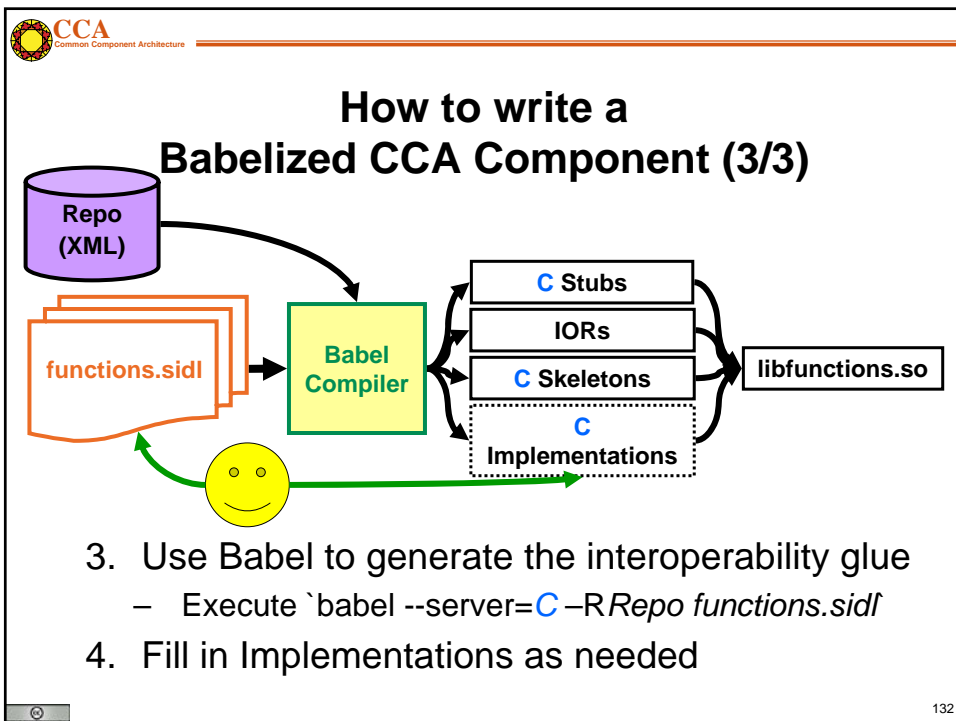
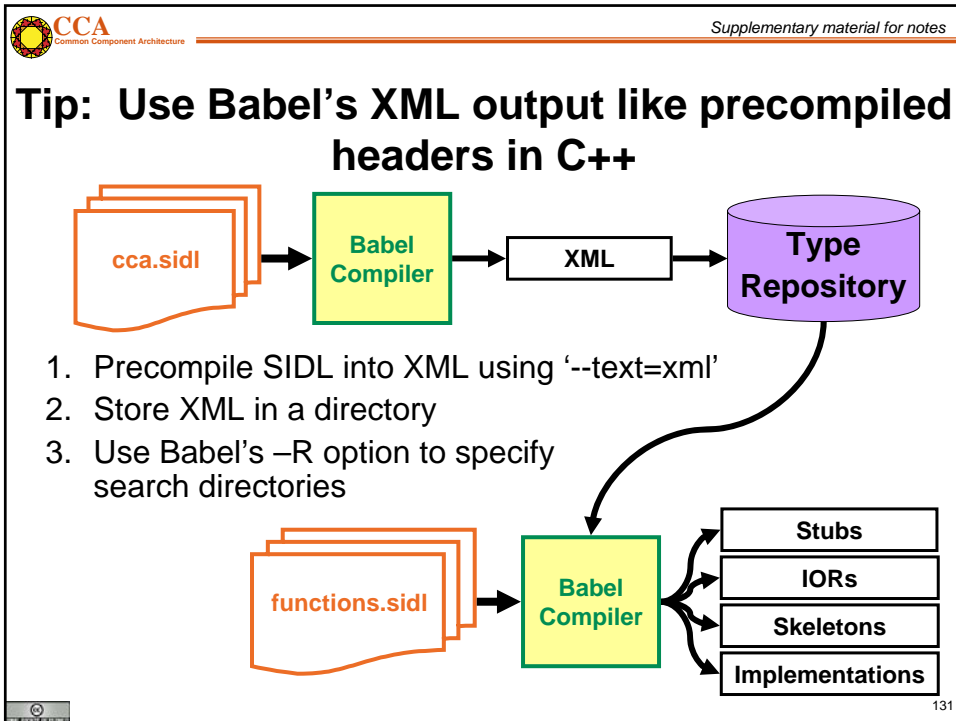
- CCA Component =
 - SIDL Class
 - implements gov.cca.Component (and any provided ports)


```
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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CCA
Common Component Architecture


Review: Goal of This Module

Learn how existing code is


- Wrapped into Babel objects, and
- Promoted to CCA components

In the process, will also covered

- Babel Basics
- Scientific Interface Definition Language (SIDL)
- Code sample (“Hello World!”)




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CCA
Common Component Architecture

Contact Information

- Project: <http://www.llnl.gov/CASC/components>
- Project Team Email: components@llnl.gov
- Mailing Lists: majordomo@lists.llnl.gov
subscribe [babel-users](#) [email address]
subscribe [babel-announce](#) [email address]
- Bug Tracking: <https://www.cca-forum.org/bugs/babel/>
or email to babel-bugs@cca-forum.org



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CCA

Common Component Architecture

Using CCA: Approaches & Experience

CCA Forum Tutorial Working Group

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



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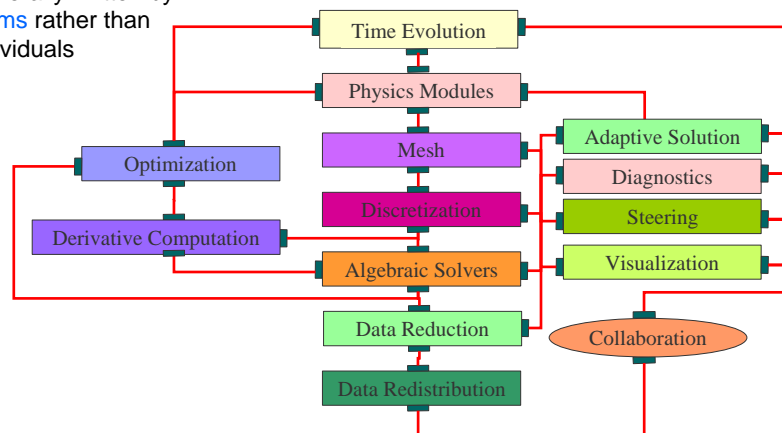
135



CCA
Common Component Architecture

Modern Scientific Software Development

- Complex codes, often **coupling** multiple types of physics, time or length scales, involving a broad range of computational and numerical techniques
- Different parts of the code require significantly **different expertise** to write (well)
- Generally written by **teams** rather than individuals



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Using CCA to Help Manage Complexity

- Application areas participating in the CCA:
astronomy, astrophysics, biological and medical simulations, chemically reacting flow, climate and weather modelling, combustion, computational chemistry, data management, fusion and plasma physics modelling, linear algebra, materials science, molecular electronics, nanoscience, nuclear power plant simulations, structured adaptive meshes, unstructured meshes, and visualization
- Research agencies sponsoring software development using the CCA:
DOE (SciDAC, Office of Science, NNSA/ASC), NASA, NIH, NSF, DoD, European Union



Outline

- Developing Components
 - Strategies for both developing new codes and wrapping existing codes
- Case Studies
 - Chemistry project
 - Moderate-sized multi-disciplinary, multi-institutional team
 - Using Ccaffeine framework, SIDL components
 - Combustion toolkit
 - Small team, both new and wrapped codes
 - Using Ccaffeine framework, C++ components





Developing Components (Both New Codes and Wrappers to Existing Codes)

- Productivity Benefits
- Application Decomposition Strategies
- Interface Design Issues
 - Social factors
 - Technical factors
- Implementation Issues and Patterns



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CCA Productivity Benefits

- Fast algorithmic **experiments** and benchmarks by substituting components
- Once ports are defined, domain-expert component implementers can **work separately** in their own **favorite languages**
- Work of **transient contributors** remains as well-defined, lasting components
- Wrapped legacy portions **need not be reimplemented or reverified**



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Components in the Small: Impacts within a Project

Benefits include:

- Rapid testing, debugging, and benchmarking
- Support for implementation-hiding discipline
- Coordination of independent workers
- Interface change effects across components are clear and usually automatically found by compilers if overlooked
- Object-orientation made simpler for C and Fortran



Components in the Large: Connecting Multiple Projects

Benefits include:

- SIDL can be used to facilitate the interface consensus processes
- Different sub-projects do not have to agree on one implementation language
- Developers who never meet in person have an excellent chance of code integration working on the first try

Costs include:

- Consensus can be expensive to obtain
- Writing code for others to use is more difficult than writing it just for yourself





Application Decomposition Strategies

- Conceptually decompose the application into
 - cutting-edge areas (*less stable*)
and
 - areas that can employ existing component-based libraries (*more stable*)
- Decompose each area into components for
 - physics
 - mathematics
 - data managementas dictated by the application; sketch a typical component layout
- Many components will encapsulate *algorithmic logic only*, with little or no private data
- Most HPC applications will have a *central data abstraction* that provides data memory management and parallel communication
- In a multilanguage application, all *I/O may need to be isolated* into components written in a single common language (file based I/O should not be affected)
- Component boundaries (and port interfaces) may be set to *isolate proprietary code or difficult contributors*



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Interface Design: Social Factors (Defining Ports to Wrap Existing Code)

- Will the port hide just one implementation, or will there need to be plug compatibility with other implementations? From other teams?
- Who defines the interface and maintains it?
 1. Project dictator? (*Fast...*)
 2. The owner of the legacy functionality? (*Slow, if not you...*)
 3. A standards committee? (*Really slow...*)
- How many iterations of redefining the ports will the customers tolerate?



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Interface Design: Technical Factors

- Do we make a single large port look like the underlying library or divide functions into groups on separate ports?
- Should a function with many optional arguments be split into several alternative functions with simpler usage?
- Do we make the ports more general than the existing code?
- Do we require the ports to work across languages?
Across networks?
 - If not, gains in efficiency or coding ease might be had
 - If so, memory management and I/O challenges may arise



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Implementation Issues in Wrapping

- Do we split large libraries into several components?
 - Splitting is difficult to do if global variables or common blocks are widely used.
- Do we expect more than one implementation instance of a port in a single run-time?
 - If not, interface contracts may include global side effects
- Do we integrate the wrapper code in the existing code's development and build processes?
 - If not, how do we ensure build consistency and on-going wrapper support?
- Code bases with large interfaces need automated wrapping tools
 - E.g., [see Chasm info in the Tools module](#) of the tutorial



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Benefits of Wrapping Code Using CCA

- Setting a language-neutral interface definition (SIDL) can greatly clarify design discussions
- Provides a chance to reorganize the interface and hide globals
- Allows testing of alternate versions if doing performance studies
- Allows easy “experimentation” with new algorithms
- Software discipline is enforced, not optional
- Implementation decisions (to split libraries, etc) can be easily revised over time if interfaces remain constant (possibly with the addition of new interfaces)



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Interface Design for New Code

- Write SIDL for each connection (port) in the sketched component layout
- If two ports must always be used together, consider merging them
- Review SIDL drafts for near-duplication of ports
- Avoid creating interface contracts that require using hidden global data
- Consider exporting tuning and/or configuration parameter inputs as a port
- All the design issues from wrapping existing code apply, also
- ***Interfaces will change.***



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Recommended Implementation Patterns

- Expect to decompose initial components further as work progresses and requirements expand
- Build systems (i.e. `make`) should be kept as simple as possible
 - Keep a subdirectory for port definitions and any implementation-independent glue code derived from the ports
 - Keep each component (and any wrapped code) in its own subdirectory
 - Keep application-wide flags in a configure script or an include file common to all components and ports
 - Consistency is key. Extract build flags from `cca-spec-babel-config` and if possible compile & link with `babel-libtool`



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Outline

- Developing Components
 - Strategies for both developing new codes and wrapping existing codes




Case Studies

- Chemistry project
 - Moderate-sized multi-disciplinary, multi-institutional team
 - Using Ccaffeine framework, SIDL components
- Combustion toolkit
 - Small team, both new and wrapped codes
 - Using Ccaffeine framework, C++ components



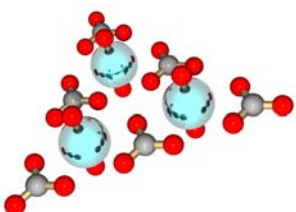
150





CCA
Common Component Architecture

Case Study 1: Chemistry Project

- Funded via SciDAC initiative
- Initial focus: Full-featured components for structure optimization
 - **Chemistry models** provided by MPQC (SNL) & NWChem (PNNL)
 - **Numerical optimization** provided by TAO (ANL) solvers
 - **Linear algebra** provided by GA (PNNL) and PETSc (ANL)
- Recent work:
 - Multi-level parallelism
 - Low-level chemistry model integration (e.g., molecular integrals)




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CCA
Common Component Architecture

CCA-Chemistry Project Participants

Pacific Northwest National Laboratory

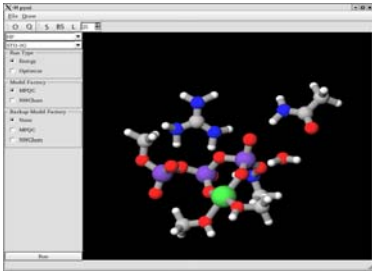
Theresa L. Windus
Yuri Alexeev
Manojkumar Krishnan
Jarek Nieplocha
Carl Fahlstrom
Elizabeth Jurrus


Argonne National Laboratory

Steve Benson
Lois Curfman McInnes
Jason Sarich


Sandia National Laboratory

Curtis L. Janssen
Joseph P. Kenney







Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy



ARGONNE NATIONAL LABORATORY
UNIVERSITY OF CHICAGO



Sandia
National
Laboratories


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CCA Impacts in Computational Chemistry

Through 4 chemistry applications we consider different facets of CCA functionality:

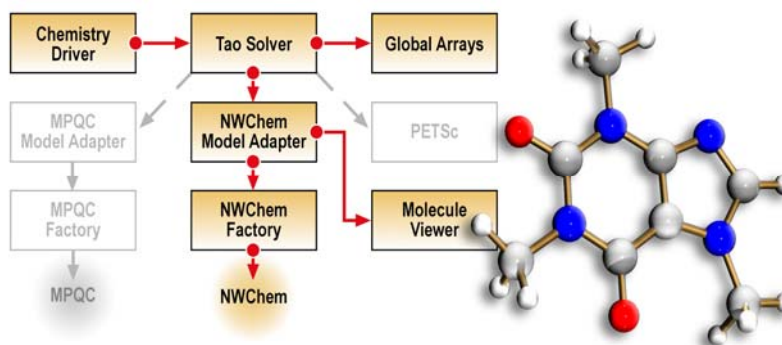
- **Molecular Geometry Optimization**
 - Combining diverse expertise of 5 different research groups
- **Lennard-Jones Molecular Dynamics**
 - Achieving good scalability and low CCA overhead
- **Multi-level Parallelism in Computational Chemistry**
 - Combining SPMD and MPMD parallelism
- **Molecular Integral Evaluation**
 - Component interoperability at deeper levels within chemistry libraries



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App 1: Molecular Geometry Optimization: Combining Diverse Expertise

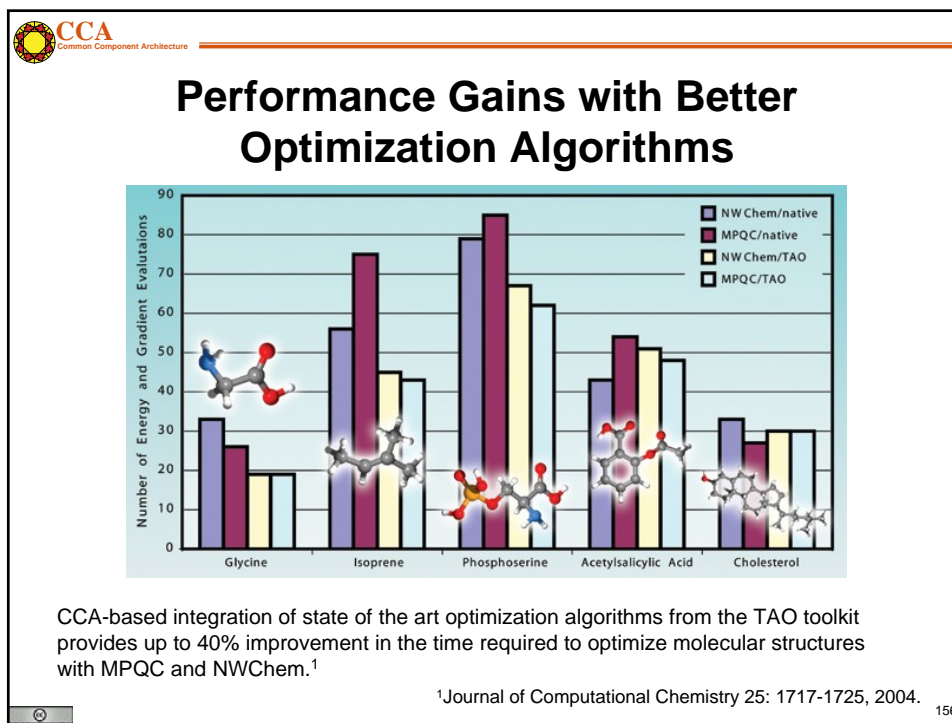
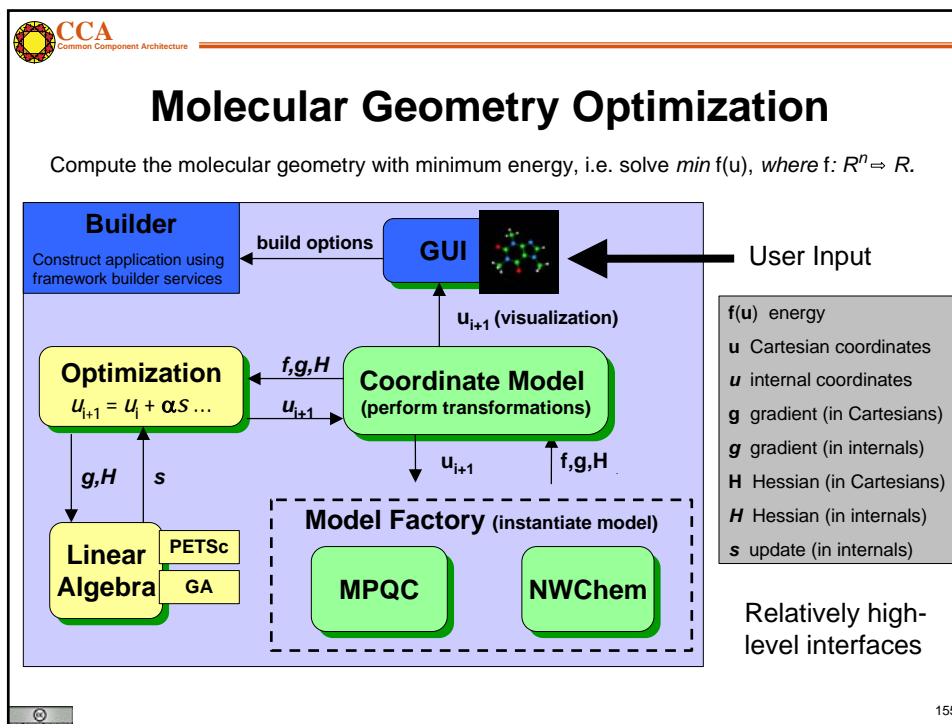


CCA quantum chemistry application using components based on:

- MPQC, NWChem (chemistry – energy evaluation)
- GA, PETSc (parallel data management and linear algebra)
- TAO (numerical optimization)



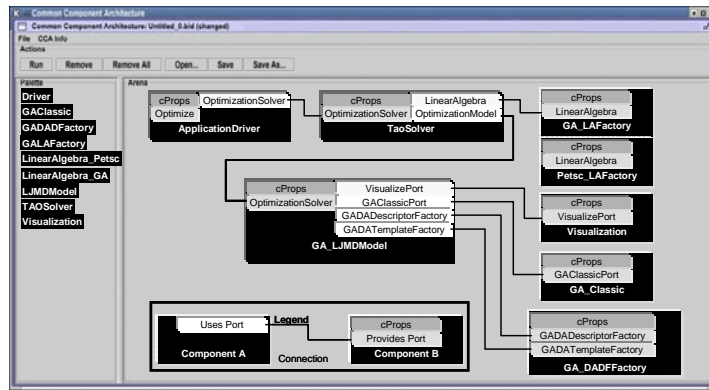
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App 2: Molecular Dynamics



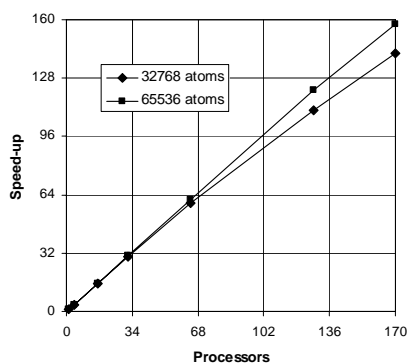
CCA component wiring diagram for Lennard-Jones energy optimization, which integrates TAO, GA and Lennard-Jones molecular dynamics components

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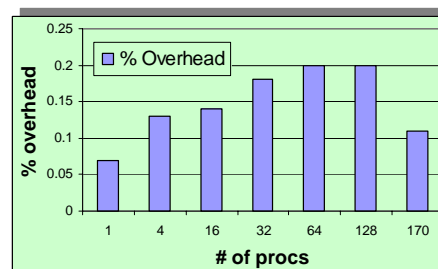
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Good CCA Scalability, Negligible Overhead



Speedup in the Lennard-Jones potential energy optimization for 32,768 and 65,536 particles

Overhead of CCA component (using SIDL) vs. "native" C++ implementation of a parallel Lennard-Jones molecular dynamics simulation



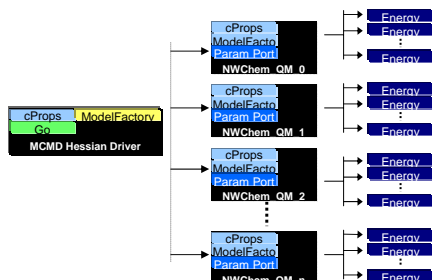
% Overhead using CCA Components

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App 3: Multilevel Parallelism Using CCA

- Massive numbers of CPUs in future systems require leading edge tools to exploit all available parallelism
- GA helps exploit multi-level parallelism
- Multi-level parallelism using CCA & GA processor groups: Combining SCMD (Single Component Multiple Data) and MCMD (Multiple Component Multiple Data) paradigms



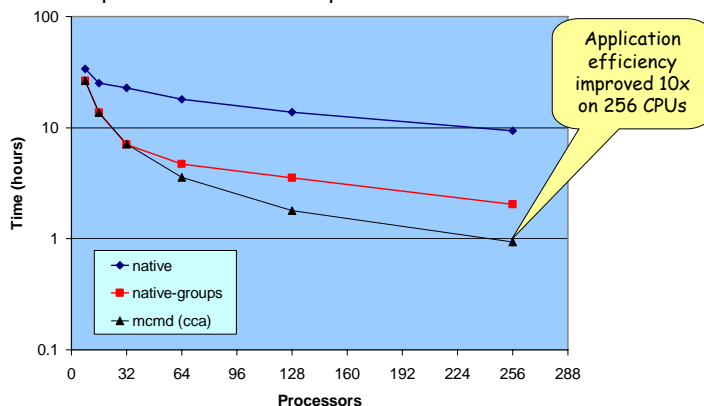
The MCMD Driver launches multiple instances of NWChem components on subsets of processors (also assigns a GA communicator for every instance). Each NWChem QM component does multiple energy computations on subgroups.

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Multilevel Parallelism - MCMD

NWChem Scalability of Numerical Hessian Computation on 11.8 TFlop/s HP Cluster at PNNL



M. Krishnan, Y. Alexeev, T. Windus, and J. Nieplocha, Multilevel Parallelism in Computational Chemistry using the Common Component Architecture and Global Arrays, Proceedings of the IEEE/ACM SC2005 Conference.

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App 4: Molecular Integrals: Deeper Levels of Interoperability among Chemistry Packages

- As a first step toward low-level integration of chemistry models, capabilities to provide and utilize molecular integral evaluator components are being added to MPQC and NWChem (also working with GAMESS developers)
- Specialized integral capabilities are provided to CCA chemistry models
 - Relativistic integrals in NWChem
 - Non-standard 2-electron integrals for linear-R12 theories in MPQC

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CCA Impacts in Computational Chemistry: Review

Through 4 chemistry applications we considered different facets of CCA functionality:

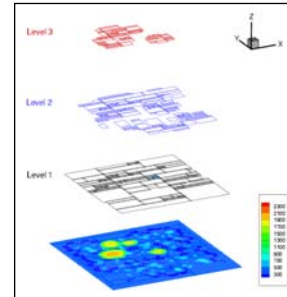
- Combining diverse expertise of 5 different research groups
- Achieving good scalability and low CCA overhead
- Implementing multi-level parallelism by combining SPMD and MPMD paradigms
- Addressing component interoperability at deeper levels within chemistry libraries

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Case Study 2: Combustion Project

- Computational Facility for Reacting Flow Science (CFRFS)
 - <http://cfrfs.ca.sandia.gov>
 - Funded via SciDAC initiative (PI: H. Najm)
- Focus: A toolkit to perform simulations of lab-sized unsteady flames
 - Solve the Navier-Stokes w/detailed chemistry
 - Various mechanisms up to ~50 species, 300 reactions
- Consequently:
 - Disparity of **length scales** :
 - use structured adaptively refined meshes
 - Disparity of **time scales** (transport versus chemistry) :
 - use an operator-split construction and solve chemistry implicitly
 - adaptive chemistry: use **computational singular perturbation** to find and follow low dimensional chemical manifolds



J. Ray, S. Lefantzi, J. Lee, C. Kennedy, W. Ashurst, K. Smith, M. Liu, N. Trebon

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Why Use CCA in the CFRFS Toolkit?

- Separate clearly the physics models, numerical algorithms, and the “CS” parts of the toolkit
 - Strictly functional!
- Realize the separation in software
- Tame **software** complexity
- Separate contributions by transient contributors
 - Form the bulk of the developers
- Create “chunks” of well-defined functionality that can be developed by experts (usually numerical analysts and combustion researchers)

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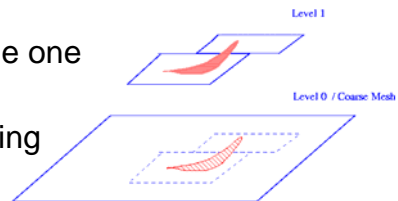
Design Principles of the Toolkit / 1

- **Principal Aim: Reduce software complexity**
 - We can deal with the rest
- Functional decomposition into components
 - “Data Object” and Mesh components
 - (Large) set of numerical algorithmic components (integrators, linear/nonlinear solvers, etc.)
 - (Large) set of physical models components (gas-phase combustion chemistry, thermodynamics, fluid dynamic quantities, e.g. viscous stress tensor)
 - Handful of adaptors



Design Principles of the Toolkit / 2

- Decomposition reflected in the port design and implementation
 - Most re-implemented port is the one that exchanges a rectangular sub-domain's data for processing by components
- Sparse connectivity between components
 - i.e., components communicate with a few others
 - Large apps (component assemblies) are composed by assembling smaller, largely independent sub-assemblies
 - Sub-assemblies usually deal with a certain physics
 - Intuitive way to assemble a *multiphysics* code



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The Code

Transport subassembly

Diffusion coefficients

Chemistry reaction subassembly

Separate component subsystems for transport (black) and for reaction (orange) in a reaction-diffusion code. They two are coupled at a relatively high level.

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Has the Toolkit Approach Helped Tame Software Complexity?

- How has the code evolved?
 - How often have new ports been added?
 - How many rewrites have been done?
- How large are the components?
- How many ports do they have?
 - How large are the ports?
- How many ports exist?
 - i.e., Is the design general enough to support many implementations?
- What is the connectivity of components in application codes?

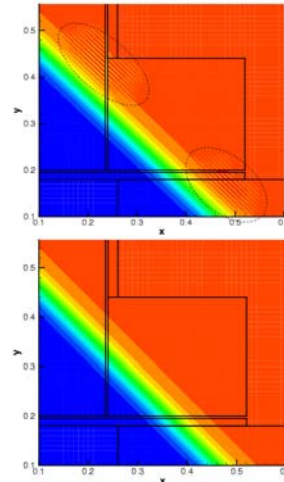
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CFRFS Toolkit Status

- Started in 2001
- 61 components today, all peers, independent, mixed and matched for combustion and shock hydrodynamics
- 7 external libraries
- Contributors: 9 in all, including 3 summer students
- Only 2 of the 9 contributors are at SNL today



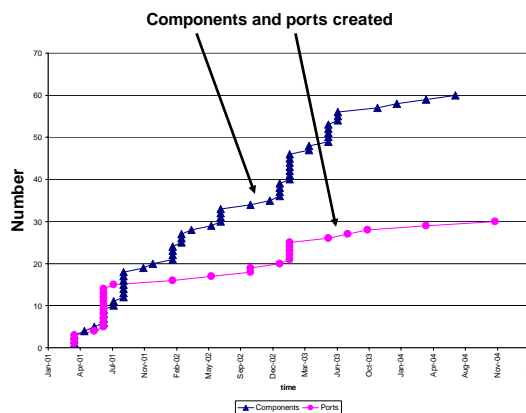
A Fitzhugh-Nagumo equation being solved on a block-structured adaptively refined mesh. The top image illustrates Runge phenomena at coarse-fine interfaces (dashed ovals) when using high-order schemes (6th order interpolations with 4th order discretizations). Filtering them with an 8th order filter removes them (bottom).

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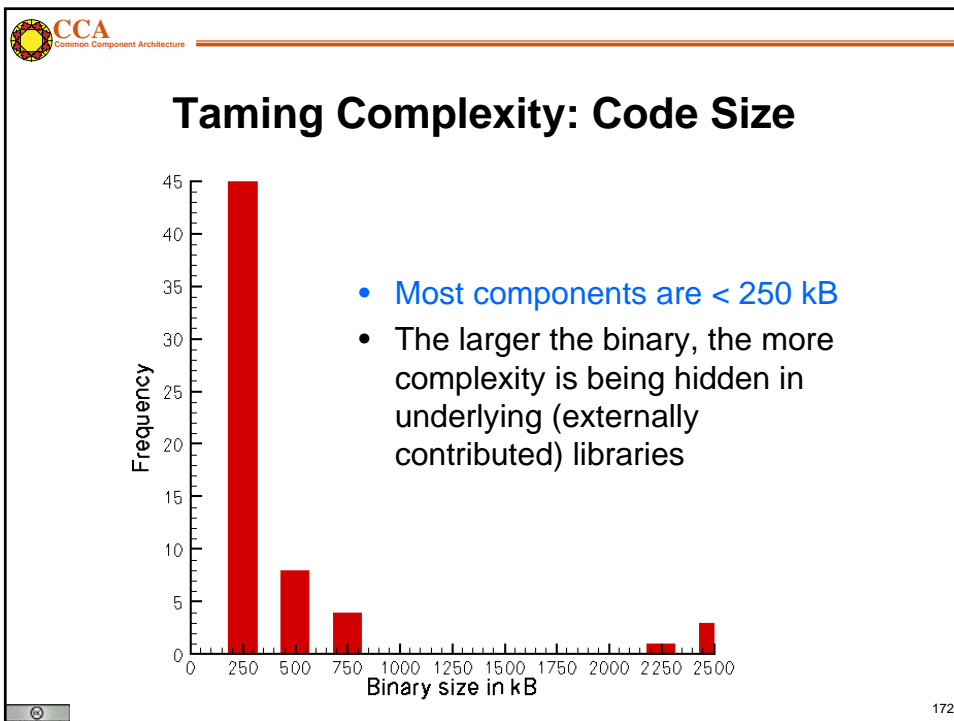
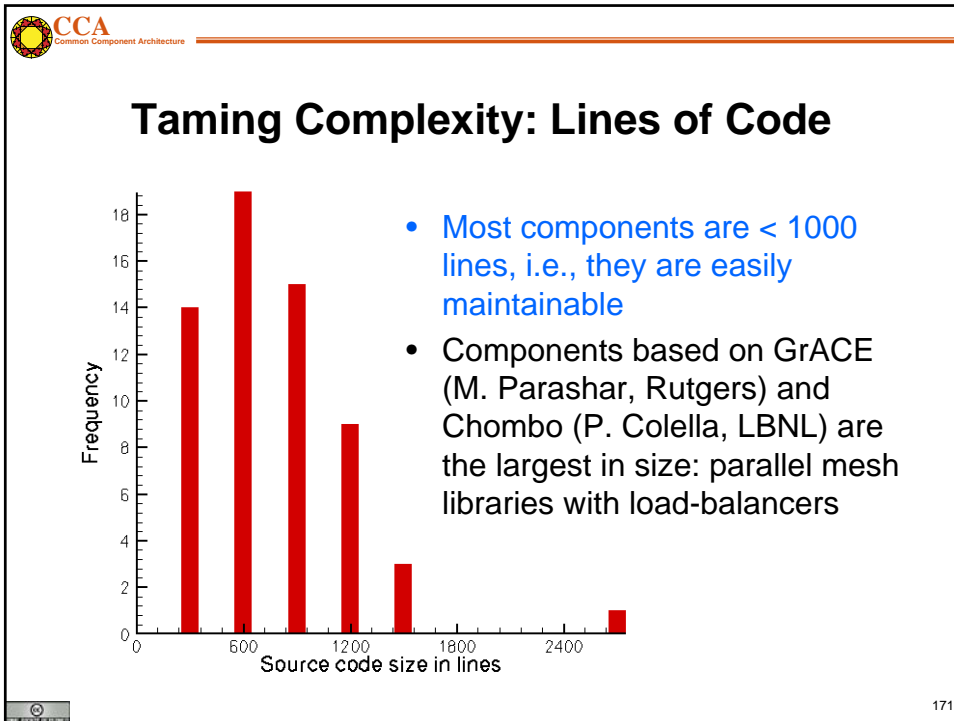
Common Component Architecture

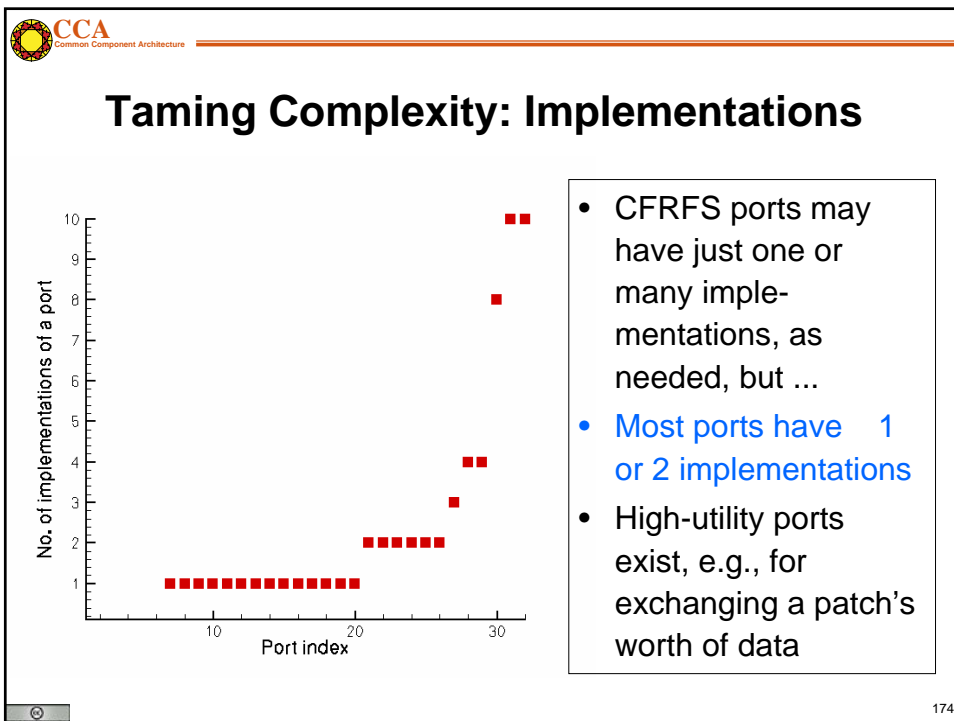
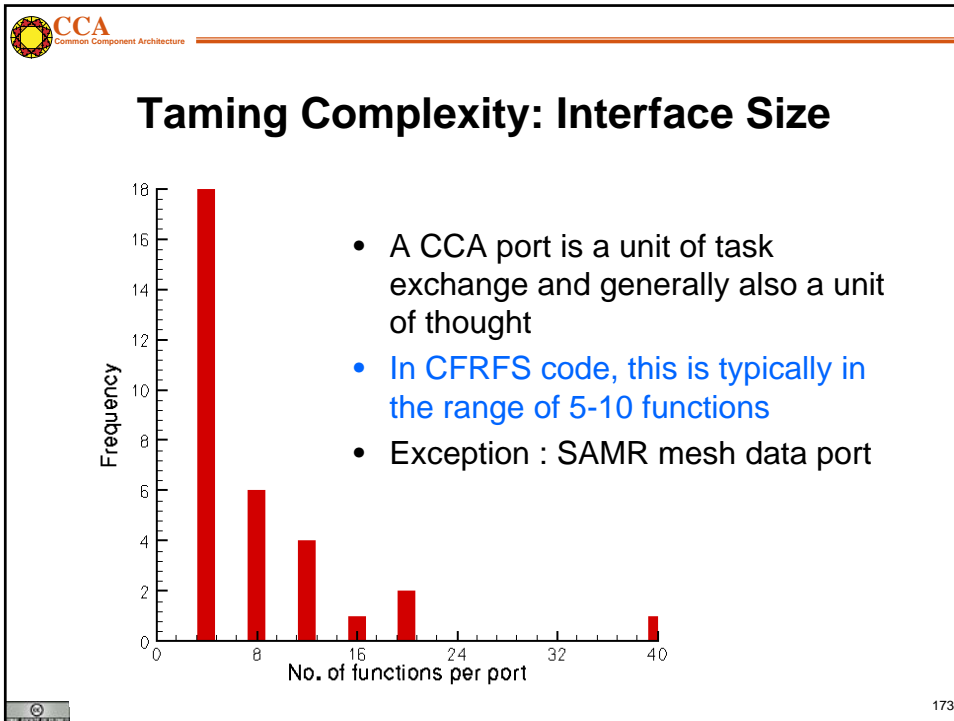
Scalability: Capability Growth without Rewrites

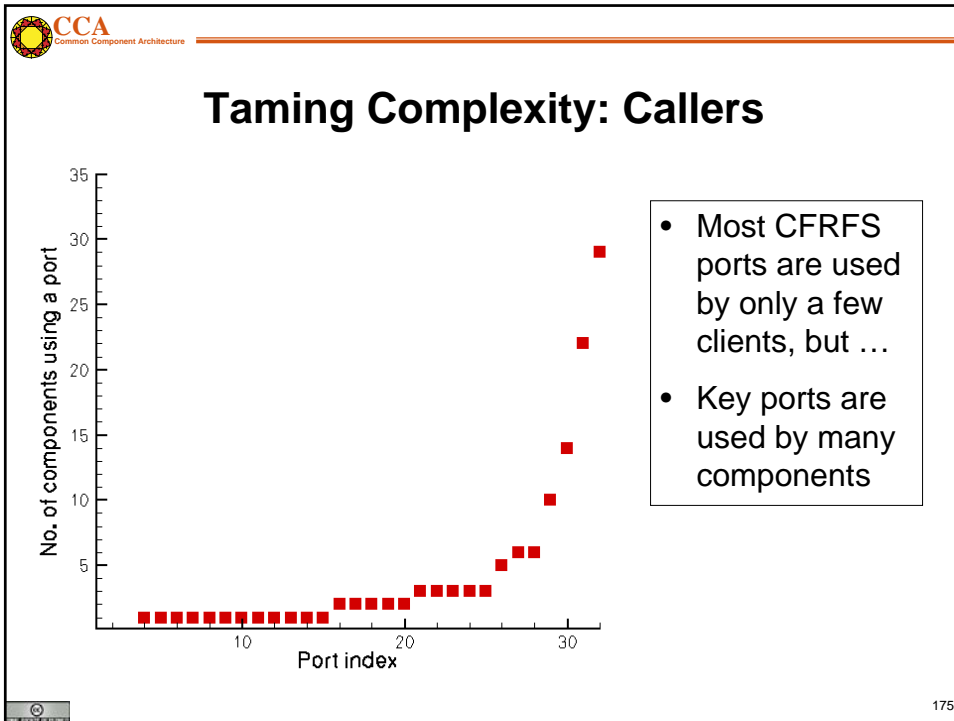


- Port designs typically occur in spurts followed by long component development times.
- Ports may have multiple implementations; hence the number of ports is typically less than the number of components.
- As the toolkit has matured, the number of ports is seen to be asymptoting to a slow growth rate.

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Adaptive Codes / Computational Quality of Service

- Can codes be optimized during runtime ?
 - CCA code is an assembly of components
 - Component applications can be non-optimal because
 - The mathematical characteristics of the simulation are different from those of the component
 - The component is badly implemented
- So, can one dynamically “re-arrange” an assembly to improve performance?
- Simplistically, 2 approaches:
 - Create performance model per component, use best one
 - Create expert system that analyzes problem and picks good solution strategy



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Requirements for CQoS codes

- A software framework within which ordinary components can be “CQoS-ified”
 - By “decorating” a given component-network with extra CQoS components
- The ‘extra’ components form a control system which monitors, tweaks and/or replaces components commensurate with the problem and the computer at hand.
 - Requires continuous performance monitoring
 - How do you monitor a component non-invasively?
 - Requires continuous querying of a performance database to analyze current situation and make predictions
- The control infrastructure/framework/software is generic, the control law is domain specific.



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Who's working on CQoS ?

- Control law work:
 - Computational chemistry: evaluation of integrals
 - Partitioning of block-structured adaptive meshes
 - Iterative sparse linear algebra: mix-and-match accelerators and preconditioners
- Infrastructure work
 - Performance measurement: Automatic performance data (statistical) analysis
 - Design of a CQoS API (to enable extraction & storage of performance data)
 - Quick-and-dirty experimentation in a CQoS world (SciPY based)
 - Infrastructural components – databases, regression-ers etc

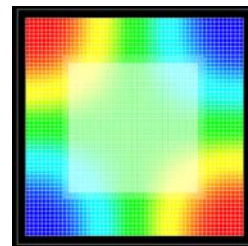


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Incorporating Other Frameworks

- Chombo (by P. Colella, LBNL) has solvers (AMRGodunov, AMRElliptic, etc.) that:
 - Work on block structured adaptive meshes
 - Accept Chombo-specific data structures
 - But fundamentally require:
 - A double pointer, an array, where variables on a patch (box) are stored in blocked format
 - Bunch of integer arrays that describe the array
- Challenge: Can Chombo be used within CCA?
- Need a standardized way of getting data into Chombo
 - Pointer aliasing, not data copy
- Implementation of this “standard” interface



Using Chombo to solve the Poisson equation (needed for CFRFS flame simulations).



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Using CCA: Summary

- Review of guidelines for developing high-performance scientific components (both new code and wrappers for existing code)
- CCA is an enabling technology for scientific applications
 - Has enabled mathematicians, chemists, combustion scientists, and computer scientists to contribute new strategies that are shrink-wrapped for easy re-use
 - Apart from **science research**, also spawned **new research directions in CS**
 - Has enabled research scientists to investigate unconventional approaches, for example multilevel parallelism and dynamic adaptivity
- For more info on the CCA applications/case studies, see:
 - Chemistry: <http://www.cca-forum.org/~cca-chem>
 - Combustion: <http://cfrfs.ca.sandia.gov>
- **Different facets of CCA components may be useful within different projects ... What are **your** needs and priorities?**



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A Few Notes in Closing

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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Resources: Its All Online

- Information about all CCA tutorials, past, present, and future:
<http://www.cca-forum.org/tutorials/>
- Specifically...
 - Latest versions of hands-on materials and code:
<http://www.cca-forum.org/tutorials/#sources>
 - Hands-On designed for self-study as well as use in an organized tutorial
 - Should work on most Linux distributions, less tested on other unixen
 - Still evolving, so please contact us if you have questions or problems
 - Archives of all tutorial presentations:
<http://www.cca-forum.org/tutorials/archives/>
- Questions...
help@cca-forum.org



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Getting Help

- We want to help insure you have a good experience with CCA, so let us know if you're having problems!
- Tutorial or "start-up" questions
 - help@cca-forum.org
- Problems with specific tools
 - *check documentation for updated contact info*
 - cca-tools bundle (includes Chasm, Babel, Ccaffeine): [Rob Armstrong, rob@sandia.gov](mailto:Rob.Armstrong@sandia.gov)
 - Chasm: [Craig Rasmussen, crasmussen@lanl.gov](mailto:crasmussen@lanl.gov)
 - Babel: babel-users@lanl.gov
 - Ccaffeine: ccafe-users@cca-forum.org
- General questions, or not sure who to ask?
 - help@cca-forum.org



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CCA is Interactive

- Collectively, CCA developers and users span a broad range of scientific interests.
 - There's a good chance we can put you in touch with others with relevant experience with CCA
- CCA Forum Quarterly Meetings
 - Meet many CCA developers and users
 - <http://www.cca-forum.org/meetings/>
- “Coding Camps”
 - Bring together CCA users & developers for a concentrated session of coding
 - Held as needed, typically 3-5 days
 - May focus on a particular theme, but generally open to all interested participants
 - If you're interested in having one, *speak up* (to individuals or cca-forum@cca-forum.org)
- Visits, Internships, etc.



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Common Component Architecture

Acknowledgements: Tutorial Working Group

- **People:** Benjamin A. Allan, Rob Armstrong, David E. Bernholdt, Randy Bramley, Tamara L. Dahlgren, Lori Freitag Diachin, Wael Elwasif, Tom Epperly, Madhusudhan Govindaraju, Ragib Hasan, Dan Katz, Jim Kohl, Gary Kurfert, Lois Curfman McInnes, Alan Morris, Boyana Norris, Craig Rasmussen, Jaideep Ray, Sameer Shende, Torsten Wilde, Shujia Zhou
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- and many more... without whom we wouldn't have much to talk about!

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Thank You!

Thanks for attending this tutorial

We welcome feedback and questions

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